

Supporting Information

***O*-substituted Groups-Controlled Selectivity in Rh(III)-Catalyzed Coupling of Benzamides
with α,α -difluoromethylene alkynes: A Computational Mechanistic Study**

Xue-Xiang Ma, Jian-Biao Liu, Fang Huang, Chuan-Zhi Sun, and De-Zhan Chen**

College of Chemistry, Chemical Engineering and Materials Science, Collaborative Innovation Center of Functionalized Probes for Chemical Imaging in Universities of Shandong, Key Laboratory of Molecular and Nano Probes, Ministry of Education, Shandong Provincial Key Laboratory of Clean Production of Fine Chemicals, Shandong Normal University, Jinan 250014, P. R. China

**E-mails: jianbiaoliu.thu@gmail.com; chendzh@sdnu.edu.cn*

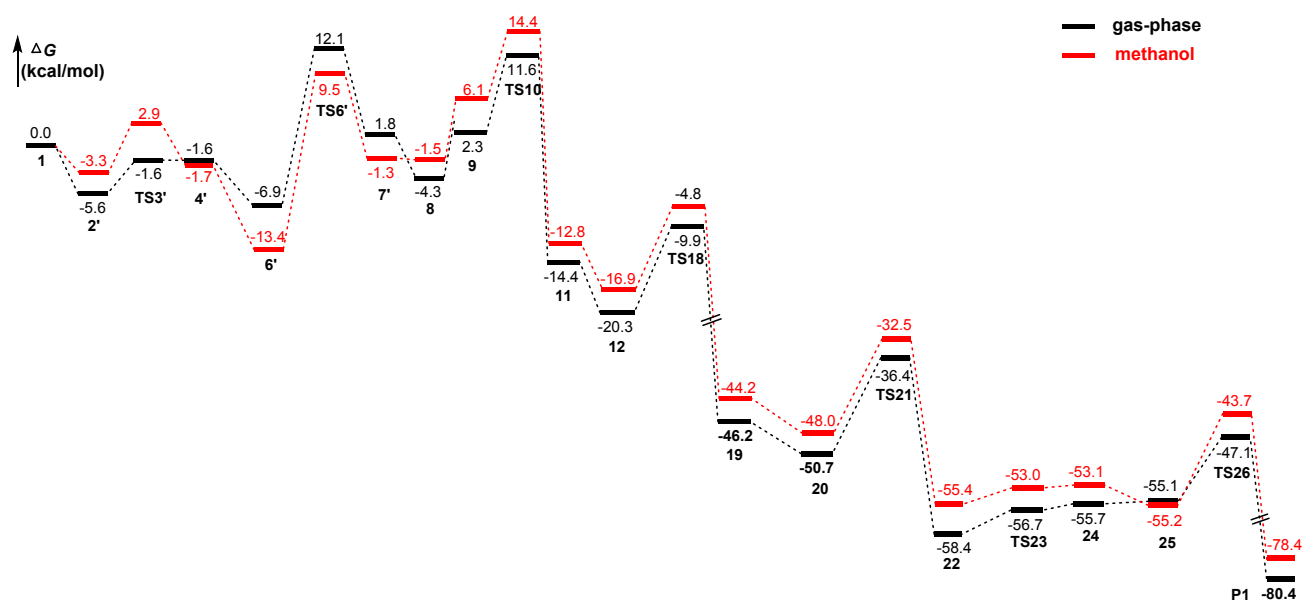


Fig. S1 Free energy profiles for the optimal path for hydroarylation products P1.

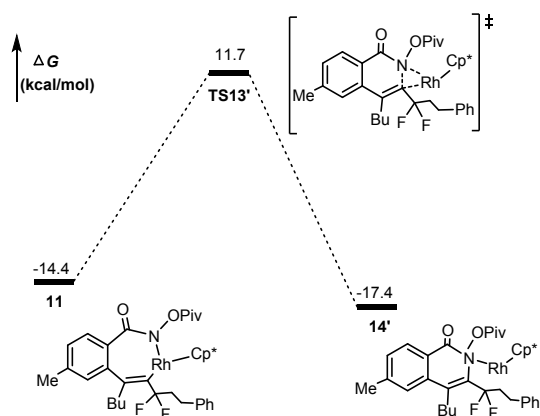


Fig. S2 Free energy profiles for direct C—N reductive elimination of 1a and 2a.

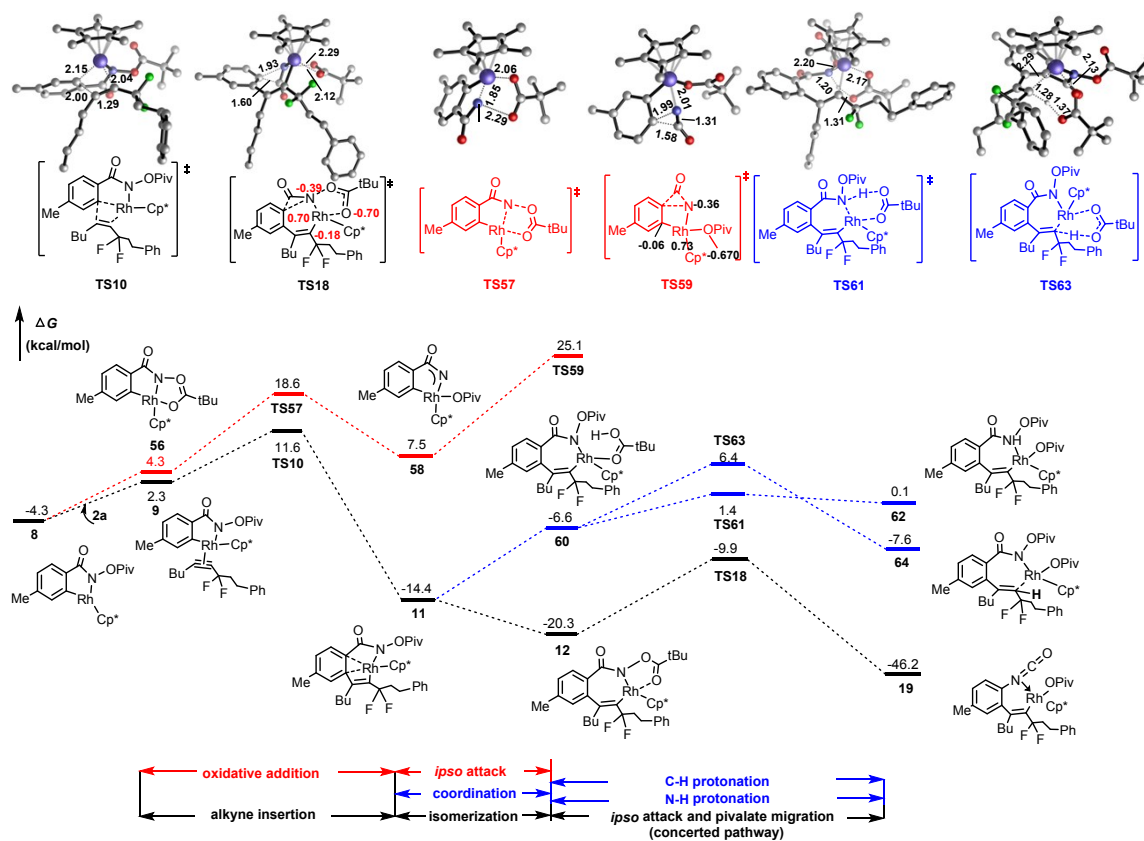


Fig. S3 Free energy profiles for Lossen rearrangement before the alkyne insertion or protonation of 11.

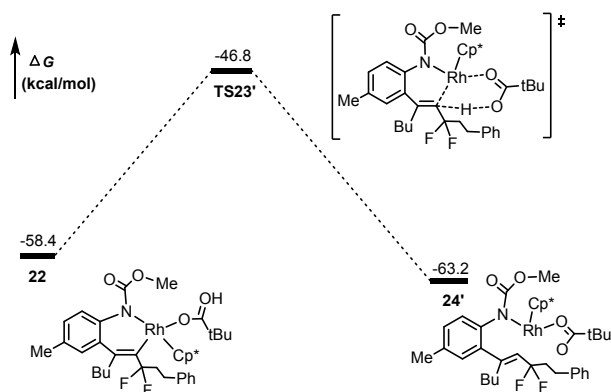


Fig. S4 Free-energy profiles for C—H protonated from 22.

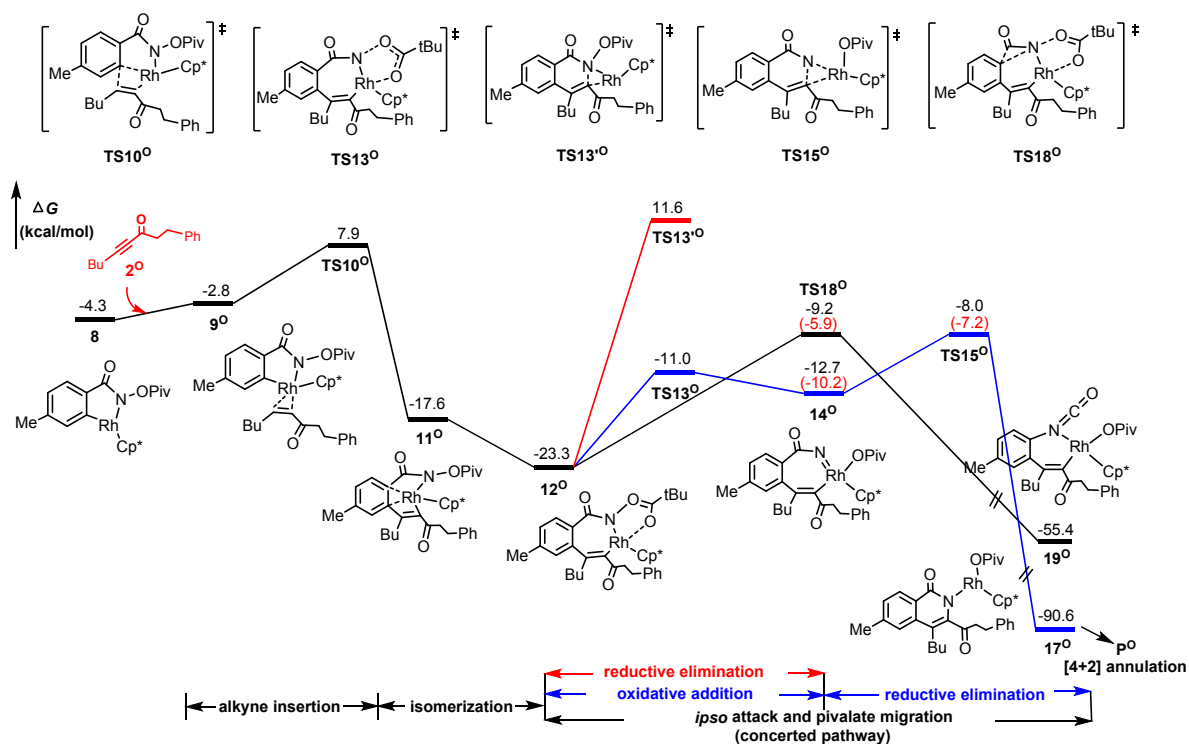


Fig. S5 Free energy profiles for the alkyne insertion and the competing pathways for the formation of 17° or 19° . Numbers in parentheses are relative free energies by optimization in MeOH (To get more accurate energies, some key structures were optimized in solvent).

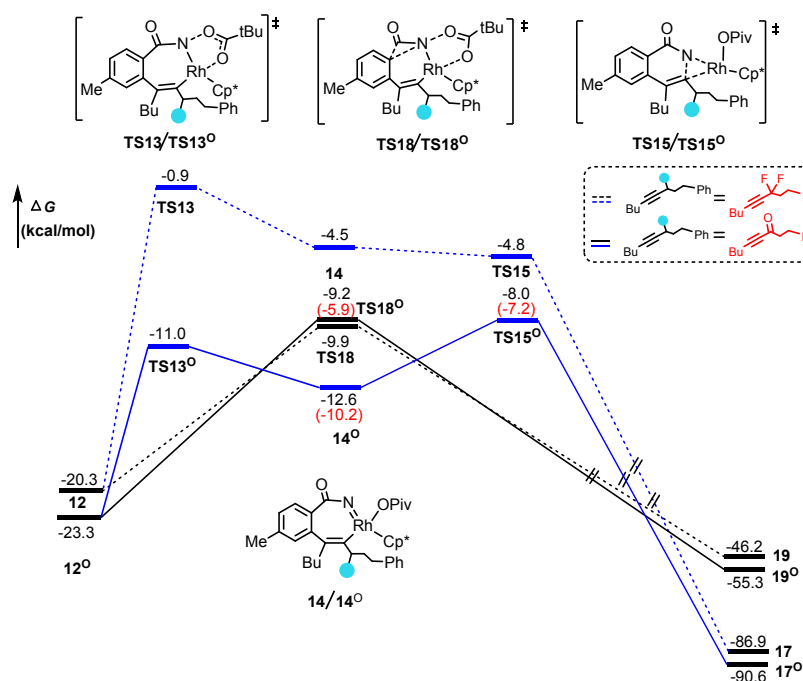


Fig. S6 Free energy profiles for the comparisons between different alkyne substrates (**2a** or **2°**) and *N*-pivaloyloxy benzamide **1a**. Numbers in parentheses are relative free energies by optimization in MeOH solution.

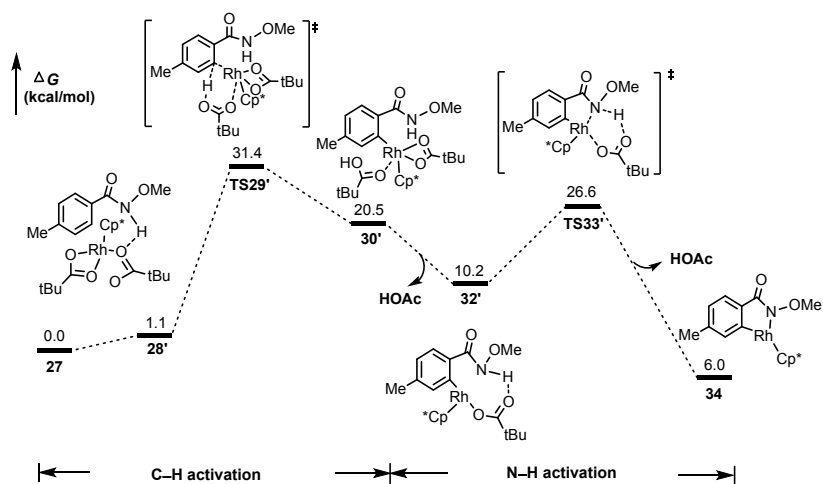


Fig. S7 Energy profiles for C–H activation, N–H deprotonation sequences of 1a'.

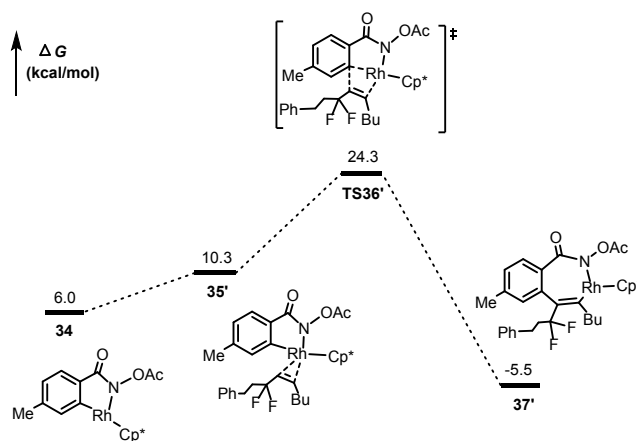


Fig. S8 Energy profiles for alkyne migratory insertion of 1a' and 2a.

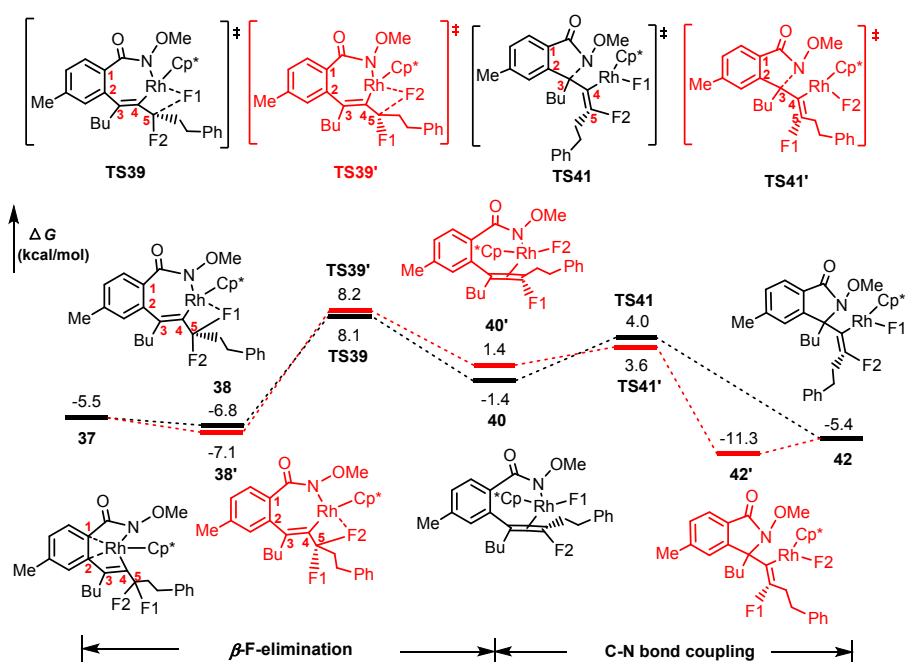


Fig. S9 The comparing pathway for β-F elimination at two different F (F1 or F2) sites.

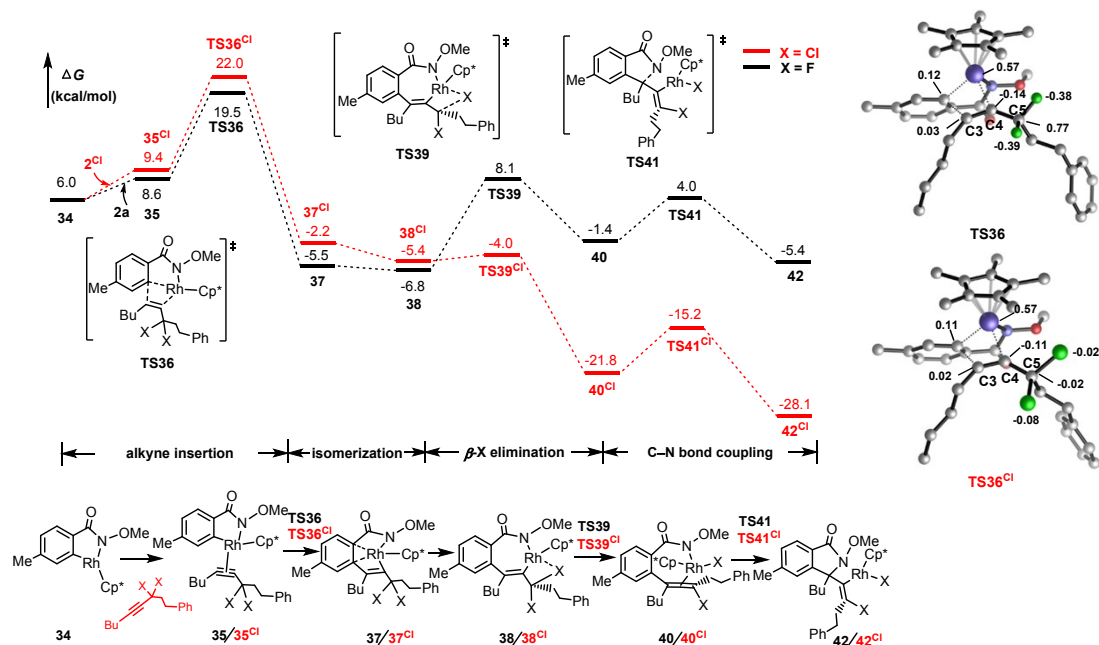


Fig. S10 Free energy profiles for the comparisons between different alkyne substrates (**2a** or **2Cl**) and *N*-methoxyl benzamide **1a'**.

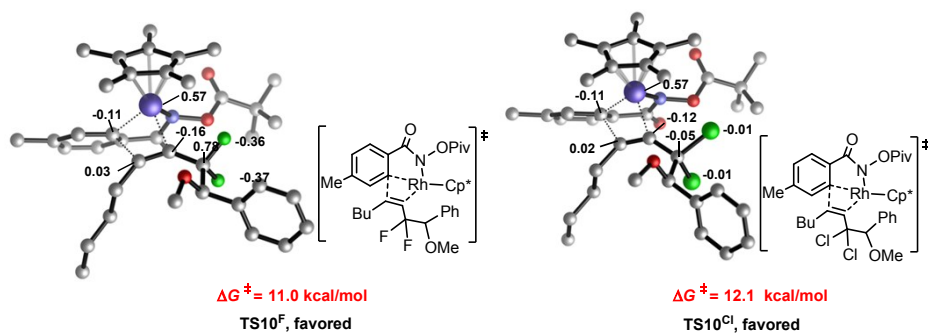


Fig. S11 Free energy profiles for alkyne insertion with different different alkyne substrates (**2'a** or **2'Cl**) in hydroarylation process.

Cartesian coordinates of all the structures

1 [Cp*Rh(OPiv)₂]

Rh	0.6754370	-0.2493740	-0.0671630
O	-1.3429300	-0.3715620	-0.4599060
O	0.1238850	1.5074340	1.0832600
C	-2.1544460	-1.0397820	0.3145600
O	-1.8228210	-1.6947800	1.3069720
C	0.1040340	2.2216770	0.0281280
O	0.4572750	1.6704270	-1.0669690
C	-3.6373840	-0.9553200	-0.1365530
C	-0.3046480	3.6936770	0.0564210
C	2.7384650	-0.6688860	-0.5565340
C	1.1880750	-2.3711650	-0.1355080
C	2.5688030	-0.7643360	0.8551020
C	1.5828020	-1.8051250	1.1243390
C	3.6456550	0.2633390	-1.3014370
H	4.5479500	-0.2656530	-1.6335190
H	3.1491430	0.6704180	-2.1856910
H	3.9591080	1.1041630	-0.6795560
C	3.2744550	0.0415840	1.9041330
H	2.5980970	0.3074900	2.7198920
H	4.1051590	-0.5346760	2.3306250
H	3.6840140	0.9672110	1.4944070
C	1.1331490	-2.2728280	2.4750130
H	1.6600140	-3.1939930	2.7568450

H	1.3388790	-1.5221260	3.2414050
H	0.0577390	-2.4585550	2.4665860
C	0.2439890	-3.5207110	-0.3148440
H	-0.1858590	-3.5316510	-1.3188210
H	0.7830390	-4.4661390	-0.1710130
H	-0.5722330	-3.4634430	0.4061290
C	1.8553890	-1.6467320	-1.1832700
C	1.7664650	-1.9124420	-2.6565590
H	0.8139370	-2.3752280	-2.9227410
H	1.8595510	-0.9881640	-3.2323960
H	2.5702170	-2.5885740	-2.9762800
C	-3.7545140	-1.5292220	-1.5647050
H	-4.7936270	-1.4779300	-1.9103120
H	-3.1274610	-0.9691390	-2.2628750
H	-3.4469030	-2.5812070	-1.5934030
C	-4.5199780	-1.7619130	0.8278330
H	-4.4450360	-1.3755980	1.8477140
H	-5.5682950	-1.7084670	0.5115630
H	-4.2191520	-2.8127660	0.8538490
C	-4.0766520	0.5237310	-0.1400210
H	-5.1257740	0.6071710	-0.4475580
H	-3.9845580	0.9642950	0.8590540
H	-3.4647220	1.1087190	-0.8308410
C	-1.4380490	3.9058240	-0.9703520
H	-2.3274550	3.3285060	-0.6996520

H	-1.7164530	4.9649190	-1.0012820
H	-1.1229870	3.5971980	-1.9700280
C	-0.7729630	4.0988180	1.4630490
H	0.0168200	3.9512400	2.2046590
H	-1.0567420	5.1569370	1.4673400
H	-1.6380230	3.5090900	1.7778490
C	0.9291910	4.5288330	-0.3574380
H	0.6686710	5.5925540	-0.3749610
H	1.7535350	4.3972230	0.3524400
H	1.2804480	4.2417130	-1.3521060

HOPIv

O	1.5272920	1.2483340	-0.0000710
C	0.9440740	0.1860250	-0.0000560
O	1.6166010	-0.9955500	-0.0000330
C	-0.5731740	-0.0101940	-0.0000030
C	-0.9726010	-0.8054840	-1.2633090
H	-2.0582630	-0.9465660	-1.2810130
H	-0.6891490	-0.2695490	-2.1751770
H	-0.4964310	-1.7887340	-1.2813040
C	-0.9724960	-0.8046170	1.2638720
H	-0.6891310	-0.2679260	2.1753190
H	-2.0581380	-0.9458250	1.2816440
H	-0.4961530	-1.7877640	1.2826020
C	-1.2509870	1.3679610	-0.0004430

H	-2.3389790	1.2466310	-0.0003680
H	-0.9669180	1.9487920	0.8809400
H	-0.9669560	1.9482070	-0.8822230
H	2.5600780	-0.7616970	0.0000440

MeOH

H	1.1336310	-0.7633740	0.0000030
C	-0.6616560	-0.0194250	0.0000000
H	-1.0382050	-0.5430860	-0.8917510
H	-1.0381990	-0.5428350	0.8918990
H	-1.0820690	0.9895260	-0.0001410
O	0.7493480	0.1220390	-0.0000010

1a

C	-3.3805940	1.2449210	-0.4707210
C	-2.0432310	0.8553440	-0.5042670
C	-1.6644900	-0.4127500	-0.0408890
C	-2.6496660	-1.2703060	0.4687440
C	-3.9818460	-0.8756710	0.4922050
C	-4.3724150	0.3882220	0.0237870
H	-3.6576070	2.2330830	-0.8280710
H	-1.2983590	1.5582240	-0.8654480
H	-2.3460170	-2.2440280	0.8376080
H	-4.7346670	-1.5566400	0.8806620
C	-0.2557320	-0.9152840	-0.0438230

O	0.1286760	-1.8470900	0.6362150	C	2.6411070	0.7694650	-0.5476350
N	0.6265180	-0.1717360	-0.8530710	C	1.5537990	1.1523060	-0.1838000
H	0.2289330	0.1490370	-1.7306220	C	3.9656000	0.3050160	-0.9551710
O	1.8066220	-0.8755940	-1.1807170	H	4.6360110	1.1701080	-1.0461040
C	2.9982530	-0.5517310	-0.5353870	H	3.8998380	-0.1363720	-1.9587570
O	3.9087170	-1.2892490	-0.8085690	C	4.5774300	-0.7218020	0.0217280
C	3.1385610	0.6835230	0.3766120	H	4.6272530	-0.2756220	1.0223050
C	4.6113010	0.7150170	0.8352080	H	3.9048570	-1.5846620	0.1005680
H	5.2946270	0.7539470	-0.0158350	C	5.9720520	-1.1854930	-0.4128970
H	4.7756170	1.5997250	1.4584010	H	6.6345300	-0.3132100	-0.4949460
H	4.8622850	-0.1734580	1.4194800	H	5.9132370	-1.6188570	-1.4205900
C	2.8390630	1.9693830	-0.4277530	C	6.5870130	-2.2066930	0.5484320
H	3.4855100	2.0454430	-1.3083110	H	7.5820520	-2.5179310	0.2153400
H	1.7983270	2.0161400	-0.7523700	H	6.6884770	-1.7903790	1.5567970
H	3.0347640	2.8413550	0.2050310	H	5.9647560	-3.1054160	0.6231710
C	2.2358610	0.5991920	1.6300020	C	0.2159290	1.5768620	0.2335270
H	1.1917780	0.8134150	1.4049930	F	-0.1079560	2.7559260	-0.4087500
H	2.2904880	-0.3868860	2.0990730	F	0.2346530	1.8750260	1.5821800
H	2.5796260	1.3402190	2.3593490	C	-0.8783320	0.5483620	-0.0318890
C	-5.8169410	0.8208790	0.0822640	H	-0.8742160	0.3211600	-1.1027040
H	-6.4913170	-0.0076680	-0.1544380	H	-0.6067650	-0.3728360	0.4933770
H	-6.0797440	1.1743790	1.0869250	C	-2.2715510	1.0338920	0.4129790
H	-6.0207370	1.6369060	-0.6162540	H	-2.5055400	1.9606790	-0.1196960
				H	-2.2326430	1.2794670	1.4787120
2a				C	-3.3438900	-0.0022790	0.1552870

C	-4.0275080	-0.0398350	-1.0673520
C	-3.6551140	-0.9680330	1.1216770
C	-4.9933720	-1.0147130	-1.3191980
H	-3.8040410	0.7066450	-1.8260190
C	-4.6201440	-1.9448890	0.8746730
H	-3.1396210	-0.9490610	2.0790950
C	-5.2923030	-1.9718210	-0.3483070
H	-5.5157830	-1.0235410	-2.2716920
H	-4.8505200	-2.6816160	1.6391320
H	-6.0464650	-2.7291960	-0.5411870

2

Rh	-1.9246030	-0.1236650	-0.3449040
O	-2.1534250	-2.0179880	0.6828680
O	-0.5926760	0.2882280	1.2437210
C	-1.1016510	-2.4899850	0.1362250
O	-0.4808230	-1.7502370	-0.6946070
C	-1.0717650	0.8215600	2.3395030
O	-2.1921420	1.3245990	2.4456230
C	-0.5989930	-3.8888680	0.4974910
C	-0.1647120	0.7729600	3.6001180
C	-2.0863630	1.2779990	-2.0143070
C	-3.7704000	0.9841520	-0.4309320
C	-2.7801410	0.0332730	-2.3158180
C	-3.8205700	-0.1391800	-1.3553040

C	-1.0288560	1.8851310	-2.8855260
H	-1.4781270	2.1588180	-3.8499730
H	-0.5972470	2.7802050	-2.4400990
H	-0.2055580	1.1941790	-3.0832100
C	-2.4490590	-0.8608580	-3.4722030
H	-2.8447680	-1.8690460	-3.3329850
H	-2.8779810	-0.4551030	-4.3973980
H	-1.3680420	-0.9369750	-3.6111530
C	-4.8049310	-1.2668190	-1.2803780
H	-5.7776120	-0.9451140	-1.6732240
H	-4.4750150	-2.1293780	-1.8628140
H	-4.9497510	-1.5945900	-0.2481250
C	-4.7471920	1.2469070	0.6730360
H	-4.2579310	1.7481370	1.5068450
H	-5.5708530	1.8720710	0.3021750
H	-5.1785170	0.3158760	1.0490090
C	-2.7167110	1.8644540	-0.8665060
C	-2.3711180	3.1782460	-0.2363160
H	-2.4437550	3.1066410	0.8499880
H	-1.3639030	3.5019360	-0.5031020
H	-3.0770000	3.9439840	-0.5849880
C	4.1251630	-2.4376740	0.6580480
C	3.4464530	-1.2478470	0.3948570
C	3.0030550	-0.9610530	-0.9032270
C	3.2661750	-1.8805010	-1.9294100

C	3.9402590	-3.0651530	-1.6575230	H	5.2022410	3.3903130	-0.7543180
C	4.3799690	-3.3672620	-0.3582440	C	0.1638490	-4.4977940	-0.6927480
H	4.4729870	-2.6409120	1.6675840	H	1.0036100	-3.8677740	-0.9923370
H	3.2873660	-0.5363310	1.1975130	H	0.5486420	-5.4860920	-0.4174930
H	2.9405630	-1.6388270	-2.9353230	H	-0.4916920	-4.6233300	-1.5613050
H	4.1372410	-3.7668700	-2.4643030	C	-1.7901000	-4.7842810	0.8866430
C	2.3234640	0.3151060	-1.2791590	H	-1.4273190	-5.7758780	1.1781600
O	2.2515860	0.7120180	-2.4315030	H	-2.3487530	-4.3569240	1.7220700
N	1.8756260	1.0831560	-0.1852330	H	-2.4821830	-4.9119080	0.0475410
H	1.2374280	0.5958580	0.4598640	C	0.3520990	-3.7365610	1.7086480
O	1.1253190	2.2114220	-0.6041490	H	-0.1672010	-3.2879650	2.5609810
C	1.7182780	3.4501180	-0.7071640	H	0.7203680	-4.7226770	2.0131960
O	0.9892520	4.2971340	-1.1742050	H	1.2146700	-3.1134260	1.4568400
C	3.1442760	3.7542070	-0.2046800	C	-0.9050920	-0.1019300	4.6372820
C	3.3958090	5.2508660	-0.4831040	H	-0.3441930	-0.1292790	5.5787190
H	2.6447120	5.8795710	-0.0001870	H	-1.9022390	0.2989400	4.8325520
H	4.3833430	5.5261520	-0.0992730	H	-1.0154410	-1.1315980	4.2790590
H	3.3680600	5.4654220	-1.5544600	C	1.2275550	0.1832100	3.3374050
C	3.2179460	3.5068630	1.3192570	H	1.8040550	0.8110050	2.6513910
H	2.4710830	4.1025140	1.8547120	H	1.7902240	0.1221950	4.2764330
H	3.0674930	2.4548130	1.5648060	H	1.1641660	-0.8218050	2.9121890
H	4.2066170	3.8056530	1.6837750	C	-0.0339080	2.2095650	4.1466390
C	4.2266070	2.9287760	-0.9393820	H	-1.0215500	2.6422020	4.3201270
H	4.2752670	1.9000930	-0.5830350	H	0.5228130	2.2097570	5.0908150
H	4.0596880	2.9122780	-2.0197220	H	0.5023890	2.8552110	3.4415910

C	5.0953980	-4.6643660	-0.0683380	H	1.9628470	-4.4315340	1.6463950
H	4.3856150	-5.4986490	-0.0069480	H	1.1564400	-3.9196800	0.1557420
H	5.8130420	-4.9099700	-0.8576930	C	3.7263830	-1.3151950	2.1965110
H	5.6352530	-4.6215400	0.8815970	H	4.1168370	-1.8429080	3.0766490
TS3				H	4.1283720	-1.8069490	1.3084540
				H	4.0902850	-0.2875870	2.2187390
Rh	0.8904600	-0.4419600	0.7520190	C	1.8415360	0.7910540	3.6730020
O	3.3253170	1.7672340	1.0350400	H	2.1968790	0.4742870	4.6626280
O	-0.0730370	1.4203900	-1.6599190	H	2.6426670	1.3128170	3.1475500
C	3.3217520	1.1854490	-0.0531760	H	1.0233240	1.4983880	3.8236990
O	2.4515570	0.2919120	-0.4372740	C	0.0149430	-0.8553280	2.7410830
C	-0.1199800	2.0680150	-0.5645000	C	-1.1727470	-0.1780900	3.3544280
O	0.0006300	1.4968090	0.5665880	H	-1.1101090	0.9062280	3.2301950
C	4.4461750	1.4435110	-1.0990920	H	-2.1136030	-0.5110210	2.9153530
C	-0.3004590	3.5922900	-0.5991910	H	-1.2017060	-0.3874630	4.4313360
C	0.0200680	-2.0724420	1.9991880	C	1.1159540	-1.6742690	-2.0830430
C	1.3856360	-0.3956410	2.8803950	C	0.0523670	-1.1760130	-1.2992980
C	1.3954370	-2.3624180	1.6245960	C	-1.1996120	-1.8426330	-1.4383880
C	2.2301150	-1.3533400	2.2222350	C	-1.3253980	-2.9474710	-2.2943250
C	-1.1410100	-2.9983810	1.8010130	C	-0.2434130	-3.4072080	-3.0370420
H	-1.1385260	-3.7410610	2.6103400	C	0.9996150	-2.7667890	-2.9512790
H	-2.1011320	-2.4825220	1.8328090	H	2.0731330	-1.1703710	-2.0001560
H	-1.0807190	-3.5411610	0.8568030	H	0.0442510	0.2005420	-1.3720820
C	1.8614940	-3.6067050	0.9287700	H	-2.2910260	-3.4374350	-2.3608650
H	2.8335300	-3.4573890	0.4538690	H	-0.3686180	-4.2641920	-3.6950310

C	-2.4642610	-1.5025260	-0.7054830	H	1.0498890	5.2900690	-0.4902530
O	-3.3907310	-2.2926250	-0.5913650	H	1.6876960	3.8337500	0.3108190
N	-2.5885430	-0.1968830	-0.2166590	H	1.6854910	3.9506420	-1.4582180
H	-1.7287560	0.2715700	0.0594290	C	-1.0951060	4.0578240	0.6353560
O	-3.4507450	-0.1216730	0.9067600	H	-2.0970100	3.6173070	0.6568710
C	-4.8013430	0.1804130	0.7438060	H	-0.5828580	3.7856260	1.5603710
O	-5.4636170	-0.0420560	1.7246230	H	-1.2071460	5.1466150	0.6081180
C	-5.3484210	0.8596620	-0.5266900	C	5.2747010	2.6659610	-0.6732450
C	-6.8225490	1.2059820	-0.2303290	H	5.7050100	2.5241030	0.3206890
H	-6.9147850	1.8495550	0.6478170	H	6.0881670	2.8347740	-1.3881700
H	-7.2501320	1.7270770	-1.0929150	H	4.6578970	3.5685830	-0.6369820
H	-7.4103380	0.3043350	-0.0421410	C	3.8490170	1.6758500	-2.5005020
C	-4.5660370	2.1646620	-0.7942370	H	4.6528480	1.8388400	-3.2279520
H	-4.5967590	2.8327590	0.0732380	H	3.2528630	0.8219150	-2.8286730
H	-3.5246180	1.9636370	-1.0495970	H	3.2028130	2.5593170	-2.5169990
H	-5.0260250	2.6919600	-1.6367220	C	5.3515400	0.1915110	-1.1325840
C	-5.3001310	-0.0591000	-1.7687930	H	4.7869220	-0.6946100	-1.4375310
H	-4.2872950	-0.1863360	-2.1486250	H	6.1716240	0.3370340	-1.8449920
H	-5.7122060	-1.0476070	-1.5523520	H	5.7954690	-0.0031760	-0.1498670
H	-5.9025930	0.3984330	-2.5609400	C	2.1698490	-3.2283810	-3.7865360
C	-1.0084340	4.0259640	-1.8942180	H	2.2251220	-4.3210480	-3.8330490
H	-1.0780530	5.1183530	-1.9248480	H	2.0812160	-2.8662900	-4.8183740
H	-0.4616800	3.6878370	-2.7769440	H	3.1168150	-2.8535220	-3.3885960
H	-2.0238260	3.6222450	-1.9524960				
C	1.1248570	4.1990700	-0.5521660	4			

Rh	0.9491040	-0.5687670	0.6149240	C	0.5906760	0.5158880	3.8368450
O	3.0236930	1.7954230	1.3845100	H	-0.3007900	1.0763080	3.5429300
O	1.0610430	2.1492460	-1.4650300	H	0.4404520	0.1757010	4.8698470
C	3.3553870	1.2834360	0.3202630	H	1.4371570	1.2051720	3.8196350
O	2.6074930	0.4213710	-0.3581760	C	-0.2275760	-1.4254890	2.2579260
C	0.0886160	2.2444810	-0.5978940	C	-1.6904740	-1.2869840	2.5559230
O	-0.1286040	1.3691280	0.2675620	H	-2.0040540	-0.2406930	2.5721160
C	4.7124410	1.6080750	-0.3557880	H	-2.3120710	-1.8097550	1.8281830
C	-0.7875150	3.4876320	-0.7357850	H	-1.9039750	-1.7088630	3.5474510
C	0.3930170	-2.4815400	1.5192150	C	1.4688760	-1.5625070	-2.1417140
C	0.8259790	-0.6455960	2.9187970	C	0.4004070	-1.2498770	-1.2777070
C	1.8186450	-2.2644800	1.5825440	C	-0.8962170	-1.6029430	-1.7240500
C	2.0640470	-1.1802050	2.5399860	C	-1.0675290	-2.2558510	-2.9613100
C	-0.2818330	-3.6627480	0.8873070	C	0.0097510	-2.5361480	-3.7875730
H	-0.3034290	-4.4892080	1.6103010	C	1.3048090	-2.1828460	-3.3866720
H	-1.3084670	-3.4515070	0.5859120	H	2.4771710	-1.3072450	-1.8313230
H	0.2570980	-4.0076150	0.0030720	H	1.6593250	1.3685300	-1.2093210
C	2.8699400	-3.1729920	1.0159740	H	-2.0727300	-2.5423600	-3.2546720
H	3.7903390	-2.6283260	0.7917660	H	-0.1521350	-3.0323300	-4.7414880
H	3.1200560	-3.9688870	1.7302320	C	-2.1948290	-1.4047950	-0.9903360
H	2.5283110	-3.6444980	0.0922580	O	-3.0584820	-2.2732440	-0.9143840
C	3.4148910	-0.7701380	3.0398770	N	-2.4181570	-0.1223930	-0.5345100
H	3.6787160	-1.3745860	3.9182070	H	-1.6495030	0.4598540	-0.2116430
H	4.1893400	-0.9367790	2.2879130	O	-3.5469230	0.0255160	0.2918220
H	3.4416820	0.2833130	3.3170800	C	-4.6391830	0.5672710	-0.3679620

O	-4.5722710	1.0698960	-1.4592250	H	-2.3468720	4.5110000	0.3553810
C	-5.9058180	0.3842660	0.4720700	C	5.4276780	2.7166220	0.4319930
C	-6.9752630	1.3629480	-0.0399830	H	5.5983630	2.4186450	1.4695250
H	-7.1501350	1.2286280	-1.1094940	H	6.3957300	2.9400640	-0.0302270
H	-7.9160080	1.1953070	0.4942540	H	4.8343140	3.6350340	0.4487150
H	-6.6723430	2.4025240	0.1208900	C	4.4796160	2.0643590	-1.8116330
C	-6.3664430	-1.0786410	0.2483620	H	5.4384550	2.3061560	-2.2836240
H	-6.6369290	-1.2455570	-0.7986070	H	3.9972430	1.2812770	-2.4021600
H	-5.5744890	-1.7858210	0.5062090	H	3.8522350	2.9609320	-1.8536580
H	-7.2465560	-1.2838650	0.8671320	C	5.5737540	0.3255600	-0.3568770
C	-5.6344060	0.6262090	1.9709180	H	5.0744500	-0.4839160	-0.8962710
H	-4.9125410	-0.0886890	2.3710330	H	6.5365190	0.5202950	-0.8424450
H	-5.2532070	1.6370370	2.1514220	H	5.7823390	-0.0133000	0.6643270
H	-6.5699990	0.5174810	2.5294140	C	2.4921480	-2.4546090	-4.2806830
C	-1.6043230	3.3437380	-2.0460280	H	3.4345330	-2.3739270	-3.7311500
H	-2.2019020	4.2494220	-2.1926570	H	2.4405470	-3.4551330	-4.7236760
H	-0.9445400	3.2254770	-2.9096570	H	2.5329760	-1.7382970	-5.1109060
H	-2.2904260	2.4922280	-2.0060460				
C	0.1260770	4.7310560	-0.8205070	5			
H	-0.4939160	5.6275230	-0.9206170	Rh	-0.3756510	-0.4929860	-0.6201250
H	0.7360360	4.8396990	0.0824690	O	-0.4506440	2.5290880	0.8781870
H	0.7945040	4.6752520	-1.6822060	C	-1.2943320	2.4065750	-0.0471570
C	-1.7345720	3.6110830	0.4687590	O	-1.4229700	1.3652440	-0.7797210
H	-2.4076830	2.7539500	0.5447900	C	-2.2471000	3.5939430	-0.3120490
H	-1.1780050	3.6915160	1.4071940	C	0.9167760	-1.2972860	-2.3656430

C	-1.4065200	-1.3135410	-2.3408010	C	-1.3133500	-0.8530310	1.1643030
C	0.4672620	-2.3558190	-1.4579650	C	-0.5122340	-0.7768140	2.3202690
C	-0.9654020	-2.4151640	-1.5377100	C	-1.0163410	-1.0928110	3.5913400
C	2.3490220	-1.0136980	-2.7096480	C	-2.3473880	-1.4585690	3.7271220
H	2.4970260	0.0262920	-3.0117990	C	-3.1916950	-1.4970900	2.6018800
H	3.0073750	-1.2252640	-1.8669430	H	-3.3280770	-1.2296560	0.4810580
H	2.6658070	-1.6489020	-3.5474090	H	-0.3542780	-1.0321970	4.4504140
C	1.3449820	-3.3947920	-0.8225820	H	-2.7483630	-1.6996920	4.7084040
H	0.8496800	-3.8582900	0.0343080	C	0.8603280	-0.2694660	2.1733250
H	1.5738440	-4.1917320	-1.5436680	O	1.7676300	-0.2974380	2.9756510
H	2.2818980	-2.9659620	-0.4691420	N	0.9723130	0.3890000	0.8729230
C	-1.8226960	-3.4966980	-0.9517320	H	0.3847830	1.3244900	0.9303480
H	-2.8539780	-3.1706620	-0.8071040	O	2.2814750	0.9297630	0.6643010
H	-1.8386290	-4.3582370	-1.6318940	C	3.3217850	0.0474940	0.6122310
H	-1.4427570	-3.8385650	0.0129370	O	3.1886760	-1.1516470	0.5410060
C	-2.8142080	-0.9736950	-2.7306630	C	4.6531860	0.8085580	0.6615420
H	-2.9769630	0.1065060	-2.6895970	C	4.7761200	1.4625120	2.0586040
H	-3.0285510	-1.3119050	-3.7528650	H	4.7100570	0.7126290	2.8518150
H	-3.5403820	-1.4476920	-2.0661690	H	5.7443620	1.9681530	2.1391510
C	-0.2172750	-0.6588310	-2.8938580	H	3.9845640	2.1971090	2.2225270
C	-0.2641620	0.4996060	-3.8443350	C	5.7946530	-0.1980800	0.4468650
H	-0.9151760	1.2903560	-3.4588830	H	5.7752260	-0.9845760	1.2049420
H	0.7277210	0.9270350	-4.0070730	H	5.7253510	-0.6782790	-0.5337810
H	-0.6585170	0.1871610	-4.8194370	H	6.7567450	0.3206140	0.5066720
C	-2.6602990	-1.1969460	1.3386090	C	4.6873850	1.8970400	-0.4338560

H	4.5842460	1.4602070	-1.4332390	C	-2.1619420	3.5698200	-0.7615270
H	3.8904540	2.6312480	-0.2961460	C	0.9331290	-1.6434510	-2.1286310
H	5.6481110	2.4212530	-0.3964570	C	-1.3906190	-1.6294510	-2.1978460
C	-3.1697910	3.3387380	-1.5126700	C	0.4294280	-2.5520110	-1.0958470
H	-3.7885350	2.4503950	-1.3590720	C	-1.0042530	-2.6062600	-1.2291180
H	-3.8342700	4.1977140	-1.6598620	C	2.3810900	-1.4303020	-2.4569100
H	-2.5969690	3.1941760	-2.4338360	H	2.5661320	-0.4260510	-2.8476620
C	-1.3853090	4.8495260	-0.5639610	H	3.0118450	-1.5802450	-1.5807740
H	-2.0279390	5.7270440	-0.6969370	H	2.6994330	-2.1473390	-3.2251890
H	-0.7124620	5.0312200	0.2768830	C	1.2645830	-3.4945560	-0.2793000
H	-0.7785370	4.7376230	-1.4698850	H	0.7079470	-3.8655550	0.5846310
C	-3.0903120	3.7966410	0.9669800	H	1.5589820	-4.3640110	-0.8832580
H	-2.4444550	3.9630630	1.8322860	H	2.1652590	-3.0061450	0.0916970
H	-3.7499270	4.6636870	0.8490800	C	-1.9039970	-3.5812280	-0.5306340
H	-3.7164070	2.9207700	1.1702990	H	-2.9352590	-3.2272810	-0.4847750
C	-4.6504010	-1.8558610	2.7624440	H	-1.9038440	-4.5339890	-1.0758680
H	-5.1617830	-1.1461220	3.4230930	H	-1.5743620	-3.7790780	0.4910460
H	-5.1730970	-1.8544920	1.8018520	C	-2.7769940	-1.3235780	-2.6824940
H	-4.7685380	-2.8498550	3.2096150	H	-2.9247040	-0.2452930	-2.7870820
TS6				H	-2.9597380	-1.7863900	-3.6610900
				H	-3.5354900	-1.6983260	-1.9912630
Rh	-0.3912600	-0.5919280	-0.5620200	C	-0.1689760	-1.0697900	-2.7843090
O	-0.3271330	2.6003560	0.4441360	C	-0.1540140	-0.0641930	-3.8968260
C	-1.2503240	2.3819520	-0.4132220	H	-0.8458460	0.7584110	-3.6915690
O	-1.4446580	1.2611360	-0.9624410	H	0.8420340	0.3604500	-4.0412040

H	-0.4608720	-0.5266190	-4.8436840	H	6.7362420	0.3121650	0.5692220
C	-2.6839410	-1.0169410	1.4750240	C	4.7085520	1.7349360	-0.6624520
C	-1.3408750	-0.6857010	1.2537430	H	4.6292120	1.1494770	-1.5851660
C	-0.5507910	-0.3900880	2.3790860	H	3.9147050	2.4850630	-0.6618240
C	-1.0625570	-0.4773980	3.6807700	H	5.6729500	2.2535950	-0.6788570
C	-2.3903200	-0.8366220	3.8720910	C	-1.2731630	4.7441970	-1.2260510
C	-3.2226310	-1.0960410	2.7689890	H	-1.8951030	5.6219010	-1.4321090
H	-3.3434530	-1.2148930	0.6329660	H	-0.5413690	5.0062670	-0.4589400
H	-0.4089030	-0.2500640	4.5181730	H	-0.7318850	4.4929040	-2.1450850
H	-2.7966560	-0.9023060	4.8784750	C	-3.1671080	3.1983120	-1.8614890
C	0.8248820	0.0974520	2.1435350	H	-3.8071670	2.3669240	-1.5542760
O	1.7088370	0.2395900	2.9673730	H	-3.8065260	4.0595080	-2.0837280
N	0.9403600	0.4827740	0.7669310	H	-2.6585600	2.9071540	-2.7855670
H	0.3022950	1.5792860	0.6345690	C	-2.9122500	3.9680300	0.5305270
O	2.2605780	0.9530360	0.4597370	H	-3.5562150	4.8321430	0.3346090
C	3.2948910	0.0789290	0.6272600	H	-3.5445150	3.1485020	0.8886170
O	3.1580810	-1.1120100	0.7871780	H	-2.2087450	4.2296490	1.3243130
C	4.6328720	0.8298790	0.5860550	C	-4.6726200	-1.4653930	2.9807380
C	4.7253370	1.6927040	1.8673720	H	-5.1771730	-0.7430660	3.6320330
H	4.6338140	1.0754360	2.7651270	H	-5.2189730	-1.5041590	2.0340070
H	5.6937600	2.2040430	1.8926110	H	-4.7661340	-2.4474700	3.4604150
H	3.9317200	2.4426540	1.8943390				
C	5.7705400	-0.2037270	0.5628000	7			
H	5.7219620	-0.8636140	1.4320610	Rh	-0.3944400	-0.6110050	-0.5601660
H	5.7241480	-0.8300400	-0.3334520	O	-0.3342690	2.6547640	0.4239020

C	-1.2841000	2.4121170	-0.4347100	H	-0.8244650	0.7124240	-3.7443660
O	-1.4589350	1.2936230	-0.9561430	H	0.8775760	0.3242900	-4.0299320
C	-2.1894030	3.6033900	-0.7570360	H	-0.3906000	-0.5857730	-4.8615770
C	0.9264780	-1.6733980	-2.1104880	C	-2.6645380	-1.0468580	1.5068590
C	-1.3977720	-1.6453780	-2.2166750	C	-1.3280060	-0.7058270	1.2664450
C	0.3976670	-2.5594220	-1.0696630	C	-0.5254710	-0.3841970	2.3741880
C	-1.0374770	-2.6113620	-1.2329930	C	-1.0207430	-0.4510560	3.6806560
C	2.3815110	-1.4817220	-2.4180230	C	-2.3446110	-0.8197390	3.8953180
H	2.5843690	-0.4906260	-2.8326740	C	-3.1872890	-1.1092950	2.8098230
H	2.9938850	-1.6140920	-1.5261060	H	-3.3312750	-1.2683380	0.6760830
H	2.7064420	-2.2232610	-3.1599410	H	-0.3581840	-0.2006620	4.5045150
C	1.2171290	-3.4846240	-0.2183280	H	-2.7376320	-0.8700160	4.9080280
H	0.6268750	-3.8826210	0.6104410	C	0.8501980	0.1103750	2.1054550
H	1.5740000	-4.3369080	-0.8128590	O	1.7232370	0.3100450	2.9377980
H	2.0794360	-2.9666350	0.2027670	N	0.9523540	0.4091640	0.7351250
C	-1.9517560	-3.5775840	-0.5407430	H	0.2058420	1.7733900	0.5883220
H	-2.9936240	-3.2543700	-0.5793450	O	2.2598430	0.8899310	0.3887820
H	-1.8900170	-4.5558900	-1.0346570	C	3.3197740	0.0601720	0.6188170
H	-1.6832950	-3.7128000	0.5085730	O	3.2244220	-1.1282970	0.8251740
C	-2.7743160	-1.3368870	-2.7277100	C	4.6346180	0.8516150	0.5685980
H	-2.9005620	-0.2637230	-2.8942700	C	4.6639810	1.7976080	1.7923640
H	-2.9619360	-1.8484390	-3.6809700	H	4.5530060	1.2376980	2.7245830
H	-3.5447980	-1.6559990	-2.0218500	H	5.6191710	2.3337730	1.8162290
C	-0.1614880	-1.0970840	-2.7857890	H	3.8530220	2.5277220	1.7441300
C	-0.1190460	-0.1070860	-3.9118890	C	5.8049090	-0.1423280	0.6415560

H	5.7548800	-0.7433920	1.5524180	C	-3.2163900	1.1055700	0.0988090
H	5.7993220	-0.8294420	-0.2100620	C	-1.8301710	1.0664470	-0.0726140
H	6.7537660	0.4041360	0.6348760	C	-1.1617470	2.2973610	-0.2128700
C	4.7179270	1.6768380	-0.7338050	C	-1.8352090	3.5144210	-0.1713790
H	4.6861830	1.0312990	-1.6186130	C	-3.2206780	3.5228510	0.0042740
H	3.8996320	2.3970850	-0.8036310	C	-3.9279660	2.3219490	0.1328660
H	5.6642790	2.2277390	-0.7575090	H	-3.7835920	0.1849310	0.2133170
C	-1.3074820	4.7750490	-1.2441860	H	-1.2694860	4.4364950	-0.2727230
H	-1.9367570	5.6476570	-1.4474830	H	-3.7569000	4.4680590	0.0405680
H	-0.5652480	5.0493620	-0.4914970	C	0.3143020	2.2341710	-0.4124920
H	-0.7805250	4.5176830	-2.1694990	O	1.0768370	3.1877260	-0.4726640
C	-3.2148680	3.2248530	-1.8357520	Rh	-0.5588550	-0.5683100	-0.1754240
H	-3.8464970	2.3931210	-1.5128090	N	0.7001260	0.8936930	-0.5180400
H	-3.8595430	4.0842080	-2.0470220	C	2.8688550	0.7131310	0.3850630
H	-2.7235380	2.9319740	-2.7683930	O	2.4260770	0.5406020	1.4989190
C	-2.9137690	4.0051280	0.5498420	O	2.0962910	0.7708450	-0.7426640
H	-3.5630700	4.8658800	0.3590290	C	4.3476610	0.9379160	0.0428830
H	-3.5368600	3.1863290	0.9244580	C	5.2125540	0.3172130	1.1525480
H	-2.1977250	4.2756270	1.3292520	H	5.1131070	-0.7736290	1.1729520
C	-4.6279310	-1.5026610	3.0440480	H	6.2667550	0.5557800	0.9778810
H	-5.2154500	-1.4395960	2.1232230	H	4.9246580	0.6992250	2.1341330
H	-4.7037210	-2.5330660	3.4139420	C	4.5447570	2.4754280	0.0116640
H	-5.1021730	-0.8590010	3.7926030	H	3.8645420	2.9440390	-0.7033010
				H	4.3502060	2.9121510	0.9956750
8				H	5.5781220	2.7054140	-0.2699560

C	4.7218710	0.3382130	-1.3265710	C	-2.9295770	-2.0629890	1.6406120
H	4.5550810	-0.7443750	-1.3498560	H	-2.8542880	-1.2296620	2.3437340
H	4.1440150	0.7905290	-2.1347180	H	-3.8312020	-1.9137220	1.0433280
H	5.7851160	0.5153230	-1.5210930	H	-3.0701740	-2.9823890	2.2227400
C	-0.3400390	-2.1525550	1.2604110	C	-5.4320920	2.3223870	0.2811380
C	0.5467840	-2.5142650	0.1711990	H	-5.9263490	2.1621860	-0.6858010
C	-0.2496030	-2.6158000	-0.9939220	H	-5.7702170	1.5255240	0.9519200
C	-1.6549090	-2.4066600	-0.6260000	H	-5.7954420	3.2750070	0.6778360
C	-1.7077840	-2.1799690	0.7770720				
C	2.0265420	-2.7311050	0.2895660	2'			
H	2.2419370	-3.7533560	0.6265240	N	-0.4504850	1.0591910	-0.3412670
H	2.5315720	-2.5872520	-0.6688420	C	1.7598820	2.1863640	-0.6887000
H	2.4699310	-2.0408240	1.0100290	C	2.7599170	2.5035020	-1.6232120
C	0.2244160	-2.9267510	-2.3813350	H	2.5452540	2.3777570	-2.6784520
H	1.2841070	-2.6948500	-2.5061600	C	3.9964470	2.9684310	-1.1991980
H	0.0835010	-3.9926400	-2.6036080	H	4.7640680	3.1987250	-1.9335450
H	-0.3345760	-2.3585820	-3.1296220	C	4.2695740	3.1485300	0.1670290
C	-2.8162070	-2.5500780	-1.5648390	C	3.2657590	2.8311210	1.0913780
H	-2.5869920	-2.1358530	-2.5501250	H	3.4545930	2.9684100	2.1527400
H	-3.0777800	-3.6077440	-1.7012310	C	2.0234060	2.3517240	0.6793350
H	-3.7015770	-2.0325750	-1.1892570	H	1.2687810	2.1344010	1.4260580
C	0.0861140	-1.9248240	2.6783260	C	-2.2507830	-2.1172910	-1.4506400
H	0.2823460	-2.8855440	3.1733760	C	-1.6854550	-1.2668510	-2.4429350
H	0.9974390	-1.3231350	2.7207220	C	-0.3181210	-1.6918540	-2.6937610
H	-0.6887900	-1.4061920	3.2467010	C	-0.0794820	-2.8659140	-1.8959110

C	-1.2405810	-3.1038220	-1.0846100	H	-4.1717240	-1.1739130	-1.1960910
O	-0.5506400	0.7293620	2.2597480	C	-2.3668950	-0.1524780	-3.1752000
O	-1.3278160	-1.1997680	1.3798120	H	-2.5480980	-0.4609210	-4.2128030
C	-1.0907210	-0.3939390	2.3580680	H	-3.3291390	0.0950780	-2.7249840
C	-1.5442160	-0.9051530	3.7489990	H	-1.7472730	0.7469170	-3.1881790
Rh	-0.4970010	-1.1584420	-0.5806100	O	1.2897030	-1.1826860	0.4820590
C	0.4354600	1.7975660	-1.2239320	O	2.6891760	-1.0450520	-1.2842660
O	0.0656260	2.0467380	-2.3579200	C	2.4664420	-1.2081120	-0.0803740
O	-1.8116490	1.4971990	-0.5053460	C	3.6270440	-1.5456630	0.8989900
H	-0.2784240	1.0864830	0.7058070	C	-2.0238300	2.7809270	-0.0374940
C	0.5988510	-1.1179620	-3.7305360	O	-1.1268250	3.4728250	0.3739540
H	1.6371250	-1.2237880	-3.4152320	C	-3.4990990	3.1773190	-0.1497760
H	0.4565160	-1.6266140	-4.6936650	C	-3.6886450	4.5105700	0.5938160
H	0.4024220	-0.0533780	-3.8758880	H	-3.0469550	5.2903820	0.1773600
C	1.1532530	-3.7139180	-1.9334690	H	-4.7314880	4.8322060	0.5077900
H	1.0511860	-4.4622480	-2.7305580	H	-3.4442730	4.4104060	1.6549620
H	2.0375380	-3.1074560	-2.1277060	C	-4.3963710	2.0884080	0.4755110
H	1.3031660	-4.2488720	-0.9931750	H	-4.2910600	1.1317050	-0.0406610
C	-1.4485680	-4.2151510	-0.1015030	H	-4.1510430	1.9323750	1.5308660
H	-2.0480280	-5.0193840	-0.5472450	H	-5.4440730	2.4012370	0.4149430
H	-0.4984260	-4.6435420	0.2237640	C	-3.8391420	3.3576560	-1.6478810
H	-1.9724200	-3.8503570	0.7854870	H	-3.2023070	4.1193850	-2.1082540
C	-3.6315080	-2.0650140	-0.8702970	H	-3.7121510	2.4262940	-2.2044660
H	-4.2117360	-2.9430590	-1.1799440	H	-4.8808660	3.6800030	-1.7478330
H	-3.5881530	-2.0534190	0.2224200	C	-0.7399240	-2.1800470	4.0827990

H	-1.0436850	-2.5709500	5.0607610	H	5.6409900	4.7852400	0.4862630
H	-0.9055470	-2.9563750	3.3315180	H	5.7815390	3.4886000	1.6779790
H	0.3338940	-1.9692170	4.1230410				
C	-1.2878460	0.1689010	4.8176560	TS3'			
H	-1.8410510	1.0865580	4.5994060	N	-0.6034780	1.0140630	-0.2049140
H	-1.6031180	-0.1992990	5.8007200	C	1.4563970	2.3233930	-0.6078100
H	-0.2280200	0.4300180	4.8678150	C	2.4018760	2.6772810	-1.5796650
C	-3.0484990	-1.2445810	3.6982160	H	2.1559840	2.5400130	-2.6264470
H	-3.3845840	-1.6145470	4.6735430	C	3.6359670	3.1995120	-1.2077430
H	-3.6474710	-0.3599510	3.4531420	H	4.3626440	3.4575020	-1.9738020
H	-3.2536360	-2.0138350	2.9493850	C	3.9544200	3.4116370	0.1415690
C	3.7254510	-3.0883430	0.9524250	C	2.9912180	3.0734080	1.1074120
H	3.9187720	-3.5057700	-0.0414190	H	3.2021960	3.2577090	2.1587190
H	4.5484320	-3.3907770	1.6102640	C	1.7599620	2.5317380	0.7451350
H	2.8020140	-3.5290900	1.3426550	H	1.0265930	2.3156100	1.5106210
C	3.3590440	-1.0038920	2.3132390	C	-1.8975550	-2.2168140	-1.6580890
H	4.1858540	-1.2756720	2.9806060	C	-1.4243850	-1.2169380	-2.5522160
H	3.2733310	0.0864340	2.3073750	C	-0.0028500	-1.4350770	-2.7647020
H	2.4318230	-1.4096220	2.7230510	C	0.3572630	-2.6587490	-2.0804360
C	4.9422900	-0.9685880	0.3488820	C	-0.7832230	-3.1103850	-1.3507090
H	4.9035580	0.1239430	0.3071970	O	-0.6852960	0.5502230	2.2635330
H	5.7797680	-1.2572650	0.9948830	O	-1.1476660	-1.4512350	1.3522140
H	5.1340110	-1.3328690	-0.6624380	C	-1.0710680	-0.6814170	2.3385680
C	5.6005560	3.6969000	0.6200110	C	-1.4739000	-1.1627380	3.7381630
H	6.4257850	3.2701600	0.0411690	Rh	-0.3052890	-1.1165450	-0.6496280

C	0.1031420	1.8971110	-1.0652330	O	2.9158850	-0.7148990	-1.1892770
O	-0.3738960	2.3170850	-2.1152860	C	2.6350750	-0.9161660	-0.0051540
O	-2.0374450	1.2290480	-0.4011500	C	3.7565050	-1.1908600	1.0358860
H	-0.4997850	0.8712680	1.0855100	C	-2.4695630	2.4099280	0.1452190
C	0.8689050	-0.6495740	-3.6961900	O	-1.7344240	3.1890500	0.7046100
H	1.8909130	-0.6216650	-3.3161330	C	-3.9729510	2.6265420	-0.0844560
H	0.8648090	-1.0993800	-4.6983480	C	-4.4305080	3.7857090	0.8174860
H	0.5093820	0.3782750	-3.7846200	H	-3.8592610	4.6931970	0.6113920
C	1.6795360	-3.3547640	-2.1676740	H	-5.4921240	3.9904280	0.6440760
H	1.6683000	-4.0343370	-3.0303250	H	-4.2950850	3.5424130	1.8754880
H	2.4918170	-2.6390000	-2.2860210	C	-4.7754070	1.3530790	0.2475840
H	1.8800870	-3.9537720	-1.2765720	H	-4.4867990	0.5177970	-0.3935830
C	-0.8818880	-4.3331660	-0.4892830	H	-4.6257120	1.0495480	1.2892450
H	-1.3650980	-5.1522120	-1.0375800	H	-5.8443770	1.5437030	0.1035780
H	0.1033940	-4.6789580	-0.1701350	C	-4.1725960	3.0101730	-1.5695360
H	-1.4740070	-4.1326560	0.4071390	H	-3.5944740	3.9032550	-1.8249170
C	-3.2940880	-2.4043140	-1.1486600	H	-3.8595220	2.2039960	-2.2367580
H	-3.7796190	-3.2416670	-1.6660570	H	-5.2311080	3.2232600	-1.7545420
H	-3.2929610	-2.6269670	-0.0784470	C	5.2942560	3.9648470	0.5510380
H	-3.9021100	-1.5125530	-1.3066190	H	5.7861900	4.4883440	-0.3015850
C	-2.2234230	-0.1449940	-3.2250190	H	5.1910950	4.6871120	1.4039560
H	-2.2610240	-0.3490740	-4.3026600	H	5.9773880	3.1436380	0.8896300
H	-3.2479220	-0.1145340	-2.8515470	C	3.9163310	-2.7277200	1.1151000
H	-1.7691860	0.8380400	-3.0742800	H	4.1772120	-3.1482310	0.1379320
O	1.4282100	-0.9881870	0.4865050	H	4.7150000	-2.9906680	1.8183630

H	2.9907040	-3.2035090	1.4613430	C	2.4170630	2.6629820	-1.5888950
C	3.3936160	-0.6437110	2.4268000	H	2.1700880	2.5192530	-2.6349860
H	4.1972860	-0.8666040	3.1389920	C	3.6478260	3.1877660	-1.2183250
H	3.2519840	0.4408920	2.3986840	H	4.3769410	3.4391730	-1.9846950
H	2.4680320	-1.0935480	2.7968860	C	3.9626570	3.4061580	0.1329630
C	5.0743130	-0.5661700	0.5483060	C	3.0056920	3.0672070	1.0972240
H	4.9865240	0.5226380	0.4837510	H	3.2213630	3.2430990	2.1481440
H	5.8862910	-0.8049850	1.2438120	C	1.7734130	2.5218590	0.7351490
H	5.3371920	-0.9359670	-0.4448410	H	1.0420970	2.2996790	1.5019300
C	-1.8579850	-2.6495640	3.7150650	C	-1.9176810	-2.2245360	-1.6325530
H	-1.0259830	-3.2702100	3.3708800	C	-1.4465300	-1.2317250	-2.5356440
H	-2.1334700	-2.9736870	4.7240830	C	-0.0275140	-1.4571310	-2.7568180
H	-2.7099190	-2.8323340	3.0540150	C	0.3324210	-2.6778920	-2.0674660
C	-0.2790330	-0.9371700	4.6914260	C	-0.8049630	-3.1209670	-1.3273910
H	0.0117630	0.1152440	4.7150220	O	-0.6776950	0.5673630	2.2575870
H	-0.5547580	-1.2467550	5.7051510	O	-1.1465710	-1.4412560	1.3654600
H	0.5906230	-1.5260600	4.3826040	C	-1.0646620	-0.6620090	2.3449010
C	-2.6759090	-0.3092600	4.2049190	C	-1.4632230	-1.1324310	3.7497600
H	-3.5395300	-0.4457710	3.5442550	Rh	-0.3147110	-1.1248990	-0.6413550
H	-2.9750890	-0.6128270	5.2136420	C	0.1169060	1.8839600	-1.0742100
H	-2.4197870	0.7526310	4.2228840	O	-0.3543000	2.2920750	-2.1312890
				O	-2.0295180	1.2353900	-0.4048420
4'				H	-0.5250020	0.8268400	1.2725710
N	-0.5975110	1.0107790	-0.2085290	C	0.8418960	-0.6809490	-3.6981290
C	1.4683100	2.3131240	-0.6154710	H	1.8670930	-0.6589870	-3.3264360

H	0.8261920	-1.1339290	-4.6987390	C	-4.4073730	3.7999060	0.8194080
H	0.4893820	0.3492990	-3.7866570	H	-3.8302780	4.7070080	0.6287740
C	1.6529730	-3.3764340	-2.1595270	H	-5.4673160	4.0131860	0.6461450
H	1.6489630	-4.0318340	-3.0406930	H	-4.2768180	3.5396460	1.8740610
H	2.4683260	-2.6598640	-2.2511590	C	-4.7653470	1.3788100	0.2101240
H	1.8419060	-4.0000370	-1.2829610	H	-4.4789070	0.5515590	-0.4422590
C	-0.9032470	-4.3377810	-0.4574380	H	-4.6229320	1.0583450	1.2476770
H	-1.3965130	-5.1571880	-0.9961370	H	-5.8323260	1.5784040	0.0636440
H	0.0825880	-4.6876840	-0.1446900	C	-4.1446810	3.0596480	-1.5787150
H	-1.4859020	-4.1278900	0.4430100	H	-3.5605890	3.9534020	-1.8174030
C	-3.3116570	-2.4019990	-1.1126730	H	-3.8329290	2.2619940	-2.2569430
H	-3.8107360	-3.2293070	-1.6333830	H	-5.2012520	3.2810510	-1.7648780
H	-3.3037710	-2.6341440	-0.0446130	C	5.2852010	4.0195720	0.5262110
H	-3.9110380	-1.5021380	-1.2570120	H	6.1152220	3.5662970	-0.0257220
C	-2.2460470	-0.1603940	-3.2089860	H	5.3017010	5.0945580	0.3071810
H	-2.3016450	-0.3767360	-4.2835060	H	5.4817010	3.8979320	1.5950270
H	-3.2645500	-0.1157230	-2.8208810	C	3.8972210	-2.7488360	1.1177140
H	-1.7806220	0.8198730	-3.0762660	H	4.6996780	-3.0112090	1.8168630
O	1.4266980	-0.9994000	0.4837360	H	2.9698980	-3.2061200	1.4783320
O	2.9048590	-0.7363770	-1.2020230	H	4.1447840	-3.1848360	0.1438110
C	2.6308860	-0.9328400	-0.0152760	C	3.4117960	-0.6426080	2.4064510
C	3.7576330	-1.2115000	1.0198730	H	4.2147930	-0.8723820	3.1171880
C	-2.4516820	2.4252290	0.1301260	H	3.2945610	0.4440420	2.3668360
O	-1.7089180	3.2056240	0.6774390	H	2.4798940	-1.0670080	2.7857850
C	-3.9535650	2.6517790	-0.0986590	C	5.0782830	-0.6073770	0.5145940

H	5.0053340	0.4810990	0.4356020	C	-1.8182440	0.9078380	-1.8973110
H	5.8923010	-0.8485010	1.2082860	C	1.5795050	0.2651980	-3.4231180
H	5.3310440	-0.9944500	-0.4746640	H	2.4575410	0.8496170	-3.1356530
C	-0.2589990	-0.9154590	4.6931090	H	1.7687670	-0.7791460	-3.1734560
H	0.0461160	0.1331050	4.7059730	H	1.4659700	0.3529780	-4.5122850
H	-0.5317850	-1.2128770	5.7112730	C	-1.0524980	-1.4303210	-2.8023930
H	0.6004610	-1.5186210	4.3831610	H	-1.9339930	-1.8321570	-2.3007780
C	-2.6522500	-0.2637560	4.2214830	H	-1.1900760	-1.5540840	-3.8842520
H	-3.5221700	-0.3937620	3.5677760	H	-0.1808550	-2.0094610	-2.4901110
H	-2.9472850	-0.5591400	5.2338640	C	-3.2454790	0.5966740	-1.5654430
H	-2.3843490	0.7953030	4.2323100	H	-3.5859960	1.1602830	-0.6947370
C	-1.8636110	-2.6151230	3.7369730	H	-3.8889490	0.8664170	-2.4138430
H	-2.1334980	-2.9318770	4.7498560	H	-3.3945100	-0.4615940	-1.3485550
H	-2.7234330	-2.7915490	3.0844070	C	-1.9273650	3.4668600	-1.3450620
H	-1.0415400	-3.2462250	3.3880260	H	-1.2200020	4.2532700	-1.0748960
5'				H	-2.5984140	3.8659110	-2.1163040
Rh	-0.0500960	0.8669260	-0.6236560	H	-2.5302470	3.2418100	-0.4619370
O	1.6437310	1.6456300	0.4623850	C	0.0913670	2.1573090	-2.3724390
C	0.9199660	1.9447890	1.4690590	C	1.0824540	3.2721970	-2.5233420
O	-0.3400430	1.7841850	1.3556720	H	1.1735640	3.5575490	-3.5786450
C	1.5395720	2.4151090	2.7820420	H	0.7832650	4.1584650	-1.9602600
C	0.3453180	0.7690090	-2.7385460	H	2.0718670	2.9699360	-2.1704220
C	-1.2271470	2.2412340	-1.8496020	C	-3.8333850	-0.5824890	1.8148370
C	-0.8571540	0.0196130	-2.4859930	C	-2.4588750	-0.6793610	1.5830840
				C	-1.9377440	-1.7742710	0.8820920

C	-2.8191920	-2.7698120	0.4343200	H	5.5040120	-1.7470050	0.8239850
C	-4.1903470	-2.6521460	0.6469760	C	2.9652120	2.9411260	2.5439500
C	-4.7225860	-1.5584400	1.3485200	H	3.4107700	3.2448900	3.4972830
H	-4.2198340	0.2666460	2.3747400	H	3.5995140	2.1750900	2.0923400
H	-2.4079070	-3.6418040	-0.0645260	H	2.9637830	3.8106100	1.8785310
H	-4.8586640	-3.4289150	0.2817990	C	1.5811420	1.1813630	3.7178720
C	-0.4601720	-2.0181660	0.7147970	H	2.0345870	1.4613710	4.6748950
O	-0.0118880	-3.1546850	0.8935520	H	0.5744050	0.8007860	3.9112130
N	0.3039250	-0.9215090	0.4196240	H	2.1718780	0.3721090	3.2788250
H	-1.7913870	0.0915680	1.9512350	C	0.6555960	3.5123930	3.4058750
O	1.6920790	-1.2525380	0.5849700	H	1.0633010	3.8090330	4.3780480
C	2.2556350	-2.0401940	-0.3647660	H	0.6201760	4.4040360	2.7701500
O	1.7625000	-2.2803310	-1.4480680	H	-0.3674200	3.1581390	3.5514380
C	3.6197340	-2.5610040	0.1130160	C	-6.2048380	-1.4632080	1.6248340
C	3.3916300	-3.4589790	1.3506970	H	-6.7956620	-1.8268420	0.7777690
H	2.6975250	-4.2722990	1.1239820	H	-6.4847280	-2.0693250	2.4957280
H	4.3468800	-3.8898770	1.6713120	H	-6.5090770	-0.4332810	1.8339650
H	2.9682830	-2.8865070	2.1785670				
C	4.2579140	-3.3790020	-1.0210270	TS6'			
H	3.6202650	-4.2185850	-1.3088560	Rh	0.5933980	-0.0220660	0.7184390
H	4.4222230	-2.7663190	-1.9123100	O	-0.0597320	1.9709320	0.4085880
H	5.2248900	-3.7735790	-0.6914190	C	0.2698790	2.6242580	-0.6306280
C	4.5317510	-1.3717320	0.4861710	O	1.0353230	2.1634120	-1.5291950
H	4.7047840	-0.7170150	-0.3750760	C	-0.2929770	4.0431420	-0.8276540
H	4.0946750	-0.7714320	1.2869810	C	-0.1963200	-0.8132170	2.6130810

C	1.9735420	0.0426940	2.4394080	C	1.7384930	-0.3333140	-1.1796140
C	0.6383260	-1.8208050	1.9800000	C	0.9672970	-1.2094100	-1.9764540
C	1.9717830	-1.3003810	1.9111880	C	1.5737830	-2.0757280	-2.8855550
C	-1.6325940	-0.9894050	3.0063070	C	2.9620910	-2.0874240	-3.0049910
H	-2.1753010	-0.0408780	2.9847780	C	3.7678710	-1.2241190	-2.2402500
H	-2.1388760	-1.6877180	2.3389930	H	3.7523980	0.3422290	-0.7747470
H	-1.6978170	-1.3859000	4.0284220	H	0.9445740	-2.7234940	-3.4887500
C	0.1926900	-3.1978880	1.5880200	H	3.4343970	-2.7648240	-3.7133680
H	0.9208140	-3.6778170	0.9302120	C	-0.5271010	-1.1642830	-1.8438310
H	0.0833820	-3.8280160	2.4804930	O	-1.3075810	-1.5834430	-2.7005270
H	-0.7670600	-3.1639510	1.0670910	N	-0.8497560	-0.5882560	-0.6548070
C	3.1802800	-2.0731560	1.4766780	H	1.3373710	0.9153890	-1.1863570
H	3.9987790	-1.4161270	1.1803890	O	-2.2298910	-0.2762440	-0.5469620
H	3.5316980	-2.6906720	2.3136670	C	-3.0616120	-1.3313810	-0.3064140
H	2.9624950	-2.7368120	0.6383320	O	-2.6947860	-2.4207780	0.0766030
C	3.1757720	0.9175140	2.6507120	C	-4.5186130	-0.9321910	-0.5779570
H	2.9059630	1.9764850	2.6327770	C	-4.6641470	-0.6518040	-2.0921020
H	3.6476120	0.7132110	3.6210180	H	-4.3553340	-1.5174660	-2.6838850
H	3.9304060	0.7555100	1.8772610	H	-5.7108180	-0.4234360	-2.3224790
C	0.6324070	0.3188740	2.8979200	H	-4.0431160	0.1930330	-2.3969440
C	0.1873500	1.5842080	3.5645840	C	-5.4309310	-2.0978750	-0.1648840
H	-0.8791700	1.7607600	3.4139870	H	-5.1853760	-3.0059880	-0.7206380
H	0.3738280	1.5246590	4.6445660	H	-5.3312200	-2.3244500	0.9008390
H	0.7264560	2.4505540	3.1760160	H	-6.4755990	-1.8378590	-0.3654670
C	3.1397150	-0.3616540	-1.3363580	C	-4.8790040	0.3355180	0.2275150

H	-4.7755010	0.1663350	1.3053380	C	-1.0144300	4.0139770	-0.8160850
H	-4.2430620	1.1788840	-0.0507450	C	0.6990160	-1.8124080	-2.0979660
H	-5.9212910	0.6097130	0.0318680	C	-1.5835850	-1.4068730	-2.3491410
C	-1.1080270	4.4958140	0.3928320	C	-0.0323470	-2.6058120	-1.1068680
H	-1.5059780	5.5011190	0.2170920	C	-1.4471700	-2.4258780	-1.3655510
H	-1.9465190	3.8211610	0.5828520	C	2.1841910	-1.8501430	-2.3021230
H	-0.4919210	4.5277270	1.2964670	H	2.5696930	-0.8954920	-2.6691260
C	-1.1954960	4.0016400	-2.0825400	H	2.7027960	-2.0938190	-1.3745850
H	-1.6008910	4.9999690	-2.2798350	H	2.4418810	-2.6195060	-3.0420980
H	-0.6307690	3.6737030	-2.9584460	C	0.5816510	-3.6278520	-0.1951300
H	-2.0365270	3.3149990	-1.9408800	H	-0.1236620	-3.9385930	0.5793200
C	0.8887890	5.0061940	-1.0696070	H	0.8740640	-4.5233860	-0.7600060
H	0.5111580	6.0160920	-1.2624750	H	1.4669720	-3.2227210	0.3000960
H	1.5463420	5.0562920	-0.1942090	C	-2.5464760	-3.2421000	-0.7547560
H	1.4849020	4.6865000	-1.9272220	H	-3.5174150	-2.7502250	-0.8403460
C	5.2679200	-1.2135240	-2.4248690	H	-2.6167230	-4.2059610	-1.2753230
H	5.7620190	-0.6120310	-1.6563980	H	-2.3653160	-3.4442100	0.3024820
H	5.6843660	-2.2260750	-2.3811790	C	-2.8591360	-0.8958600	-2.9545560
H	5.5449270	-0.7948560	-3.3998260	H	-2.7848670	0.1680800	-3.1955540
				H	-3.0957660	-1.4290540	-3.8850660
7'				H	-3.7058610	-1.0245000	-2.2756110
Rh	-0.5073510	-0.5858930	-0.5937660	C	-0.2393550	-1.0582960	-2.8221340
O	-0.8590950	1.5958110	-1.0213130	C	0.0376620	-0.0667770	-3.9123650
C	-1.0633870	2.5767910	-0.2994540	H	1.1029680	0.1629670	-3.9845160
O	-1.3350090	2.4854380	0.9908090	H	-0.2873430	-0.4593190	-4.8843860

H	-0.4974860	0.8716930	-3.7392910	H	5.6174050	1.6880450	2.0415830
C	-2.9332620	-0.7127550	1.3753300	C	5.7178930	-0.8020170	0.8605820
C	-1.5511370	-0.5605100	1.1860330	H	5.5993530	-1.4102310	1.7601100
C	-0.7532470	-0.3673050	2.3316610	H	5.7075510	-1.4776860	-0.0003340
C	-1.3052680	-0.3778230	3.6159450	H	6.6949010	-0.3086170	0.8975540
C	-2.6752770	-0.5660770	3.7757230	C	-0.8074480	4.0200870	-2.3379620
C	-3.5093370	-0.7250900	2.6572970	H	-0.7575310	5.0534010	-2.6951920
H	-3.5923740	-0.8219290	0.5164240	H	0.1209150	3.5148030	-2.6163460
H	-0.6442990	-0.2218730	4.4640320	H	-1.6321020	3.5208320	-2.8552990
H	-3.1097050	-0.5713250	4.7726810	C	0.1713620	4.7202230	-0.1141280
C	0.6979040	-0.0601770	2.1171380	H	0.2367230	5.7548710	-0.4659240
O	1.5111130	0.1628670	3.0152400	H	0.0410730	4.7297010	0.9704960
N	0.9272570	-0.0072720	0.7725470	H	1.1194640	4.2227030	-0.3421690
H	-1.3321670	1.5383810	1.2632650	C	-2.3370160	4.7254190	-0.4516480
O	2.2462740	0.4177960	0.4544790	H	-2.3031200	5.7602310	-0.8070820
C	3.2481700	-0.4616000	0.7580710	H	-3.1953440	4.2356930	-0.9241370
O	3.0786980	-1.6382730	0.9885230	H	-2.4990380	4.7356570	0.6283210
C	4.6063070	0.2544160	0.7581080	C	-4.9972390	-0.9262750	2.8322710
C	4.7807860	1.0854380	-0.5312780	H	-5.5435370	-0.7011170	1.9112890
H	4.0063240	1.8504870	-0.6208160	H	-5.2280900	-1.9637710	3.1058010
H	5.7568730	1.5825040	-0.5177090	H	-5.3971600	-0.2888350	3.6275780
H	4.7427510	0.4509700	-1.4239650				
C	4.6438730	1.1872770	1.9917980	9			
H	3.8578270	1.9430400	1.9353540	C	1.6079030	-2.1410730	-0.9789780
H	4.4913400	0.6230980	2.9153540	C	0.3236590	-1.5965540	-0.8828450

C	-0.5743130	-1.8255150	-1.9306210	H	-4.6893720	1.9030210	-1.5214890
C	-0.2061480	-2.5855460	-3.0444860	H	-6.3653100	2.1686340	-1.0122580
C	1.0708970	-3.1299520	-3.1189600	C	0.3441070	-1.9829570	2.2549000
C	1.9957770	-2.9133970	-2.0858410	C	-1.0893910	-2.0221180	2.1984860
H	2.3401350	-1.9748710	-0.1938530	C	-1.5860330	-0.7404070	2.6718020
H	-0.9382540	-2.7291430	-3.8341400	C	-0.4657520	0.0890500	2.9376620
H	1.3601520	-3.7231890	-3.9832440	C	0.7380280	-0.6619450	2.6390320
C	-1.9288970	-1.2237070	-1.8271630	C	-1.9370500	-3.2218000	1.8918090
O	-2.7802640	-1.2199010	-2.7164670	H	-2.3172750	-3.6692190	2.8197290
Rh	-0.4564540	-0.4917480	0.6982010	H	-2.7896120	-2.9489580	1.2644690
N	-2.0831910	-0.7094580	-0.5657110	H	-1.3605450	-3.9864820	1.3663930
C	-4.4196390	-0.6510470	-0.2836190	C	-3.0258240	-0.4251900	2.9504820
O	-4.4477680	-1.7974640	0.1060900	H	-3.6862330	-1.0055930	2.3059450
O	-3.2747060	0.0723900	-0.4703980	H	-3.2694510	-0.6748540	3.9916480
C	-5.6747640	0.1503310	-0.6587210	H	-3.2484720	0.6350050	2.8057030
C	-6.7682400	-0.1486440	0.3843150	C	-0.4805540	1.4652240	3.5346400
H	-6.5067520	0.2639480	1.3656730	H	0.2015140	2.1419560	3.0110240
H	-7.7153550	0.3033860	0.0719700	H	-1.4804570	1.9037020	3.5127000
H	-6.9125430	-1.2252050	0.4955400	H	-0.1604620	1.4278730	4.5836820
C	-6.1029350	-0.3925480	-2.0462290	C	1.2483680	-3.1663950	2.0844680
H	-5.2951420	-0.2773720	-2.7731050	H	2.2877190	-2.8684750	1.9342120
H	-6.3496440	-1.4558140	-1.9834490	H	1.2113420	-3.7827880	2.9919990
H	-6.9870970	0.1522950	-2.3951780	H	0.9523790	-3.7924540	1.2409080
C	-5.4276390	1.6655380	-0.7522570	C	2.1326400	-0.1943170	2.9413110
H	-5.0815340	2.0800440	0.2006960	H	2.8794220	-0.7155510	2.3384710

H	2.2434010	0.8767150	2.7550910	H	-3.2505280	4.6167030	-0.7044590
H	2.3787670	-0.3706720	3.9968320	H	-2.4487970	5.2120730	0.7406320
F	1.7620260	0.8376190	-2.2817000	C	6.2226030	-0.2014140	-0.7148970
F	1.8116740	2.8093920	-1.3079090	H	5.7276200	-0.9259690	-1.3576920
C	-0.5164200	1.6060260	0.0942280	C	7.4016240	-0.5521350	-0.0554670
C	0.5882180	1.1410560	-0.2800440	H	7.8174190	-1.5475740	-0.1855330
C	3.1476930	1.1034300	-0.3805960	C	8.0504930	0.3760140	0.7613030
H	3.1410230	0.0383330	-0.1398850	H	8.9707590	0.1062940	1.2714580
H	3.1960350	1.6528890	0.5650230	C	-1.9567090	6.3142950	-1.0542950
C	5.6700590	1.0791220	-0.5710590	H	-2.7458460	7.0612230	-0.9203740
C	-1.5725730	2.6258290	0.2346860	H	-1.8343120	6.1476140	-2.1301760
H	-1.7494970	2.8278440	1.2993380	H	-1.0218510	6.7451020	-0.6782710
H	-2.5058160	2.2152840	-0.1608140	C	3.3929160	-3.4839310	-2.1769190
C	4.3701880	1.4425240	-1.2558690	H	3.9703480	-2.9960270	-2.9721340
H	4.2804290	0.9049410	-2.2046470	H	3.9432330	-3.3546410	-1.2397690
H	4.3521000	2.5114850	-1.4902150	H	3.3743500	-4.5546550	-2.4090800
C	1.8249010	1.4451410	-1.0491930				
C	-1.2095660	3.9383860	-0.4922610	TS10			
H	-0.2524650	4.3156090	-0.1127570	C	-1.8636980	-3.0859220	0.2971390
H	-1.0540340	3.7230840	-1.5558020	C	-1.6228500	-1.7940030	-0.2063950
C	6.3335620	2.0017730	0.2493860	C	-2.2917240	-1.3995340	-1.3804260
H	5.9247780	3.0033180	0.3638060	C	-3.1371210	-2.2871000	-2.0498160
C	7.5130530	1.6558940	0.9106930	C	-3.3548530	-3.5633550	-1.5389860
H	8.0153160	2.3877530	1.5373750	C	-2.7321940	-3.9740430	-0.3458380
C	-2.2959460	5.0084520	-0.3286070	H	-1.3525290	-3.4180020	1.1981760

H	-3.6170600	-1.9487590	-2.9635550	C	-0.4560160	0.6954400	3.0058760
H	-4.0167330	-4.2508510	-2.0601030	C	-1.0489190	-0.6037480	3.1634090
C	-2.0963740	-0.0018640	-1.8669830	C	-3.9950580	1.3836860	1.8627030
O	-2.2459880	0.3512360	-3.0367190	H	-4.3943470	2.0735180	2.6176620
Rh	-1.1087710	-0.0700190	0.9790770	H	-3.8761370	1.9318130	0.9241180
N	-1.7664650	0.7926650	-0.8031020	H	-4.7385220	0.5988950	1.7053750
C	-2.0784060	3.0689560	-1.3624140	C	-1.2965110	3.0364580	2.1901760
O	-3.1961020	3.0878270	-0.8927910	H	-2.0051410	3.3771610	1.4336710
O	-1.2117270	2.0270360	-1.2601580	H	-1.4968360	3.5979470	3.1128570
C	-1.4476390	4.2030760	-2.1845600	H	-0.2888500	3.2898440	1.8537060
C	-2.2554700	5.4899080	-1.9524880	C	0.9271980	1.0861680	3.4382720
H	-2.1926720	5.8175050	-0.9094230	H	1.6135220	0.2354890	3.4060540
H	-1.8620730	6.2927620	-2.5849930	H	1.3373140	1.8748360	2.8068460
H	-3.3108410	5.3412540	-2.1911010	H	0.9100630	1.4516640	4.4734040
C	-1.5412850	3.7760120	-3.6706110	C	-3.4691850	-1.5945520	2.9334640
H	-1.0399580	2.8204550	-3.8372240	H	-3.9177460	-1.5650840	3.9348230
H	-2.5848710	3.6616600	-3.9790440	H	-4.2736830	-1.4891720	2.2027230
H	-1.0780370	4.5433470	-4.3010550	H	-3.0305500	-2.5852200	2.7970400
C	0.0291560	4.4223730	-1.7964070	C	-0.3953730	-1.7904880	3.8133780
H	0.1241470	4.7131950	-0.7442980	H	-0.8548650	-2.7294690	3.4950840
H	0.6265450	3.5233060	-1.9540180	H	0.6711680	-1.8437120	3.5793640
H	0.4465290	5.2321800	-2.4051910	H	-0.4895900	-1.7378790	4.9062050
C	-2.4475240	-0.5057050	2.7883500	F	1.7826420	1.0966580	-1.6347830
C	-2.6887990	0.8115990	2.3259380	F	1.5918550	1.9556960	0.3833860
C	-1.4396000	1.5630480	2.4357650	C	0.3419070	-1.3993620	-0.2258020

C	0.6649010	-0.1692960	-0.0245860	H	8.1835240	-1.1021300	-1.4103070
C	3.1813380	0.2393060	0.0660070	C	8.1935130	-0.4428880	0.6430540
H	3.3515260	-0.6815370	-0.5007190	H	9.1664920	-0.8725370	0.8634420
H	3.1820900	-0.0311820	1.1271440	C	1.2747580	-4.9155530	-3.8169870
C	5.6755650	0.6807190	0.0686120	H	1.8169710	-5.8432010	-4.0275140
C	0.9874770	-2.7048550	-0.5890530	H	1.6187030	-4.1584580	-4.5303650
H	0.6575090	-3.4898170	0.0987630	H	0.2125450	-5.0963200	-4.0154240
H	2.0660190	-2.5797570	-0.4238550	C	-3.0027810	-5.3467210	0.2263590
C	4.3065550	1.2518160	-0.2312630	H	-2.9187580	-6.1229490	-0.5417700
H	4.2418870	1.5446750	-1.2835740	H	-2.3034810	-5.5923100	1.0310310
H	4.1354910	2.1548000	0.3628060	H	-4.0174990	-5.4122930	0.6377010
C	1.7930410	0.7647040	-0.2936850				
C	0.7462930	-3.1576870	-2.0416240	11			
H	-0.3260160	-3.2974360	-2.2090070	C	0.8962450	-3.5080840	0.1982220
H	1.0666870	-2.3592030	-2.7223640	C	0.9200900	-2.1708730	0.6607000
C	6.2433330	0.8050100	1.3441030	C	2.1828620	-1.5630940	0.9079610
H	5.7056050	1.3507900	2.1164080	C	3.3616210	-2.3105890	0.6967550
C	7.4907800	0.2489370	1.6313210	C	3.3016950	-3.6165060	0.2433510
H	7.9165110	0.3614620	2.6246530	C	2.0587640	-4.2415560	-0.0097420
C	1.4955290	-4.4548470	-2.3726350	H	-0.0692180	-3.9794210	0.0301300
H	2.5705730	-4.3147890	-2.1930090	H	4.3191840	-1.8511720	0.9237550
H	1.1718460	-5.2460290	-1.6819690	H	4.2205540	-4.1801450	0.0994350
C	6.3929330	-0.0145760	-0.9147130	C	2.2351110	-0.2043120	1.5964020
H	5.9718290	-0.1121280	-1.9128680	O	2.4229400	-0.0884360	2.8022340
C	7.6407240	-0.5721330	-0.6325110	Rh	1.1309260	-0.1713650	-0.9964010

N	2.0178430	0.7515260	0.6557760	H	4.6421630	0.7058740	-2.4105130
C	2.2241340	3.0886560	1.0058180	C	0.9106220	2.7180350	-2.5231560
O	3.1109170	3.1926790	0.1834280	H	1.6465460	3.2054780	-1.8813030
O	1.5532500	1.9491840	1.2862170	H	0.9766300	3.1730230	-3.5214320
C	1.6988710	4.2274560	1.8957100	H	-0.0838170	2.9197370	-2.1221040
C	2.3916480	5.5352900	1.4832280	C	-1.2349000	0.4712730	-3.2977110
H	2.1623580	5.7977150	0.4460820	H	-1.8355450	-0.4354020	-3.1941360
H	2.0504540	6.3523580	2.1275300	H	-1.6634490	1.2455220	-2.6612460
H	3.4779630	5.4536240	1.5712630	H	-1.3186720	0.8049440	-4.3404570
C	2.0416510	3.8790580	3.3636980	C	3.3964870	-1.7828450	-3.0039910
H	1.6036810	2.9215840	3.6537950	H	3.1899250	-2.6379580	-2.3530240
H	3.1251200	3.8135680	3.5089150	H	3.4509540	-2.1575050	-4.0339720
H	1.6583740	4.6621100	4.0271200	H	4.3793370	-1.3910910	-2.7359350
C	0.1684430	4.3595920	1.7309710	C	0.3255460	-2.3462040	-3.4246450
H	-0.0974480	4.5995660	0.6956620	H	0.8506960	-3.1637240	-2.9235260
H	-0.3496260	3.4398070	2.0079260	H	-0.7319910	-2.4179470	-3.1592310
H	-0.1959880	5.1738260	2.3671280	H	0.4107070	-2.5131560	-4.5068620
C	2.3319190	-0.7347290	-2.8889720	F	-1.7381540	1.0688110	1.6991640
C	2.5049100	0.6395300	-2.6584680	F	-1.3778060	1.8013260	-0.3446820
C	1.1741760	1.2453450	-2.6116420	C	-0.3571680	-1.4363940	0.9805690
C	0.2043880	0.2238170	-2.9637790	C	-0.5110200	-0.3316840	0.2318430
C	0.8989440	-1.0121490	-3.0433980	C	-3.0283340	0.1445180	-0.0545610
C	3.7895750	1.3865680	-2.4656880	H	-3.2612770	-0.7625390	0.5100990
H	3.9627530	2.0682500	-3.3081730	H	-2.9669790	-0.1503780	-1.1058950
H	3.7630450	1.9798550	-1.5477600	C	-5.4912590	0.6849160	-0.3234700

C	-1.2289090	-1.9822990	2.0972740	H	-0.1403800	-1.9910760	6.2094030
H	-1.6766850	-2.9384550	1.7833900	H	0.1278060	-3.6778560	5.7586340
H	-2.0551760	-1.2915640	2.2814600	C	2.0106920	-5.6811130	-0.4642710
C	-4.1435370	1.1922710	0.1409300	H	2.4120560	-6.3499950	0.3060570
H	-4.1848670	1.4634640	1.2004800	H	0.9877250	-5.9990330	-0.6823180
H	-3.8764170	2.1003080	-0.4084640	H	2.6135080	-5.8364810	-1.3662660
C	-1.6490420	0.6411530	0.3787920				
C	-0.4674530	-2.2057350	3.4191240	9'			
H	0.3239130	-2.9514170	3.2669600	C	1.6079030	-2.1410730	-0.9789780
H	0.0429230	-1.2782760	3.7033560	C	0.3236590	-1.5965540	-0.8828450
C	-5.9428370	0.9341320	-1.6267420	C	-0.5743130	-1.8255150	-1.9306210
H	-5.3278760	1.5292290	-2.2984750	C	-0.2061480	-2.5855460	-3.0444860
C	-7.1715370	0.4408460	-2.0685740	C	1.0708970	-3.1299520	-3.1189600
H	-7.5055390	0.6511540	-3.0809930	C	1.9957770	-2.9133970	-2.0858410
C	-1.3876680	-2.6695220	4.5551820	H	2.3401350	-1.9748710	-0.1938530
H	-2.1749330	-1.9190480	4.7111950	H	-0.9382540	-2.7291430	-3.8341400
H	-1.9037450	-3.5928400	4.2552000	H	1.3601520	-3.7231890	-3.9832440
C	-6.3076050	-0.0720750	0.5288130	C	-1.9288970	-1.2237070	-1.8271630
H	-5.9787020	-0.2673570	1.5470780	O	-2.7802640	-1.2199010	-2.7164670
C	-7.5365860	-0.5680470	0.0920620	Rh	-0.4564540	-0.4917480	0.6982010
H	-8.1565010	-1.1478550	0.7704050	N	-2.0831910	-0.7094580	-0.5657110
C	-7.9727370	-0.3136940	-1.2098230	C	-4.4196390	-0.6510470	-0.2836190
H	-8.9311880	-0.6952960	-1.5499520	O	-4.4477680	-1.7974640	0.1060900
C	-0.6410950	-2.9051200	5.8720440	O	-3.2747060	0.0723900	-0.4703980
H	-1.3223970	-3.2268960	6.6669370	C	-5.6747640	0.1503310	-0.6587210

C	-6.7682400	-0.1486440	0.3843150	C	-0.4805540	1.4652240	3.5346400
H	-6.5067520	0.2639480	1.3656730	H	0.2015140	2.1419560	3.0110240
H	-7.7153550	0.3033860	0.0719700	H	-1.4804570	1.9037020	3.5127000
H	-6.9125430	-1.2252050	0.4955400	H	-0.1604620	1.4278730	4.5836820
C	-6.1029350	-0.3925480	-2.0462290	C	1.2483680	-3.1663950	2.0844680
H	-5.2951420	-0.2773720	-2.7731050	H	2.2877190	-2.8684750	1.9342120
H	-6.3496440	-1.4558140	-1.9834490	H	1.2113420	-3.7827880	2.9919990
H	-6.9870970	0.1522950	-2.3951780	H	0.9523790	-3.7924540	1.2409080
C	-5.4276390	1.6655380	-0.7522570	C	2.1326400	-0.1943170	2.9413110
H	-5.0815340	2.0800440	0.2006960	H	2.8794220	-0.7155510	2.3384710
H	-4.6893720	1.9030210	-1.5214890	H	2.2434010	0.8767150	2.7550910
H	-6.3653100	2.1686340	-1.0122580	H	2.3787670	-0.3706720	3.9968320
C	0.3441070	-1.9829570	2.2549000	F	1.7620260	0.8376190	-2.2817000
C	-1.0893910	-2.0221180	2.1984860	F	1.8116740	2.8093920	-1.3079090
C	-1.5860330	-0.7404070	2.6718020	C	-0.5164200	1.6060260	0.0942280
C	-0.4657520	0.0890500	2.9376620	C	0.5882180	1.1410560	-0.2800440
C	0.7380280	-0.6619450	2.6390320	C	3.1476930	1.1034300	-0.3805960
C	-1.9370500	-3.2218000	1.8918090	H	3.1410230	0.0383330	-0.1398850
H	-2.3172750	-3.6692190	2.8197290	H	3.1960350	1.6528890	0.5650230
H	-2.7896120	-2.9489580	1.2644690	C	5.6700590	1.0791220	-0.5710590
H	-1.3605450	-3.9864820	1.3663930	C	-1.5725730	2.6258290	0.2346860
C	-3.0258240	-0.4251900	2.9504820	H	-1.7494970	2.8278440	1.2993380
H	-3.6862330	-1.0055930	2.3059450	H	-2.5058160	2.2152840	-0.1608140
H	-3.2694510	-0.6748540	3.9916480	C	4.3701880	1.4425240	-1.2558690
H	-3.2484720	0.6350050	2.8057030	H	4.2804290	0.9049410	-2.2046470

H	4.3521000	2.5114850	-1.4902150
C	1.8249010	1.4451410	-1.0491930
C	-1.2095660	3.9383860	-0.4922610
H	-0.2524650	4.3156090	-0.1127570
H	-1.0540340	3.7230840	-1.5558020
C	6.3335620	2.0017730	0.2493860
H	5.9247780	3.0033180	0.3638060
C	7.5130530	1.6558940	0.9106930
H	8.0153160	2.3877530	1.5373750
C	-2.2959460	5.0084520	-0.3286070
H	-3.2505280	4.6167030	-0.7044590
H	-2.4487970	5.2120730	0.7406320
C	6.2226030	-0.2014140	-0.7148970
H	5.7276200	-0.9259690	-1.3576920
C	7.4016240	-0.5521350	-0.0554670
H	7.8174190	-1.5475740	-0.1855330
C	8.0504930	0.3760140	0.7613030
H	8.9707590	0.1062940	1.2714580
C	-1.9567090	6.3142950	-1.0542950
H	-2.7458460	7.0612230	-0.9203740
H	-1.8343120	6.1476140	-2.1301760
H	-1.0218510	6.7451020	-0.6782710
C	3.3929160	-3.4839310	-2.1769190
H	3.9703480	-2.9960270	-2.9721340
H	3.9432330	-3.3546410	-1.2397690

H	3.3743500	-4.5546550	-2.4090800
TS10'			
C	0.1951620	-3.2587870	-0.5985470
C	-0.3037100	-1.9608690	-0.8144680
C	-0.9339380	-1.6838260	-2.0462990
C	-1.0026470	-2.6572730	-3.0429640
C	-0.4873260	-3.9297210	-2.8143040
C	0.1069220	-4.2487600	-1.5817990
H	0.7107200	-3.4874610	0.3274110
H	-1.4863160	-2.3980550	-3.9802490
H	-0.5503570	-4.6879800	-3.5910470
C	-1.5834460	-0.3560720	-2.2307610
O	-1.7957380	0.1757070	-3.3217270
Rh	-1.0526320	-0.6627980	0.7204180
N	-1.9352740	0.1337300	-1.0003300
C	-3.5880160	1.8013100	-1.2702120
O	-4.4847170	1.0112390	-1.0716690
O	-2.2646000	1.5269640	-1.1037000
C	-3.8036790	3.2283260	-1.7966780
C	-5.1406780	3.7576410	-1.2486620
H	-5.0962110	3.9072760	-0.1639130
H	-5.3770620	4.7212340	-1.7118580
H	-5.9512550	3.0574550	-1.4597770
C	-3.8786150	3.0834300	-3.3386450

H	-2.9804240	2.5959620	-3.7265920	H	-1.1562280	-4.2161240	1.5796960
H	-4.7420990	2.4768160	-3.6264580	H	-2.5590030	-4.2633400	2.6525970
H	-3.9816460	4.0733080	-3.7969520	H	-2.7674170	-3.9422020	0.9249540
C	-2.6586820	4.1864020	-1.4223540	C	0.3095490	-2.3649500	3.3340550
H	-2.5243920	4.2509270	-0.3371540	H	0.5762290	-3.2555330	2.7609660
H	-1.7124660	3.8730620	-1.8684800	H	1.1910610	-1.7210100	3.3741690
H	-2.8926950	5.1912200	-1.7905590	H	0.0870460	-2.6891780	4.3597740
C	-1.9894730	-2.2843050	2.0646080	C	0.6815170	-5.6258320	-1.3421510
C	-2.9521910	-1.2863600	1.7847860	H	0.9174330	-5.7851730	-0.2860010
C	-2.4636180	-0.0215630	2.3357680	H	-0.0147950	-6.4108670	-1.6563110
C	-1.2147750	-0.2779040	2.9769200	H	1.6080040	-5.7697660	-1.9113020
C	-0.8731520	-1.6535350	2.7407870	F	2.5579780	-1.9857100	0.7524900
C	-4.2851980	-1.4764870	1.1247210	F	2.5101200	-1.9419090	-1.4477240
H	-5.0895480	-1.4084430	1.8690810	C	0.4721820	0.5703400	0.0677490
H	-4.4612540	-0.7193090	0.3566730	C	0.9515360	-0.5893390	-0.2472940
H	-4.3551610	-2.4583010	0.6511080	C	3.4350510	-0.0826340	-0.3547800
C	-3.2751780	1.2398470	2.4025420	H	3.3398500	0.5285310	0.5471160
H	-3.9055110	1.3466070	1.5179560	H	3.2584050	0.5703970	-1.2150230
H	-3.9367410	1.2220130	3.2792230	C	5.9207930	0.3843190	-0.4458300
H	-2.6446560	2.1289540	2.4842540	C	0.7101520	2.0336980	-0.0347530
C	-0.4321410	0.6577940	3.8505890	H	-0.0237820	2.4219470	-0.7520380
H	0.6428350	0.5903560	3.6615230	H	1.7019440	2.1993310	-0.4768260
H	-0.7348240	1.6963930	3.7111180	C	4.8516640	-0.6869900	-0.4381100
H	-0.5932900	0.4048650	4.9068720	H	4.9984820	-1.3594930	0.4128710
C	-2.1224480	-3.7515760	1.7850860	H	4.9215340	-1.2963130	-1.3440440

C	2.3426750	-1.1486310	-0.3393500	C	0.5043610	-1.2059020	1.9153660
C	0.5910890	2.8395270	1.2668940	C	0.7764480	-2.3822700	2.6422240
H	-0.4188630	2.7081730	1.6710620	C	-0.1264760	-3.4310360	2.6665610
H	1.2859270	2.4403530	2.0171900	C	-1.3467540	-3.3498800	1.9609300
C	6.3481990	0.9617240	-1.6495240	H	-2.5545600	-2.1104790	0.7042580
H	5.9267510	0.6107350	-2.5888130	H	1.7035590	-2.4384780	3.2045390
C	7.3107180	1.9721430	-1.6576970	H	0.0986720	-4.3239530	3.2451340
H	7.6323770	2.4034270	-2.6015850	C	1.5070570	-0.0646880	1.9933950
C	0.8717510	4.3323700	1.0548620	O	1.7552970	0.5387960	3.0340220
H	1.8796230	4.4561270	0.6361020	Rh	1.0284110	-0.9494820	-0.7091710
H	0.1776750	4.7257300	0.3006050	N	2.0702220	0.0652640	0.7734220
C	6.4848490	0.8453310	0.7515230	C	4.1753770	1.0785620	1.0322440
H	6.1718770	0.4014030	1.6940740	O	4.7104230	0.0037590	1.1901700
C	7.4478860	1.8555700	0.7484860	O	2.8703900	1.2432930	0.6618940
H	7.8775440	2.1950420	1.6869580	C	4.8537460	2.4332620	1.2781500
C	7.8634150	2.4231080	-0.4574340	C	6.3705930	2.2665370	1.0851690
H	8.6154710	3.2068370	-0.4623420	H	6.6169420	2.0388200	0.0422350
C	0.7507430	5.1542680	2.3418470	H	6.8833090	3.1945770	1.3586280
H	0.9563990	6.2137730	2.1592290	H	6.7566850	1.4553480	1.7055970
H	1.4574230	4.8057100	3.1038410	C	4.5405220	2.7969940	2.7521730
H	-0.2573330	5.0812540	2.7666210	H	3.4629340	2.8100550	2.9321890
				H	4.9840370	2.0657650	3.4342100
11'				H	4.9580690	3.7833270	2.9827230
C	-1.6136630	-2.1909050	1.2415880	C	4.3162270	3.5336490	0.3446900
C	-0.7216210	-1.0903740	1.2068740	H	4.4712540	3.2762190	-0.7091260

H	3.2504670	3.7078520	0.5006890	H	-1.5964860	-2.5355460	-2.6495550
H	4.8505290	4.4694780	0.5413400	H	-0.7450800	-4.0211480	-3.0930710
C	1.6586650	-3.0774620	-1.4445850	C	-2.3403960	-4.4860260	2.0201100
C	2.7532980	-2.2243100	-1.6255560	H	-1.8680670	-5.4452610	1.7805350
C	2.2920190	-1.0866780	-2.4288760	H	-2.7666300	-4.5823110	3.0257240
C	0.9365790	-1.3664170	-2.8674990	H	-3.1683270	-4.3324940	1.3225550
C	0.5066730	-2.5298790	-2.1767570	F	-2.4117790	0.6411460	2.4283590
C	4.1412610	-2.3734910	-1.0781030	F	-2.0066920	2.3215700	1.0550720
H	4.8796730	-2.3179530	-1.8869280	C	-0.3638200	0.5364730	-0.5435970
H	4.3735140	-1.5929330	-0.3462410	C	-1.1149680	0.1894690	0.5153350
H	4.2681180	-3.3385890	-0.5820950	C	-3.6472340	0.7537060	0.4249170
C	3.1881980	-0.0038770	-2.9528380	H	-3.8929800	-0.3115340	0.4841660
H	3.9601370	0.2510150	-2.2235230	H	-3.5497720	0.9970730	-0.6383150
H	3.6926010	-0.3337090	-3.8714560	C	-6.1170950	1.3280210	0.4184660
H	2.6302290	0.9060050	-3.1853920	C	-0.5199580	1.7670650	-1.3952840
C	0.1830310	-0.6336540	-3.9363140	H	-1.5494510	2.1417540	-1.3293300
H	-0.8889990	-0.5894980	-3.7284060	H	-0.3516480	1.5085540	-2.4462280
H	0.5469920	0.3879610	-4.0620090	C	-4.7750410	1.5867020	1.0674280
H	0.3141700	-1.1465520	-4.8982140	H	-4.8199230	1.3466360	2.1342620
C	1.6084110	-4.3498140	-0.6543140	H	-4.5149800	2.6468240	0.9899520
H	1.4043760	-5.2029070	-1.3133960	C	-2.2890520	0.9653280	1.0906610
H	2.5504980	-4.5391620	-0.1368400	C	0.4296600	2.9221190	-1.0178190
H	0.8151380	-4.3213800	0.1002770	H	0.2433560	3.1963650	0.0262950
C	-0.8124650	-3.2289140	-2.3353230	H	1.4682240	2.5776190	-1.0665850
H	-1.1319060	-3.6937060	-1.3990450	C	-6.5334520	2.0713110	-0.6947610

H	-5.8956220	2.8672830	-1.0726620
C	-7.7556530	1.8106300	-1.3160460
H	-8.0622410	2.4024950	-2.1741980
C	0.2341120	4.1479650	-1.9196890
H	0.4210790	3.8663050	-2.9662910
H	-0.8169840	4.4651370	-1.8752960
C	-6.9619010	0.3157700	0.8949330
H	-6.6597760	-0.2642370	1.7642220
C	-8.1852010	0.0511370	0.2774420
H	-8.8280520	-0.7336300	0.6668930
C	-8.5859980	0.7979550	-0.8320190
H	-9.5398200	0.5966770	-1.3112970
C	1.1344840	5.3285420	-1.5420270
H	0.9623630	6.1889740	-2.1975240
H	2.1942200	5.0601300	-1.6157530
H	0.9476230	5.6520880	-0.5119580

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C	-2.7327500	3.1244370	-0.1823820
C	-1.8177730	2.1694040	0.3020120
C	-2.0667150	1.6152630	1.5710030
C	-3.1833110	2.0274960	2.3113070
C	-4.0795000	2.9593690	1.7993320
C	-3.8635260	3.5240050	0.5339710
H	-2.5594860	3.5657740	-1.1605570

H	-3.3304450	1.6170150	3.3063210
H	-4.9421960	3.2619690	2.3881910
C	-1.0958560	0.6787500	2.2449450
O	-0.4700480	1.0165570	3.2464680
Rh	-1.2521520	-1.1399630	-0.3290910
N	-1.0938770	-0.5592590	1.6631250
C	0.7226350	-2.0388270	1.5929880
O	-0.0845870	-1.3697470	2.3747550
O	0.6095670	-2.0524090	0.3527550
C	1.8248160	-2.7855100	2.3450370
C	2.8108310	-1.7216730	2.8897780
H	2.2953870	-0.9955480	3.5233430
H	3.5863160	-2.2179360	3.4823430
H	3.3057160	-1.1828810	2.0754320
C	2.5482780	-3.7443280	1.3862290
H	1.8680620	-4.5053210	0.9912900
H	2.9818290	-3.2099330	0.5377430
H	3.3541650	-4.2543650	1.9232350
C	1.2032650	-3.5700190	3.5214580
H	0.7027990	-2.9019340	4.2253530
H	0.4743300	-4.3077010	3.1685960
H	1.9936020	-4.1079230	4.0546020
C	-2.4636150	-1.2550170	-2.1764560
C	-3.3024060	-1.0179550	-1.0223080
C	-3.2605380	-2.2178890	-0.1870950

C	-2.3446280	-3.1161380	-0.7590200	C	-0.2415200	0.5970880	-0.8553690
C	-1.8145330	-2.5060390	-1.9825300	C	2.3447430	0.4997390	-1.0200880
C	-4.3203370	0.0727310	-0.8749250	H	2.3673870	-0.2321390	-0.2089240
H	-4.4688260	0.3491480	0.1709160	H	2.4010170	1.4878110	-0.5569070
H	-4.0271930	0.9747020	-1.4122360	C	4.8647380	0.3582350	-1.2214490
H	-5.2873590	-0.2612460	-1.2764550	C	0.2020900	3.1238310	-0.8599290
C	-4.0516750	-2.3831640	1.0755520	H	-0.4630400	3.8358870	-1.3662130
H	-5.1250570	-2.4253640	0.8545060	H	0.9899680	2.9053730	-1.5785720
H	-3.7821520	-3.2984950	1.6069470	C	3.5474970	0.2859880	-1.9623370
H	-3.8813180	-1.5411740	1.7531260	H	3.4462310	-0.6887070	-2.4494990
C	-1.9459530	-4.4739460	-0.2594420	H	3.5164680	1.0425600	-2.7527670
H	-0.8570950	-4.5859750	-0.2421900	C	0.9924830	0.3522240	-1.7133730
H	-2.3204040	-4.6601980	0.7497480	C	0.8037920	3.8236160	0.3754220
H	-2.3433670	-5.2609940	-0.9125990	H	0.0070460	4.0672880	1.0885100
C	-2.3450950	-0.3629870	-3.3770820	H	1.4707670	3.1264840	0.9005570
H	-3.0881010	-0.6462650	-4.1339350	C	5.5122440	1.5850920	-1.0193740
H	-2.5159680	0.6822080	-3.1121990	H	5.0762640	2.4920100	-1.4323830
H	-1.3543460	-0.4303190	-3.8299910	C	6.7076630	1.6570310	-0.3029010
C	-0.8812230	-3.2019630	-2.9277440	H	7.1947380	2.6178970	-0.1609520
H	-1.4163860	-3.9865020	-3.4790680	C	1.5760730	5.1003710	0.0187470
H	-0.4511590	-2.5090320	-3.6507200	H	2.3726160	4.8572660	-0.6985130
H	-0.0556650	-3.6768200	-2.3905230	H	0.9040880	5.7968860	-0.5017100
F	0.9525010	-0.9337670	-2.2517130	C	5.4526150	-0.7976540	-0.6881850
F	0.9764010	1.1616300	-2.8518110	H	4.9719700	-1.7604440	-0.8484100
C	-0.5891120	1.8594580	-0.5054770	C	6.6480420	-0.7313220	0.0296180

H	7.0892890	-1.6403280	0.4294870	N	0.9335030	-0.2975620	-1.4434570
C	7.2795020	0.4981740	0.2258410	C	-0.9881580	-2.3815560	-1.4834480
H	8.2113150	0.5524190	0.7814610	O	-0.1756260	-2.3106660	-2.4107980
C	2.1841530	5.7944270	1.2418870	O	-0.8261930	-1.9086940	-0.2779620
H	2.7269820	6.7030150	0.9600510	C	-2.3667220	-3.0632500	-1.7407010
H	2.8864170	5.1337120	1.7626890	C	-2.1394870	-4.3022900	-2.6272670
H	1.4074620	6.0786650	1.9608070	H	-1.5307850	-5.0531650	-2.1107560
C	-4.8141140	4.5581280	-0.0236000	H	-3.1001890	-4.7655230	-2.8786500
H	-5.8578880	4.2433990	0.0839070	H	-1.6250680	-4.0288310	-3.5502870
H	-4.7122370	5.5148040	0.5034250	C	-3.2287670	-2.0342210	-2.5069320
H	-4.6258270	4.7458470	-1.0845370	H	-3.4393410	-1.1502870	-1.8963420
TS13				H	-2.7224400	-1.7103470	-3.4202880
				H	-4.1888440	-2.4847280	-2.7838460
C	2.9184790	3.1325170	0.2479100	C	-3.0665690	-3.4719050	-0.4355880
C	2.1052090	2.1084790	-0.2862130	H	-2.4757860	-4.2066950	0.1219850
C	2.6076400	1.4420230	-1.4308310	H	-3.2294950	-2.6135410	0.2193120
C	3.8140800	1.8607400	-2.0175270	H	-4.0373370	-3.9279460	-0.6627450
C	4.5695440	2.8885740	-1.4756980	C	3.1415680	-1.2616810	1.0991360
C	4.1365970	3.5286600	-0.3064320	C	3.0423440	-2.3607610	0.1795030
H	2.5897720	3.6392230	1.1488990	C	1.9697930	-3.2034180	0.6205450
H	4.1379680	1.3336230	-2.9085220	C	1.4642740	-2.6769700	1.8750850
H	5.5004070	3.1885250	-1.9504470	C	2.1776140	-1.4858220	2.1652450
C	2.0268200	0.2040750	-2.0786090	C	3.9275930	-2.5920790	-1.0090030
O	2.5192850	-0.3026680	-3.0901050	H	4.9603750	-2.7601880	-0.6796270
Rh	1.0798530	-1.1786040	0.1891520	H	3.6068010	-3.4680680	-1.5753420

H	3.9254310	-1.7438860	-1.6997000	C	0.0271850	3.2138180	0.6330170
C	1.5206630	-4.4833370	-0.0217920	H	0.6495640	3.9226800	1.1900520
H	1.6164240	-4.4419210	-1.1085610	H	-0.8515800	3.0593410	1.2530240
H	2.1172900	-5.3288900	0.3446880	C	-3.5626830	0.6614580	1.7483890
H	0.4745380	-4.6916450	0.2134380	H	-3.6082570	-0.3283950	2.2128780
C	0.4009590	-3.3327690	2.7040480	H	-3.4426410	1.3880290	2.5585350
H	0.0792900	-2.6911590	3.5248630	C	-1.0092690	0.5621030	1.5870080
H	-0.4802060	-3.5663170	2.0999410	C	-0.3956280	3.8730930	-0.6959180
H	0.7764970	-4.2711090	3.1311470	H	0.4891570	4.0611270	-1.3162560
C	4.2443460	-0.2460260	1.1190230	H	-1.0220050	3.1717930	-1.2636490
H	3.9287610	0.6897750	1.5827520	C	-5.2697700	2.2572910	0.7689950
H	5.0963380	-0.6340080	1.6939580	H	-4.6832450	3.0816750	1.1690800
H	4.5980630	-0.0155250	0.1125460	C	-6.4345770	2.5240640	0.0490320
C	2.0546790	-0.6440690	3.4009210	H	-6.7474610	3.5523570	-0.1104640
H	2.2640100	0.4060000	3.1868350	C	-1.1580900	5.1877240	-0.4850190
H	1.0525580	-0.7016870	3.8269950	H	-2.0439790	4.9988680	0.1370830
H	2.7720350	-0.9831200	4.1594790	H	-0.5289610	5.8832160	0.0877400
F	-1.0374870	-0.6690620	2.2271890	C	-5.6249770	-0.1054340	0.4812340
F	-0.9709980	1.4619550	2.6541060	H	-5.3173390	-1.1339660	0.6535400
C	0.7772620	1.8921400	0.4028790	C	-6.7920190	0.1561250	-0.2392820
C	0.2740180	0.6913260	0.7753290	H	-7.3837550	-0.6692580	-0.6255620
C	-2.3223720	0.7323160	0.8324110	C	-7.2002470	1.4725040	-0.4590240
H	-2.3506280	-0.0509010	0.0724520	H	-8.1090600	1.6776820	-1.0175100
H	-2.3009600	1.6911500	0.3074690	C	-1.5876660	5.8491060	-1.7985040
C	-4.8451770	0.9398310	0.9941670	H	-2.1281450	6.7841030	-1.6174760

H	-2.2455600	5.1903250	-2.3763380	C	-1.8848880	-4.8574750	-2.2959540
H	-0.7203900	6.0817600	-2.4266400	H	-1.4211820	-5.6243110	-1.6688060
C	4.9536290	4.6338640	0.3190250	H	-2.8764700	-5.2131760	-2.5991380
H	4.5597780	4.9223470	1.2972520	H	-1.2656310	-4.7454040	-3.1889380
H	5.9985140	4.3320820	0.4496130	C	-2.6487540	-2.4655240	-2.4703870
H	4.9559120	5.5282700	-0.3156030	H	-2.7829520	-1.5107030	-1.9567590
14				H	-2.0212600	-2.2895050	-3.3503050
C	2.4799350	3.4694840	0.1994480	H	-3.6300210	-2.8089770	-2.8182220
C	1.8123990	2.3394920	-0.3242960	C	-2.8913580	-3.7172710	-0.2874240
C	2.3798750	1.7580210	-1.4824840	H	-2.4738010	-4.4877210	0.3713400
C	3.5003250	2.3481380	-2.0935480	H	-2.9673780	-2.7919540	0.2880230
C	4.1122360	3.4705790	-1.5614180	H	-3.8997890	-4.0382750	-0.5741070
C	3.6162860	4.0372810	-0.3780100	C	3.4597880	-1.2785800	0.4417390
H	2.1051340	3.9229730	1.1099800	C	2.9391730	-2.6222630	0.2998180
H	3.8770720	1.8773250	-2.9952150	C	2.0238870	-2.8632120	1.3790780
H	4.9789800	3.9040610	-2.0539230	C	1.9614880	-1.6877450	2.1847280
C	1.9459670	0.4748120	-2.1169350	C	2.8594190	-0.7056220	1.6049210
O	2.4730030	0.0268820	-3.1460880	C	3.3804000	-3.6120040	-0.7315800
Rh	1.2302980	-1.1164610	0.0822990	H	4.1941620	-4.2288660	-0.3252760
N	0.9542340	-0.2526090	-1.5406920	H	2.5549510	-4.2563350	-1.0311050
C	-0.6063560	-3.0291090	-1.1200470	H	3.7537750	-3.1097250	-1.6267210
O	0.4133660	-3.6232130	-1.4803110	C	1.2965870	-4.1498040	1.6288620
O	-0.6272710	-1.9609250	-0.3690730	H	1.0255800	-4.6256020	0.6854630
C	-2.0159120	-3.5244610	-1.5421890	H	1.9335190	-4.8387550	2.1986050
				H	0.3836760	-3.9842690	2.2048770

C	1.2976540	-1.5572460	3.5233270	H	-3.5822850	0.8787060	2.4706360
H	0.9268900	-0.5463320	3.6995250	C	-1.1028530	0.3444870	1.4558960
H	0.4529780	-2.2393970	3.6227590	C	-0.8720150	3.8362700	-0.5777000
H	2.0193540	-1.7949030	4.3166240	H	-0.0252450	4.1956250	-1.1746430
C	4.5652010	-0.7015610	-0.3926010	H	-1.4030290	3.1102610	-1.2079670
H	4.7131670	0.3597840	-0.1888680	C	-5.5056940	1.8521660	0.9061890
H	5.5057990	-1.2218570	-0.1727870	H	-5.0256760	2.6131350	1.5178860
H	4.3661210	-0.8119740	-1.4627270	C	-6.6728430	2.1624590	0.2068100
C	3.2413610	0.5833280	2.2655450	H	-7.0937320	3.1619900	0.2746500
H	3.6569980	1.2995970	1.5572890	C	-1.8037040	5.0126330	-0.2561750
H	2.3861830	1.0505160	2.7571370	H	-2.6585760	4.6490810	0.3301700
H	4.0012540	0.3826270	3.0325890	H	-1.2750570	5.7280160	0.3891770
F	-1.0634440	-0.9223330	1.9973590	C	-5.5872540	-0.3986940	0.0572320
F	-1.1251620	1.1619860	2.5932410	H	-5.1709490	-1.4013240	-0.0000910
C	0.5391520	1.9203070	0.3685410	C	-6.7548080	-0.0932570	-0.6438790
C	0.1810500	0.6509000	0.6766630	H	-7.2393570	-0.8588080	-1.2436580
C	-2.4149660	0.4884100	0.6934890	C	-7.3015470	1.1893870	-0.5721220
H	-2.3713920	-0.2307550	-0.1269780	H	-8.2116710	1.4274290	-1.1152730
H	-2.4619440	1.4842140	0.2476280	C	-2.3128440	5.7326630	-1.5087960
C	-4.9443710	0.5691410	0.8413460	H	-2.9722980	6.5674490	-1.2496560
C	-0.3586540	3.1278320	0.6922730	H	-2.8768380	5.0509400	-2.1550800
H	0.1878070	3.8555800	1.3016660	H	-1.4818100	6.1350820	-2.0992070
H	-1.2037250	2.8322650	1.3056630	C	4.2837900	5.2419490	0.2408340
C	-3.6593970	0.2521090	1.5763430	H	3.8137840	5.5209160	1.1875760
H	-3.6655210	-0.7883000	1.9160630	H	5.3458970	5.0531160	0.4330320

H 4.2295950 6.1085940 -0.4283910

TS13'

C -1.5841630 3.6641810 -1.2270600

C -1.4218850 2.4351510 -0.5282980

C -2.6064750 1.6793800 -0.2728100

C -3.8560790 2.1575420 -0.7249040

C -3.9632570 3.3355620 -1.4342140

C -2.8095510 4.1127520 -1.6937880

H -0.7034160 4.2670390 -1.4276680

H -4.7353140 1.5706410 -0.4795490

H -4.9343970 3.6779030 -1.7826380

C -2.6479300 0.5018700 0.6034300

O -3.6627580 0.0958970 1.1686010

Rh -0.4515160 -1.0631240 -0.8331440

N -1.4075420 -0.1657110 0.7973350

C -1.8435690 -2.1305570 2.1005870

O -2.0980290 -2.7830040 1.1145860

O -1.4213780 -0.8320730 2.0772110

C -1.9142870 -2.6232630 3.5534650

C -2.3876960 -4.0853270 3.5483530

H -1.6980990 -4.7253210 2.9909120

H -2.4469950 -4.4551150 4.5772960

H -3.3753060 -4.1799070 3.0893450

C -2.9184710 -1.7401360 4.3290860

H -2.5829000 -0.7018900 4.3713360

H -3.9044860 -1.7537080 3.8556470

H -3.0204050 -2.1174750 5.3523990

C -0.5123700 -2.5189320 4.1959200

H 0.2135420 -3.1454560 3.6663960

H -0.1451890 -1.4901890 4.1886170

H -0.5600180 -2.8635930 5.2344470

C -1.4686670 -0.9351790 -2.7208830

C -1.8245730 -2.2847960 -2.2504530

C -0.6423210 -3.0113760 -2.1114980

C 0.4762140 -2.1365520 -2.5093150

C -0.0480090 -0.9060410 -2.9921480

C -3.2241120 -2.7176280 -1.9359120

H -3.2444500 -3.7110700 -1.4858360

H -3.6968630 -2.0309270 -1.2273330

H -3.8372120 -2.7403780 -2.8457120

C -0.4785520 -4.4156140 -1.6105840

H 0.3614890 -4.4946670 -0.9132470

H -1.3716790 -4.7575420 -1.0850590

H -0.2792190 -5.1092160 -2.4382530

C 1.9080070 -2.5860530 -2.5636530

H 2.5975790 -1.7423010 -2.6442830

H 2.1820110 -3.1631950 -1.6754300

H 2.0749850 -3.2338600 -3.4343720

C -2.4612630 0.0756440 -3.2100730

H	-2.7223260	-0.1484040	-4.2542180	C	5.5865480	-1.2340340	-0.3657260
H	-3.3822380	0.0562350	-2.6263510	H	5.0092220	-2.1480560	-0.4871610
H	-2.0653770	1.0923110	-3.1728410	C	6.8074490	-1.0932520	-1.0277050
C	0.6925410	0.2216690	-3.6475070	H	7.1722560	-1.8948030	-1.6641010
H	0.3434830	1.1909210	-3.2790510	C	1.2156670	5.0290180	2.1361130
H	1.7674520	0.1619740	-3.4571840	H	2.1896320	4.5914930	2.3977000
H	0.5484280	0.2050480	-4.7358180	H	1.4065780	5.7102850	1.2949030
F	1.3056150	0.4845420	2.2833080	C	5.8668140	0.9429620	0.6232980
F	1.0131190	-1.3241340	1.0197450	H	5.5079050	1.7371310	1.2742730
C	-0.1358150	2.0201060	-0.0128900	C	7.0876980	1.0886140	-0.0366030
C	0.0472090	0.6599870	0.2365920	H	7.6711870	1.9945980	0.1015700
C	2.6170350	0.2480340	0.3142800	C	7.5617290	0.0702130	-0.8658970
H	2.8199470	1.3029950	0.1273550	H	8.5137580	0.1800540	-1.3770830
H	2.5626400	-0.2359100	-0.6635910	C	0.6811250	5.8291890	3.3286200
C	5.0978350	-0.2186600	0.4675830	H	1.3793470	6.6174940	3.6297360
C	0.8102880	3.1089990	0.4829050	H	0.5154660	5.1813440	4.1968760
H	1.0504780	3.8061670	-0.3323870	H	-0.2757700	6.3058320	3.0873360
H	1.7694950	2.6899410	0.7897080	C	-2.9275720	5.4069620	-2.4629140
C	3.7583700	-0.3578110	1.1588140	H	-3.3639440	5.2421300	-3.4552680
H	3.7835920	0.1448780	2.1306140	H	-3.5818680	6.1167710	-1.9427150
H	3.5453130	-1.4139540	1.3511240	H	-1.9540090	5.8859220	-2.5989740
C	1.2459720	0.1012120	0.9705110				
C	0.2635410	3.9166070	1.6801960	14'			
H	-0.7082370	4.3509860	1.4161760	C	-3.9371920	0.6488180	1.0822770
H	0.0791150	3.2245140	2.5123080	C	-2.5405490	0.5393460	1.2568620

C	-2.0893790	0.1466640	2.5300120	H	3.6427470	-1.9378360	0.9685240
C	-2.9869250	-0.1000290	3.5794620	H	3.9845400	-3.6552110	1.2319090
C	-4.3502590	0.0387230	3.3823890	C	-0.1425570	-2.4189680	-2.4711870
C	-4.8417370	0.4033890	2.1144310	C	0.1489210	-1.1398110	-2.9708090
H	-4.3310590	0.9350280	0.1131920	C	-1.1049190	-0.3938480	-3.0071230
H	-2.5811470	-0.4158390	4.5345650	C	-2.1880230	-1.3047260	-2.6549580
H	-5.0429560	-0.1460780	4.1991380	C	-1.5899420	-2.5121520	-2.2430560
C	-0.6794260	-0.2075660	2.7337070	C	1.4697710	-0.6161300	-3.4545950
O	-0.2727830	-0.8283370	3.7078620	H	1.4984770	-0.5735080	-4.5520130
Rh	-0.8445810	-0.8349240	-0.8942870	H	1.6554130	0.3935050	-3.0800490
N	0.1954330	0.1111830	1.6755010	H	2.2974090	-1.2527550	-3.1306570
C	0.9328500	-2.0675580	1.3873980	C	-1.2761940	0.8991690	-3.7517910
O	-0.1126200	-2.3180670	0.8023340	H	-0.4536530	1.5901660	-3.5585420
O	1.3007360	-0.7922620	1.6926450	H	-1.2977050	0.7011870	-4.8325390
C	1.9801300	-3.0860320	1.8347030	H	-2.2099530	1.4018520	-3.4947980
C	1.3876430	-4.5005030	1.7213070	C	-3.6554000	-1.0048030	-2.7607200
H	1.0936510	-4.7374900	0.6963890	H	-4.2414120	-1.6152300	-2.0686080
H	2.1367610	-5.2317520	2.0401840	H	-3.8701400	0.0438700	-2.5365580
H	0.5068810	-4.6113340	2.3599030	H	-4.0273800	-1.2026840	-3.7753110
C	2.3872300	-2.8001940	3.2984760	C	0.8053660	-3.5670030	-2.2935340
H	2.8822760	-1.8318010	3.3916290	H	0.6136860	-4.1027450	-1.3601620
H	1.5163520	-2.7911520	3.9572620	H	0.6962980	-4.2936890	-3.1101650
H	3.0794410	-3.5798340	3.6326640	H	1.8476780	-3.2372610	-2.2872500
C	3.2167100	-2.9430950	0.9129380	C	-2.2813900	-3.7488160	-1.7443130
H	2.9673940	-3.1603510	-0.1299330	H	-1.7807670	-4.1548250	-0.8597520

H	-3.3198760	-3.5457230	-1.4717310	H	-2.0942150	4.6563050	-1.6457630
H	-2.2860440	-4.5355150	-2.5106520	H	-3.7571890	4.1446670	-1.4067620
F	0.7647280	1.9840750	-1.3985770	C	5.5381880	1.4311670	-1.0679370
F	0.6758730	2.8959300	0.6081720	H	5.0772960	1.1842330	-2.0219330
C	-1.5857630	0.8781200	0.1680310	C	6.8697970	1.0846840	-0.8326970
C	-0.1423250	0.6628890	0.3774040	H	7.4373800	0.5679100	-1.6019030
C	2.3852600	1.3475350	0.1727890	C	7.4733380	1.4084920	0.3837320
H	2.5985820	0.4010840	-0.3315730	H	8.5107600	1.1437710	0.5672680
H	2.5517540	1.1891970	1.2398490	C	-3.1543560	5.7915530	-0.1429800
C	4.7854380	2.1050450	-0.0963890	H	-3.4913410	6.5697780	-0.8361090
C	-2.0722440	2.0544350	-0.6956320	H	-2.2631540	6.1671630	0.3723270
H	-2.9838260	1.7507490	-1.2245800	H	-3.9376900	5.6556600	0.6116130
H	-1.3397880	2.2707390	-1.4667950	C	-6.3289630	0.5367300	1.8876420
C	3.3326930	2.4515850	-0.3415380	H	-6.7559320	1.3213870	2.5234140
H	3.1628950	2.6051870	-1.4114960	H	-6.5578620	0.7863240	0.8481000
H	3.0813870	3.3917030	0.1592900	H	-6.8520300	-0.3940700	2.1349820
C	0.9155410	1.6917910	-0.0468880				
C	-2.3743620	3.3634450	0.0653010	TS15			
H	-3.1356940	3.1892520	0.8347830	C	2.6194820	3.3865890	0.1623350
H	-1.4700250	3.6917350	0.5856620	C	1.8532590	2.3082320	-0.3311440
C	5.4049190	2.4249370	1.1199960	C	2.2930830	1.7168200	-1.5333030
H	4.8387720	2.9544300	1.8830190	C	3.3975200	2.2432700	-2.2224960
C	6.7357950	2.0810270	1.3602240	C	4.1149250	3.3164800	-1.7191320
H	7.1981890	2.3430680	2.3079200	C	3.7443950	3.8913190	-0.4933640
C	-2.8552120	4.4782460	-0.8733700	H	2.3308340	3.8510890	1.0990810

H	3.6745800	1.7675160	-3.1573820	C	1.9344690	-1.8861440	2.1478420
H	4.9686720	3.7071200	-2.2669260	C	2.7774560	-0.8019330	1.6957900
C	1.7088060	0.4783500	-2.1194930	C	3.4580080	-3.3985840	-0.9571860
O	2.0674740	0.0196360	-3.2131090	H	4.1413600	-4.1801470	-0.5996190
Rh	1.1917490	-1.1620140	0.1356190	H	2.6013900	-3.8718650	-1.4419030
N	0.7631940	-0.2270090	-1.4377750	H	3.9861680	-2.8018200	-1.7033110
C	-0.6538340	-3.0460050	-1.0900490	C	1.4392130	-4.3132540	1.3307830
O	0.3590930	-3.5466130	-1.5867290	H	1.3201580	-4.7747470	0.3506710
O	-0.6650140	-2.0554710	-0.2396780	H	2.0582680	-4.9666520	1.9594270
C	-2.0677130	-3.5692180	-1.4631570	H	0.4522180	-4.2429300	1.7938870
C	-1.9385620	-4.9184570	-2.1883360	C	1.2163250	-1.9521820	3.4628540
H	-1.4695470	-5.6704420	-1.5460240	H	0.8469010	-0.9743580	3.7747230
H	-2.9309020	-5.2852910	-2.4753390	H	0.3594800	-2.6260680	3.4151660
H	-1.3249290	-4.8240020	-3.0865650	H	1.8948410	-2.3235740	4.2426570
C	-2.7157380	-2.5345140	-2.4098260	C	4.5154180	-0.4747480	-0.2436780
H	-2.8420610	-1.5664480	-1.9181580	H	4.5346250	0.5850060	0.0129990
H	-2.1013210	-2.3819940	-3.3030080	H	5.4908810	-0.9031090	0.0202250
H	-3.7028150	-2.8859890	-2.7325320	H	4.4022650	-0.5536850	-1.3278010
C	-2.9296010	-3.7355350	-0.1969420	C	3.0567880	0.4465280	2.4766190
H	-2.5006460	-4.4850590	0.4784080	H	3.3460910	1.2757930	1.8303430
H	-3.0076330	-2.7967850	0.3555990	H	2.1889590	0.7573910	3.0609420
H	-3.9378090	-4.0720190	-0.4663730	H	3.8828280	0.2574740	3.1750870
C	3.4259860	-1.2061350	0.4829560	F	-1.0830750	-0.8552700	2.0212580
C	2.9968230	-2.5557070	0.1901440	F	-1.1250400	1.2319850	2.5801460
C	2.0787110	-2.9627660	1.2141580	C	0.5948270	1.9407400	0.4031640

C	0.1871150	0.6763900	0.6762460	H	-7.1990860	-0.7342140	-1.3562000
C	-2.4024430	0.5581900	0.6743280	C	-7.2619690	1.3076880	-0.6657560
H	-2.3558460	-0.1541810	-0.1525210	H	-8.1612060	1.5559970	-1.2222920
H	-2.4260830	1.5599780	0.2372000	C	-2.0157220	6.0148270	-1.2714260
C	-4.9332510	0.6608640	0.7820590	H	-2.6037770	6.8864480	-0.9659670
C	-0.2244990	3.1850430	0.7845450	H	-2.6436630	5.4028650	-1.9285420
H	0.3756260	3.8472800	1.4195930	H	-1.1692560	6.3756370	-1.8668010
H	-1.0837410	2.9169430	1.3900920	C	4.5254250	5.0485820	0.0819180
C	-3.6627670	0.3292510	1.5355150	H	4.2155710	5.2757370	1.1054280
H	-3.6825580	-0.7129120	1.8691540	H	5.6002410	4.8380950	0.0911600
H	-3.5941020	0.9506090	2.4342310	H	4.3822070	5.9552030	-0.5182200
C	-1.1050220	0.3986970	1.4547900				
C	-0.7033060	3.9816110	-0.4469500	TS16			
H	0.1558190	4.3013730	-1.0482720	C	-1.5462200	3.8551170	0.2287630
H	-1.3011290	3.3247260	-1.0931490	C	-1.0878780	2.5531930	0.4893550
C	-5.4886650	1.9461800	0.8498920	C	-1.6383350	1.9116880	1.6205040
H	-5.0149200	2.6985620	1.4768500	C	-2.6323140	2.5060940	2.4123910
C	-6.6418510	2.2696660	0.1335320	C	-3.0582450	3.7936840	2.1248890
H	-7.0585420	3.2707900	0.2038740	C	-2.5188630	4.4806920	1.0211260
C	-1.5362080	5.2108610	-0.0587690	H	-1.1494230	4.3953070	-0.6218680
H	-2.4031970	4.8908670	0.5350230	H	-3.0542360	1.9467900	3.2395160
H	-0.9403000	5.8585760	0.5991870	H	-3.8161630	4.2680230	2.7380070
C	-5.5675220	-0.2960080	-0.0223550	C	-0.9006330	0.5786650	2.2066890
H	-5.1557840	-1.3004190	-0.0820110	O	-0.0025300	0.4445650	3.0157760
C	-6.7209570	0.0227600	-0.7406170	Rh	-1.5932400	-0.7060200	-0.3119020

N	-1.8549400	0.0157450	1.4815080	H	-5.6564960	0.4785260	-0.6172600
C	-0.4495170	-2.8299660	1.3936050	C	-4.3683990	-2.6728860	0.2431970
O	-1.6152950	-3.2874520	1.4546410	H	-4.9767240	-2.0465270	0.9024690
O	-0.0828280	-1.7917750	0.6378120	H	-5.0386860	-3.3611150	-0.2894750
C	0.6640780	-3.4328060	2.2783840	H	-3.6672830	-3.2434070	0.8564820
C	0.3535510	-2.9620860	3.7278410	C	-2.1058300	-3.7266980	-1.7166160
H	-0.6396830	-3.3142980	4.0235720	H	-1.1494080	-3.7863130	-2.2424890
H	1.1010560	-3.3717650	4.4174520	H	-1.9745550	-4.1157320	-0.7042740
H	0.3755260	-1.8685550	3.7768010	H	-2.8362630	-4.3505180	-2.2502800
C	2.0658920	-2.9617970	1.8655660	C	-2.7229980	1.3496560	-2.6297660
H	2.2713240	-3.2280030	0.8232590	H	-3.4953560	1.4813800	-3.4001870
H	2.1514300	-1.8782010	1.9722340	H	-2.8478920	2.1345750	-1.8785510
H	2.8155900	-3.4393300	2.5077040	H	-1.7427020	1.4829620	-3.0932600
C	0.5536340	-4.9707090	2.1936740	C	-1.2886760	-1.2901890	-3.7053070
H	-0.4700300	-5.2751720	2.4230940	H	-1.9391700	-1.2732960	-4.5912040
H	0.8049290	-5.3190080	1.1842180	H	-0.5833610	-0.4604200	-3.7724300
H	1.2439930	-5.4364390	2.9061060	H	-0.7123750	-2.2163570	-3.7217580
C	-2.8294480	-0.0174270	-2.0096130	F	0.7695500	-1.3546840	-1.8647740
C	-3.7287670	-0.4100110	-0.9426070	F	1.2508620	0.6631330	-2.7001740
C	-3.5964150	-1.8271730	-0.7305510	C	-0.0348010	1.9083170	-0.3501000
C	-2.5877240	-2.3048930	-1.6439050	C	-0.0560950	0.5943940	-0.6834330
C	-2.1378150	-1.2055130	-2.4650530	C	2.4288250	-0.1184490	-0.7370350
C	-4.6465990	0.5101900	-0.1868930	H	2.2810520	-0.7740550	0.1215250
H	-4.7073800	0.2170160	0.8647110	H	2.7148200	0.8675350	-0.3714670
H	-4.2863840	1.5414410	-0.2281460	C	4.8923630	-0.6129570	-1.0015590

C	1.0747180	2.8777330	-0.7997400	H	4.3784560	3.9962260	1.6351890
H	0.6159700	3.7368160	-1.3072070	H	3.3234480	5.4186800	1.7554590
H	1.6952410	2.3892510	-1.5475180	C	-2.9875310	5.8857460	0.6987330
C	3.5343630	-0.6736070	-1.6731140	H	-2.5768030	6.5984140	1.4255850
H	3.2803240	-1.7036370	-1.9408640	H	-2.6609440	6.1918110	-0.2991290
H	3.5351920	-0.0764040	-2.5902890	H	-4.0800260	5.9541140	0.7440830
C	1.0867460	-0.0327070	-1.4477620				
C	1.9351210	3.3984710	0.3780280	17			
H	1.3006980	3.9598630	1.0750000	C	-1.4965940	-4.6067750	-0.0067260
H	2.3435070	2.5440480	0.9321980	C	-0.7859350	-3.3807970	-0.1031450
C	5.7282310	0.4974770	-1.1835290	C	0.5331200	-3.3524100	0.4018350
H	5.4105450	1.2993850	-1.8429210	C	1.0964010	-4.4997380	0.9919970
C	6.9624160	0.5765550	-0.5352680	C	0.3747390	-5.6732140	1.0805180
H	7.5997290	1.4398770	-0.6906260	C	-0.9413970	-5.7400260	0.5695460
C	3.0950660	4.2969870	-0.1046730	H	-2.5039450	-4.6755900	-0.4009300
H	3.7333730	3.7198600	-0.7873200	H	2.1104970	-4.4241520	1.3688530
H	2.6864810	5.1408440	-0.6774250	H	0.8174980	-6.5542840	1.5389790
C	5.3185180	-1.6437430	-0.1525420	C	1.3414340	-2.1358990	0.3051370
H	4.6793250	-2.5076160	-0.0021600	O	2.5125920	-2.0986170	0.7398560
C	6.5515320	-1.5673850	0.4974040	Rh	2.2255480	0.6004380	-0.1234340
H	6.8680980	-2.3738040	1.1492690	N	0.7791300	-1.0281150	-0.2974410
C	7.3775940	-0.4566540	0.3079000	C	0.9205810	1.3243010	1.9754730
H	8.3360820	-0.3982310	0.8105970	O	1.8887740	0.5055590	2.0408660
C	3.9432920	4.8284870	1.0703410	O	0.6364050	1.8157870	0.8315830
H	4.7600290	5.4644750	0.7113580	C	0.0987070	1.6551490	3.2228000

C	1.0389600	1.7438970	4.4410150	C	2.5961370	3.4076330	-1.7091280
H	1.7537150	2.5671480	4.3320330	H	1.6451080	3.2731330	-2.2281270
H	0.4542250	1.9251080	5.3493390	H	2.4106320	4.0208660	-0.8250510
H	1.6044470	0.8181570	4.5669460	H	3.2714520	3.9626220	-2.3727940
C	-0.9011760	0.4908880	3.4266230	C	4.0139720	-1.5675720	-1.8873750
H	-1.5788140	0.3950580	2.5725400	H	3.1995950	-1.8837200	-2.5429640
H	-0.3746370	-0.4587930	3.5553800	H	4.9499510	-1.6334120	-2.4579290
H	-1.5070240	0.6764720	4.3201940	H	4.0538620	-2.2598080	-1.0466330
C	-0.6628960	2.9785920	3.0381750	C	2.4550990	0.7269410	-3.4629430
H	0.0254990	3.8138450	2.8720620	H	1.9633340	-0.2410500	-3.5776440
H	-1.3490500	2.9358940	2.1891860	H	1.7100970	1.4998770	-3.6513310
H	-1.2473060	3.1965080	3.9387150	H	3.2300200	0.8041050	-4.2370580
C	3.8077510	-0.1635670	-1.4083320	F	0.0407690	1.0243580	-1.8436650
C	4.3670090	0.4135850	-0.2191140	F	-1.4798000	-0.1996270	-2.7934380
C	3.9976110	1.8163880	-0.1734630	C	-1.3323090	-2.1865210	-0.7143410
C	3.2028740	2.0873940	-1.3427650	C	-0.5045720	-1.0782330	-0.8071920
C	3.0783380	0.8697280	-2.1071660	C	-2.0669420	1.0085400	-0.8270050
C	5.1820860	-0.3221960	0.7977640	H	-1.6024460	1.3849620	0.0873910
H	6.2040150	-0.4700420	0.4254790	H	-2.8955550	0.3611590	-0.5361560
H	5.2391220	0.2302790	1.7375550	C	-3.6342560	2.9942350	-0.9426260
H	4.7299220	-1.2946340	1.0012970	C	-2.7715460	-2.2389350	-1.2053310
C	4.4260080	2.8031630	0.8724390	H	-2.9112100	-3.1570330	-1.7914210
H	4.4492820	2.3424690	1.8628860	H	-2.9804560	-1.4313680	-1.9039680
H	5.4305490	3.1886650	0.6564150	C	-2.5923400	2.1816900	-1.6805060
H	3.7453770	3.6565620	0.9187360	H	-1.7496330	2.8226260	-1.9581060

H	-3.0143270	1.7862870	-2.6098860
C	-1.0085110	0.1770390	-1.5405520
C	-3.8293660	-2.2118160	-0.0788560
H	-3.6389530	-3.0201000	0.6368950
H	-3.7270860	-1.2816260	0.4960150
C	-4.9974070	2.6887180	-1.0546940
H	-5.3093440	1.8757570	-1.7066880
C	-5.9570400	3.4159050	-0.3484080
H	-7.0091590	3.1652080	-0.4528780
C	-5.2641830	-2.3256250	-0.6096590
H	-5.4482550	-1.5196040	-1.3338320
H	-5.3689480	-3.2637890	-1.1721910
C	-3.2567570	4.0526020	-0.1039340
H	-2.2035430	4.3076540	-0.0111790
C	-4.2124070	4.7822500	0.6048440
H	-3.8992840	5.6012370	1.2466830
C	-5.5670850	4.4655920	0.4851600
H	-6.3125020	5.0346520	1.0333720
C	-6.3237010	-2.2706230	0.4954980
H	-7.3355710	-2.3586260	0.0859420
H	-6.2695900	-1.3260110	1.0486030
H	-6.1855920	-3.0831630	1.2180100
C	-1.7196440	-7.0317550	0.6552930
H	-1.8470650	-7.3495400	1.6970080
H	-2.7140000	-6.9338740	0.2109540

H	-1.1979460	-7.8445630	0.1362660
TS18			
C	-2.4759350	3.4202380	0.0211780
C	-1.6690550	2.3168620	0.3490330
C	-2.0195510	1.6199880	1.5241300
C	-3.1551850	1.9507760	2.2811470
C	-3.9268720	3.0436880	1.9189110
C	-3.5924860	3.7953590	0.7772510
H	-2.2400980	3.9981100	-0.8670240
H	-3.4007190	1.3566400	3.1560690
H	-4.7948230	3.3169600	2.5130250
C	-0.9409860	0.6457890	2.1935310
O	-0.0772450	0.9165410	2.9891850
Rh	-1.3561940	-1.0083040	-0.3068570
N	-1.6022710	-0.2655920	1.5521240
C	0.3666900	-2.3228730	1.6539320
O	-0.5663330	-2.0956620	2.4474240
O	0.4131660	-1.9118620	0.4303120
C	1.6026700	-3.1153760	2.1572570
C	2.5558560	-2.0804930	2.8009430
H	2.0440720	-1.5120370	3.5823420
H	3.4142250	-2.5946300	3.2483480
H	2.9380030	-1.3726680	2.0588910
C	2.3139670	-3.8394890	1.0026360

H	1.6606020	-4.5867090	0.5383620	H	-2.7670610	-0.6970380	-4.3297780
H	2.6243800	-3.1392680	0.2244990	H	-2.2818550	0.6813340	-3.3311500
H	3.2007040	-4.3613620	1.3805490	H	-1.0725280	-0.4906730	-3.8475990
C	1.1543740	-4.1325890	3.2224380	C	-0.8003200	-3.2378500	-2.7705350
H	0.6355420	-3.6342750	4.0433190	H	-1.2998410	-4.0940860	-3.2424730
H	0.4732440	-4.8781850	2.7973340	H	-0.3536050	-2.6288650	-3.5560900
H	2.0253620	-4.6629610	3.6233590	H	0.0102610	-3.6251870	-2.1474930
C	-2.3753560	-1.1975750	-2.2843880	F	0.9130110	-0.9273000	-2.2172980
C	-3.3245520	-0.8750490	-1.2474070	F	1.0699400	1.1635170	-2.7926470
C	-3.3991490	-2.0169530	-0.3413490	C	-0.4813420	1.9457530	-0.4762650
C	-2.4482810	-2.9694810	-0.7585040	C	-0.2165320	0.6575230	-0.8249050
C	-1.7850200	-2.4541290	-1.9551350	C	2.3521520	0.4032400	-0.9258220
C	-4.2649080	0.2949730	-1.2350560	H	2.2868220	-0.3152510	-0.1050620
H	-4.5152890	0.5962060	-0.2149800	H	2.4642540	1.3937310	-0.4776020
H	-3.8340200	1.1619870	-1.7399670	C	4.8730570	0.1876480	-1.0774920
H	-5.2035140	0.0422220	-1.7468290	C	0.3759200	3.1622150	-0.8514730
C	-4.3148850	-2.1055560	0.8422270	H	-0.2411950	3.8895760	-1.3963640
H	-5.3467890	-2.2893900	0.5177070	H	1.1584180	2.8791060	-1.5510720
H	-4.0210760	-2.9123980	1.5160790	C	3.5633720	0.0919990	-1.8295950
H	-4.3039520	-1.1763520	1.4182750	H	3.4451070	-0.9124550	-2.2475800
C	-2.1521310	-4.3041410	-0.1426450	H	3.5646940	0.7903100	-2.6729500
H	-1.0749150	-4.4896240	-0.1132140	C	1.0179120	0.3408030	-1.6623030
H	-2.5306540	-4.3722470	0.8788770	C	1.0035900	3.8672240	0.3673410
H	-2.6089940	-5.1113580	-0.7296490	H	0.2159320	4.2001500	1.0547940
C	-2.1048910	-0.3807990	-3.5133950	H	1.6082860	3.1455800	0.9323390

C	5.5662600	1.4031320	-0.9930170	C	-3.0724710	-0.6201060	0.1336820
H	5.1696300	2.2787540	-1.5023420	C	-4.2772430	-1.2922700	-0.0727000
C	6.7574580	1.5026680	-0.2728590	C	-5.3760680	-0.6193370	-0.5985550
H	7.2808020	2.4537070	-0.2234740	C	-5.2679490	0.7342770	-0.9333960
C	1.8725740	5.0683430	-0.0282680	H	-3.9899360	2.4335590	-0.9564250
H	2.6594550	4.7353990	-0.7190820	H	-4.3420190	-2.3509050	0.1639140
H	1.2619830	5.7883860	-0.5909860	H	-6.3091820	-1.1525930	-0.7581500
C	5.4093660	-0.9293580	-0.4217640	C	-1.9839420	-2.1222590	1.5807120
H	4.8897200	-1.8827970	-0.4823300	O	-2.0097070	-2.8261270	2.5090100
C	6.6004670	-0.8352730	0.2995730	Rh	-0.1031430	-0.9796480	-0.5528060
H	7.0004400	-1.7142620	0.7976660	N	-1.9376790	-1.3598120	0.6088330
C	7.2787940	0.3824580	0.3771710	C	0.9851370	-2.8519840	1.4758450
H	8.2072890	0.4569900	0.9360610	O	0.3756730	-3.7381110	0.8592010
C	2.5117500	5.7689730	1.1749870	O	0.9234890	-1.5799260	1.2079070
H	3.1231320	6.6225630	0.8637530	C	1.8903630	-3.2535610	2.6739990
H	3.1568650	5.0825140	1.7345820	C	2.5688500	-2.0487460	3.3418120
H	1.7481810	6.1404120	1.8678340	H	1.8317220	-1.3405130	3.7307180
C	-4.4274150	4.9880640	0.3807850	H	3.1893230	-2.3875250	4.1799450
H	-5.4952930	4.7446270	0.3789060	H	3.2133780	-1.5112150	2.6403050
H	-4.2885830	5.8137260	1.0893780	C	2.9622770	-4.2254670	2.1355590
H	-4.1595070	5.3554170	-0.6131730	H	2.4932460	-5.0838910	1.6485310
				H	3.6176190	-3.7322690	1.4080660
19				H	3.5903450	-4.5889300	2.9567700
C	-4.0494750	1.3821950	-0.7017600	C	1.0083400	-3.9935430	3.7022310
C	-2.9122050	0.7507950	-0.1559330	H	0.2512670	-3.3270370	4.1283800

H	0.4935540	-4.8343400	3.2317260	H	0.3346480	1.8984750	-2.5490780
H	1.6253960	-4.3730520	4.5248930	H	0.0089240	1.2461470	-4.1669230
C	-0.8986330	-1.3210680	-2.6036570	F	1.0510190	2.6954320	-0.3438130
C	-0.1741210	-2.5408050	-2.2559910	F	0.4066490	2.5576910	1.7745900
C	1.1674270	-2.1849720	-2.0217170	C	-1.6656180	1.5130510	0.1760760
C	1.3051980	-0.7416260	-2.1944740	C	-0.4335970	0.9285630	0.2217460
C	0.0229590	-0.2321980	-2.6224920	C	2.0549120	1.0866370	1.0857140
C	-0.7496800	-3.9246390	-2.1889980	H	2.3861970	0.4190970	0.2924490
H	-0.5093720	-4.4935260	-3.0965350	H	1.8031190	0.4414540	1.9265900
H	-0.3555650	-4.4583950	-1.3217480	C	4.0912030	2.5312730	0.3665720
H	-1.8388670	-3.8989830	-2.1005370	C	-1.9178060	2.9966680	0.4746140
C	2.2854990	-3.1227080	-1.6830160	H	-2.5202840	3.4257460	-0.3357260
H	1.9234820	-3.9668620	-1.0957000	H	-0.9846930	3.5513800	0.4554170
H	2.7448210	-3.5046270	-2.6043740	C	3.1854280	2.0671920	1.4915300
H	3.0699670	-2.6209650	-1.1111090	H	2.7455930	2.9293150	2.0008910
C	2.6038370	0.0046640	-2.2792550	H	3.8036850	1.5539170	2.2366370
H	2.4919410	1.0572860	-2.0138940	C	0.7599460	1.7685970	0.6766340
H	3.3668100	-0.4246330	-1.6265170	C	-2.6316080	3.2529100	1.8145000
H	2.9928410	-0.0406490	-3.3058450	H	-3.5806330	2.7011860	1.8442990
C	-2.3195140	-1.2744130	-3.0797170	H	-2.0074570	2.8490010	2.6200750
H	-2.3555870	-1.5139560	-4.1508090	C	5.1998490	1.7589680	-0.0106050
H	-2.9496900	-1.9987630	-2.5603210	H	5.4082990	0.8324330	0.5208300
H	-2.7635860	-0.2873390	-2.9413790	C	6.0456740	2.1642540	-1.0448160
C	-0.2495900	1.1624930	-3.1030570	H	6.9009550	1.5506970	-1.3154760
H	-1.3039630	1.4247000	-2.9932820	C	-2.9013920	4.7406950	2.0727230

H	-1.9498220	5.2884660	2.0466900	H	3.4096770	1.6596380	-2.6389190
H	-3.5095560	5.1491420	1.2530260	H	4.0784320	4.0509920	-2.4652700
C	3.8619210	3.7335590	-0.3166930	C	1.1206670	-0.1307490	-2.3587500
H	3.0072920	4.3439480	-0.0420840	O	0.7811050	-0.7259850	-3.3017870
C	4.7063100	4.1457580	-1.3487520	Rh	1.3381120	-0.4882470	0.6314820
H	4.5105390	5.0836000	-1.8618690	N	1.4367570	0.4718410	-1.3288340
C	5.8007620	3.3617340	-1.7193880	C	0.1560840	-2.8380820	-0.9097080
H	6.4601570	3.6842820	-2.5203140	O	1.2964310	-3.1828580	-1.2703100
C	-3.6054430	5.0010630	3.4084190	O	-0.1347120	-1.7571030	-0.2636890
H	-3.7829450	6.0699070	3.5680740	C	-1.0612110	-3.7409150	-1.2454160
H	-3.0052460	4.6341390	4.2487160	C	-0.5881570	-5.0305360	-1.9347740
H	-4.5756630	4.4925760	3.4503940	H	0.0941050	-5.5963840	-1.2942280
C	-6.4482980	1.4907360	-1.4972940	H	-1.4493130	-5.6670460	-2.1688380
H	-7.0347430	0.8671470	-2.1793540	H	-0.0577890	-4.8103880	-2.8646360
H	-7.1241360	1.8203890	-0.6983900	C	-2.0018810	-2.9655010	-2.1933440
H	-6.1290590	2.3827560	-2.0435660	H	-2.3825620	-2.0562310	-1.7225310
20				H	-1.4843180	-2.6799620	-3.1153250
				H	-2.8585000	-3.5913620	-2.4686830
C	1.4542540	4.0252070	-0.3098030	C	-1.8054950	-4.0866110	0.0605980
C	1.0408510	2.6820160	-0.3834440	H	-1.1680730	-4.6691880	0.7363070
C	1.7826850	1.8626860	-1.2554390	H	-2.1143760	-3.1816410	0.5881710
C	2.8616430	2.3423040	-1.9964660	H	-2.6934700	-4.6916790	-0.1574720
C	3.2352830	3.6804570	-1.8886380	C	3.5935230	-0.6416950	1.0656080
C	2.5334250	4.5409010	-1.0367230	C	3.0412710	-1.9106130	1.3426900
H	0.9189610	4.6997770	0.3499220	C	1.9857370	-1.7198570	2.3260880

C	1.9710520	-0.3373630	2.7188750	C	-0.1963690	0.8989920	0.8538400
C	2.9133940	0.3565030	1.8804910	C	-2.6720820	0.1747970	0.7284760
C	3.5286800	-3.2311720	0.8258870	H	-2.3997810	-0.5910460	-0.0014060
H	4.0429990	-3.1151880	-0.1293550	H	-2.8923890	1.0878590	0.1701440
H	4.2299260	-3.6785960	1.5439130	C	-5.1296060	-0.4410050	0.6614200
H	2.7067740	-3.9300060	0.6668290	C	-1.2451090	3.2216850	0.5720060
C	1.1931930	-2.8295480	2.9479970	H	-0.8379590	4.0875550	1.1124530
H	0.9193650	-3.5807800	2.2034120	H	-2.0254400	2.8372670	1.2244920
H	1.7902310	-3.3306410	3.7215640	C	-3.9117530	-0.2548680	1.5406170
H	0.2766450	-2.4589770	3.4071860	H	-3.6851490	-1.1854170	2.0701840
C	1.2273540	0.2557220	3.8778030	H	-4.1137800	0.5041380	2.3031630
H	0.9318630	1.2881640	3.6815020	C	-1.4323970	0.4022560	1.5886130
H	0.3245240	-0.3075950	4.1108130	C	-1.8787560	3.7168430	-0.7429910
H	1.8742800	0.2527620	4.7651830	H	-1.1061010	4.1379600	-1.3978100
C	4.7207270	-0.3604760	0.1178790	H	-2.3019200	2.8603180	-1.2858710
H	4.6512590	-0.9793730	-0.7803470	C	-5.4099820	-1.6816770	0.0720280
H	4.7332660	0.6886820	-0.1862670	H	-4.7580980	-2.5276210	0.2761570
H	5.6783450	-0.5697160	0.6131990	C	-6.5136060	-1.8450960	-0.7665440
C	3.3284100	1.7903780	2.0376410	H	-6.7146970	-2.8163470	-1.2103950
H	3.6859590	2.2173110	1.0983830	C	-2.9752450	4.7656090	-0.5142100
H	2.4964650	2.4062990	2.3844550	H	-3.7537880	4.3414600	0.1345870
H	4.1392940	1.8762870	2.7735710	H	-2.5524870	5.6160650	0.0385890
F	-1.1675090	-0.7987560	2.2391210	C	-5.9896610	0.6323170	0.3897540
F	-1.7530920	1.2619200	2.6464160	H	-5.7936230	1.6004030	0.8457470
C	-0.1399050	2.1754120	0.3846270	C	-7.0942870	0.4742530	-0.4483710

H	-7.7504820	1.3185090	-0.6420730	H	-1.0302670	4.6149650	-0.5731000
C	-7.3595880	-0.7664440	-1.0309880	H	-3.6676390	1.7887410	2.4749260
H	-8.2204570	-0.8926020	-1.6814210	H	-4.2778690	4.1657220	2.1707420
C	-3.6106400	5.2664400	-1.8151460	C	-1.7096190	0.0325400	2.4924620
H	-4.3882140	6.0124460	-1.6204210	O	-1.4952000	0.1300450	3.6471960
H	-4.0714310	4.4432760	-2.3729230	Rh	-1.4001770	-0.6172990	-0.5184870
H	-2.8620710	5.7286700	-2.4688620	N	-1.7172350	0.4613470	1.2955180
C	2.9103510	5.9999800	-0.9236530	C	0.0717180	-2.8848210	1.0434400
H	3.9849900	6.1478810	-1.0665410	O	-1.0132160	-3.4057870	1.4189760
H	2.3958770	6.6013710	-1.6836470	O	0.1800360	-1.7416600	0.4851120
H	2.6388600	6.4096750	0.0536460	C	1.3885470	-3.6645390	1.2858800
H	2.6966760	-2.4188840	-1.9635860	C	1.0946770	-5.0313190	1.9253560
C	3.6507120	-2.6622900	-3.6565320	H	0.4561690	-5.6434000	1.2824450
H	2.7806230	-2.5658770	-4.3212220	H	2.0332130	-5.5719250	2.0936040
H	4.5117320	-2.2046780	-4.1543390	H	0.5840550	-4.9191270	2.8851090
H	3.8648390	-3.7327270	-3.5235070	C	2.2763810	-2.8337780	2.2383320
O	3.4561750	-1.9948820	-2.4222610	H	2.5101480	-1.8534160	1.8183040
TS21				H	1.7817200	-2.6800080	3.2039030
C	-1.5973590	3.9835110	0.1016730	H	3.2190410	-3.3597590	2.4263390
C	-1.2047260	2.6398230	0.2591660	C	2.1066740	-3.8651700	-0.0645090
C	-1.9875960	1.8630830	1.1381070	H	1.5169720	-4.5044850	-0.7318410
C	-3.0804400	2.4184080	1.8127050	H	2.2694340	-2.9131680	-0.5724940
C	-3.4250840	3.7551910	1.6365420	H	3.0739750	-4.3564670	0.0917610
C	-2.6855140	4.5596740	0.7644020	C	-3.6089700	-0.9580180	-1.0001130
				C	-2.9745880	-2.2001030	-1.1959500

C	-1.9144740	-2.0006330	-2.1802200	C	-0.0026000	2.1014310	-0.4453250
C	-1.9788760	-0.6531000	-2.6508250	C	0.0926920	0.7969720	-0.8174230
C	-2.9681410	0.0349510	-1.8573730	C	2.6216130	0.2184080	-0.6912850
C	-3.3759220	-3.5266850	-0.6226910	H	2.4233280	-0.5113340	0.0964380
H	-4.0710670	-3.4037180	0.2103160	H	2.7945030	1.1774240	-0.1992660
H	-3.8770140	-4.1312580	-1.3904110	C	5.1268370	-0.1964830	-0.6800850
H	-2.5150430	-4.0848640	-0.2501090	C	1.0852180	3.1527830	-0.7008500
C	-1.0601510	-3.1015490	-2.7334020	H	0.6664920	3.9750260	-1.2964420
H	-0.7661100	-3.8026200	-1.9484830	H	1.8729020	2.7442230	-1.3285910
H	-1.6171620	-3.6689990	-3.4909790	C	3.8652110	-0.1775340	-1.5158790
H	-0.1535570	-2.7110850	-3.1955270	H	3.6986030	-1.1609820	-1.9661710
C	-1.2542650	-0.0759880	-3.8296770	H	3.9782850	0.5328920	-2.3409110
H	-1.0115820	0.9774100	-3.6782960	C	1.3466090	0.3017730	-1.5271460
H	-0.3224240	-0.6035690	-4.0294520	C	1.7076220	3.7396080	0.5815010
H	-1.8913040	-0.1509590	-4.7210390	H	0.9259780	4.1866940	1.2073090
C	-4.7605570	-0.6759710	-0.0823480	H	2.1415870	2.9253570	1.1779370
H	-4.7519420	-1.3433930	0.7806130	C	5.5568520	-1.3696330	-0.0449670
H	-4.7270410	0.3513910	0.2885790	H	4.9862630	-2.2856120	-0.1771250
H	-5.7112750	-0.8035210	-0.6161860	C	6.7073740	-1.3780110	0.7454080
C	-3.4658550	1.4300810	-2.1027020	H	7.0257580	-2.2996570	1.2250480
H	-3.8880820	1.8745520	-1.1992910	C	2.7882800	4.7891370	0.2903520
H	-2.6612250	2.0833510	-2.4466570	H	3.5727980	4.3398860	-0.3344080
H	-4.2496830	1.4281520	-2.8724220	H	2.3530290	5.6003380	-0.3099300
F	1.1430970	-0.9643100	-2.0689310	C	5.8842590	0.9700080	-0.5025630
F	1.5937470	1.0840020	-2.6636630	H	5.5713150	1.8878770	-0.9957430

C	7.0345690	0.9673710	0.2872600
H	7.6093810	1.8816750	0.4075450
C	7.4503350	-0.2084300	0.9151250
H	8.3476330	-0.2139660	1.5274140
C	3.4183940	5.3730040	1.5589500
H	4.1840600	6.1185570	1.3199120
H	3.8925880	4.5897680	2.1610850
H	2.6640230	5.8598610	2.1874920
C	-3.0278840	6.0179430	0.5656200
H	-2.4906540	6.6529840	1.2814640
H	-2.7583400	6.3609110	-0.4378600
H	-4.0970320	6.2010840	0.7094590
H	-2.0056970	-2.3947780	1.8543070
C	-2.9351740	-2.3270780	3.6171550
H	-2.2633240	-1.9263790	4.3844390
H	-3.9664490	-2.0852000	3.8910800
H	-2.8156370	-3.4133240	3.5667730
O	-2.6472720	-1.7514980	2.3425160

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C	2.0625040	3.7867490	0.0557360
C	1.5317920	2.5027010	-0.1909000
C	2.2524380	1.6463570	-1.0569940
C	3.4515250	2.1211660	-1.6291400
C	3.9391790	3.3927500	-1.3636710

C	3.2491020	4.2560670	-0.5037670
H	1.5304910	4.4499940	0.7287600
H	3.9949660	1.4808360	-2.3124150
H	4.8698540	3.7135130	-1.8266380
C	2.1228100	-0.2253200	-2.4703990
O	2.3555460	0.3298330	-3.5342290
Rh	1.3351340	-0.7516620	0.4774690
N	1.8423900	0.3056110	-1.2634710
C	-0.6830320	-2.8220690	-1.1362840
O	0.2617230	-3.2976600	-1.9246180
O	-0.5270350	-1.8090120	-0.4484610
C	-2.0072030	-3.5930720	-1.1750600
C	-1.8140900	-5.0116070	-1.7419440
H	-1.1158450	-5.5954830	-1.1340810
H	-2.7765180	-5.5333790	-1.7438910
H	-1.4330070	-4.9898810	-2.7651870
C	-2.9539240	-2.7905990	-2.1033520
H	-3.1541370	-1.7915010	-1.7084820
H	-2.5302720	-2.6880190	-3.1076660
H	-3.9089800	-3.3183430	-2.1921140
C	-2.5956120	-3.6665060	0.2465260
H	-1.9845890	-4.3058350	0.8929940
H	-2.6479250	-2.6800660	0.7088110
H	-3.6009200	-4.0984450	0.2072730
C	3.4594030	-1.4445770	0.8920100

C	2.6518140	-2.5801980	1.0676990	F	-1.4437940	1.2418290	2.6679700
C	1.6717710	-2.2781330	2.1161470	C	0.2551470	2.0936480	0.4596720
C	1.9282510	-0.9768190	2.6141920	C	0.0154560	0.8059450	0.8176490
C	2.9728210	-0.3952590	1.7901930	C	-2.5653600	0.5032480	0.6982280
C	2.8021190	-3.9150840	0.3973970	H	-2.4613500	-0.2493020	-0.0860750
H	3.4636560	-3.8532450	-0.4692930	H	-2.6263480	1.4704750	0.1969990
H	3.2319210	-4.6493550	1.0912180	C	-5.0991740	0.3802220	0.6822450
H	1.8439930	-4.3148040	0.0540290	C	-0.7324980	3.2441540	0.6884070
C	0.6982830	-3.2741860	2.6720710	H	-0.2554200	4.0277140	1.2900330
H	0.3031130	-3.9249730	1.8877620	H	-1.5745280	2.9191500	1.2946560
H	1.1909790	-3.9187440	3.4122540	C	-3.8468750	0.2649290	1.5249040
H	-0.1457300	-2.7813540	3.1551830	H	-3.7994600	-0.7241330	1.9914010
C	1.3116430	-0.3288190	3.8179670	H	-3.8774820	0.9957840	2.3393310
H	1.1323570	0.7353930	3.6536130	C	-1.2821920	0.4453980	1.5273040
H	0.3563520	-0.7864950	4.0746030	C	-1.2528920	3.8754160	-0.6180140
H	1.9850280	-0.4300010	4.6792750	H	-0.4089980	4.2381250	-1.2162120
C	4.6328070	-1.2903920	-0.0279090	H	-1.7403540	3.0997460	-1.2251230
H	4.6165350	-2.0273030	-0.8329140	C	-5.7248490	-0.7566470	0.1531420
H	4.6527600	-0.2958810	-0.4802160	H	-5.3198050	-1.7398360	0.3805420
H	5.5693960	-1.4174910	0.5302690	C	-6.8618450	-0.6446260	-0.6497320
C	3.6660320	0.9087990	2.0545960	H	-7.3339860	-1.5398220	-1.0456100
H	4.0623440	1.3484810	1.1371870	C	-2.2383670	5.0256020	-0.3739630
H	2.9815960	1.6345510	2.4973500	H	-3.0848040	4.6603620	0.2247170
H	4.5024170	0.7617810	2.7518300	H	-1.7498350	5.7983390	0.2359260
F	-1.2157440	-0.8415330	2.0647340	C	-5.6493690	1.6364500	0.3880430

H	-5.1849080	2.5306370	0.7981160	C	-5.3201430	-0.4093980	-1.0382800
C	-6.7844220	1.7543610	-0.4142570	C	-4.9991370	0.5175130	-2.0301270
H	-7.1955100	2.7374650	-0.6267710	H	-3.4583080	1.8069520	-2.7432580
C	-7.3948390	0.6124960	-0.9378720	H	-4.6755560	-1.4994130	0.6814290
H	-8.2805150	0.7022310	-1.5603630	H	-6.3070590	-0.8661380	-1.0181480
C	-2.7627550	5.6531750	-1.6695860	C	-2.3829140	-1.5714870	1.8867970
H	-3.4610650	6.4720430	-1.4661150	O	-3.3253490	-2.3449000	1.9318260
H	-3.2873560	4.9122920	-2.2835970	Rh	-0.1940160	-1.1280540	-0.1511620
H	-1.9417810	6.0572810	-2.2727390	N	-2.0873640	-0.5926720	0.9221840
C	3.7599400	5.6478960	-0.2140490	C	0.3890220	0.6135330	2.3157600
H	4.8319990	5.6443130	0.0130650	O	-0.7954230	1.0814460	2.2407190
H	3.6179180	6.3148710	-1.0739860	O	0.8477950	-0.2845470	1.5467170
H	3.2390180	6.0960940	0.6372820	C	1.2842750	1.1786990	3.4328870
H	1.0081010	-2.6240370	-1.9692060	C	1.3425840	2.7145540	3.2792770
C	2.5915610	-2.2202850	-3.7001150	H	0.3422580	3.1489810	3.3401680
H	1.9260750	-1.9198850	-4.5110630	H	1.9591670	3.1425200	4.0773770
H	3.6068310	-1.8997410	-3.9399740	H	1.7747720	2.9990620	2.3162490
H	2.5582910	-3.3014450	-3.5538650	C	2.7000950	0.5865150	3.3731560
O	2.1723780	-1.6456390	-2.4451630	H	2.6842900	-0.5017130	3.4800800
TS23				H	3.1936830	0.8209750	2.4261040
C	-3.7242130	1.0833070	-1.9800340	H	3.3076770	1.0019070	4.1845600
C	-2.7624280	0.7554910	-1.0085000	C	0.6254580	0.8233410	4.7850770
C	-3.0994460	-0.2240320	-0.0407580	H	-0.3924880	1.2162400	4.8373230
C	-4.3934870	-0.7741640	-0.0636730	H	0.5845890	-0.2612670	4.9327140
				H	1.2093830	1.2526890	5.6064390

C	-0.7176200	-3.3553660	-0.5554550	F	1.0232980	2.2735620	-2.2382930
C	0.5931790	-3.3005540	-0.0539580	F	1.0130340	2.6966670	-0.0594410
C	1.3870990	-2.4663230	-0.9540150	C	-1.4485310	1.4693390	-1.0483080
C	0.5408400	-2.0404720	-2.0286740	C	-0.2688360	0.8322130	-0.8445110
C	-0.7931730	-2.4948960	-1.7343760	C	2.3740820	0.9686440	-0.8682570
C	1.1526320	-3.9977450	1.1510180	H	2.4321650	0.2223570	-1.6585290
H	0.3623270	-4.4171430	1.7772710	H	2.4324070	0.4437540	0.0847070
H	1.8157300	-4.8210430	0.8556470	C	4.8821940	1.2379290	-1.0683640
H	1.7386670	-3.3079960	1.7662120	C	-1.5886080	2.9807360	-1.2709090
C	2.8814740	-2.3692820	-0.8499690	H	-2.2116230	3.1786700	-2.1506430
H	3.1954810	-1.9830700	0.1238680	H	-0.6271340	3.4389540	-1.4774980
H	3.3199390	-3.3694660	-0.9610980	C	3.5511190	1.9566200	-1.0187790
H	3.3207910	-1.7326520	-1.6176010	H	3.4082160	2.5386030	-1.9341050
C	0.9444870	-1.3670530	-3.3086270	H	3.5371920	2.6653210	-0.1855040
H	0.8654410	-2.0814460	-4.1378960	C	1.0174400	1.6435270	-0.9848920
H	0.3017640	-0.5142100	-3.5387340	C	-2.2217200	3.6837120	-0.0530550
H	1.9765030	-1.0139800	-3.2808620	H	-3.2048140	3.2449710	0.1616240
C	-1.8479020	-4.2064170	-0.0640050	H	-1.5954300	3.4926570	0.8264800
H	-1.6665850	-4.5947010	0.9398860	C	5.3852700	0.7468390	-2.2824850
H	-2.7968520	-3.6684780	-0.0393900	H	4.8276950	0.9251410	-3.1996850
H	-1.9667190	-5.0650610	-0.7379920	C	6.5930590	0.0488770	-2.3320950
C	-1.9796440	-2.3928420	-2.6480640	H	6.9673160	-0.3163460	-3.2847440
H	-2.9135020	-2.3146410	-2.0866460	C	-2.3749550	5.1960170	-0.2598180
H	-1.9097490	-1.5154430	-3.2940040	H	-1.3910030	5.6329150	-0.4784500
H	-2.0467280	-3.2809290	-3.2916530	H	-2.9941620	5.3821020	-1.1487380

C	5.6303470	1.0151960	0.0958030	C	-4.1589770	-1.5493580	0.5420400
H	5.2651770	1.4008500	1.0448120	C	-5.3834820	-0.8875650	0.5066710
C	6.8392680	0.3179390	0.0521820	C	-5.4328400	0.5050690	0.5749260
H	7.4052610	0.1616260	0.9665510	H	-4.2727160	2.2719380	0.7617740
C	7.3240940	-0.1702020	-1.1625040	H	-4.1468130	-2.6297090	0.4959750
H	8.2664430	-0.7093260	-1.1990250	H	-6.2999830	-1.4678630	0.4389140
C	-2.9919640	5.9073310	0.9489350	C	-1.7080750	-2.9626310	0.5685880
H	-3.0872910	6.9848890	0.7766080	O	-2.2483910	-3.5771240	-0.3278070
H	-2.3773490	5.7662030	1.8453330	Rh	-0.2835760	-0.6937560	-0.7798640
H	-3.9914290	5.5156900	1.1708270	N	-1.6855060	-1.5391920	0.7049750
C	-5.9966610	0.9238640	-3.0889790	C	1.2265150	-1.5721640	1.7661940
H	-6.6632500	1.7165960	-2.7257160	O	0.2913000	-1.1884910	2.4949530
H	-5.4979190	1.3051630	-3.9852430	O	1.2189440	-1.5476840	0.4721750
H	-6.6303060	0.0823060	-3.3870430	C	2.5006650	-2.1457630	2.4440110
H	-1.4770660	0.3514260	1.5287510	C	2.9409550	-1.1556950	3.5429680
C	-1.6633420	-2.5032560	3.9248450	H	2.1280960	-0.9803880	4.2505000
H	-2.6187470	-2.3024810	4.4155070	H	3.8058580	-1.5554400	4.0845200
H	-1.6675660	-3.5326640	3.5568310	H	3.2277670	-0.1878080	3.1180430
H	-0.8384470	-2.3534190	4.6214010	C	3.6474820	-2.3793940	1.4493100
O	-1.4334940	-1.5753580	2.8580470	H	3.3555740	-3.0811720	0.6632060
24				H	3.9641280	-1.4496470	0.9681110
				H	4.5149020	-2.7965600	1.9743620
C	-4.2228870	1.1941930	0.6870330	C	2.1076350	-3.4847890	3.1062920
C	-2.9565300	0.5750650	0.7026740	H	1.2523240	-3.3475950	3.7728690
C	-2.9579430	-0.8393030	0.6276810	H	1.8464510	-4.2349140	2.3518010

H	2.9479140	-3.8779280	3.6899320	H	-2.3341020	1.4013660	-3.8760150
C	-1.3362220	-1.3076600	-2.7045800	F	0.5363890	3.1301380	0.1110740
C	-0.0685680	-1.9639530	-2.6735740	F	0.8136520	2.1465400	2.0807570
C	0.9418160	-0.9346700	-2.6263990	C	-1.7197680	1.4045570	0.8716450
C	0.2964590	0.3497860	-2.6580030	C	-0.4972050	1.0008920	0.4226220
C	-1.1270500	0.1178360	-2.6451060	C	2.1216380	1.4141650	0.3073300
C	0.1862750	-3.4409630	-2.7670250	H	2.1127750	1.1553650	-0.7487120
H	-0.6112080	-4.0122890	-2.2859000	H	2.3576260	0.4960800	0.8411930
H	0.2503150	-3.7686300	-3.8132730	C	4.5614320	2.0476620	0.0718090
H	1.1298840	-3.7070780	-2.2825710	C	-1.9650090	2.7417460	1.5930610
C	2.4172340	-1.2021660	-2.6000820	H	-1.0853470	3.0079360	2.1739420
H	2.6776960	-1.8300620	-1.7424770	H	-2.7731550	2.5979890	2.3202010
H	2.7250200	-1.7264050	-3.5128320	C	3.2032340	2.4824240	0.5782300
H	3.0014340	-0.2831680	-2.5262180	H	2.9106320	3.4179540	0.0929710
C	0.9291050	1.6891920	-2.9089780	H	3.2455550	2.6815310	1.6534130
H	0.6118110	2.4445370	-2.1864450	C	0.7276780	1.8714570	0.7185110
H	2.0194700	1.6366130	-2.8889760	C	-2.3122580	3.9464240	0.6865950
H	0.6398610	2.0406980	-3.9077690	H	-1.4545650	4.1533870	0.0417280
C	-2.6746420	-1.9536640	-2.8900400	H	-3.1489950	3.7129390	0.0157300
H	-2.6543740	-3.0130270	-2.6414590	C	4.9626730	2.3392820	-1.2402790
H	-3.4406000	-1.4805390	-2.2713960	H	4.3033430	2.9222620	-1.8800540
H	-2.9788540	-1.8419030	-3.9394890	C	6.1985580	1.9108550	-1.7281360
C	-2.1794310	1.1741790	-2.8122610	H	6.4920680	2.1549010	-2.7456750
H	-3.1376250	0.8556040	-2.3969600	C	-2.6574420	5.2027410	1.4977420
H	-1.8921590	2.0999690	-2.3088160	H	-3.5153090	4.9928860	2.1520640

H	-1.8188020	5.4396240	2.1660460	C	-2.9619640	-0.5426490	0.4833510
C	5.4409050	1.3202340	0.8859690	C	-4.2152380	-1.1514340	0.7565560
H	5.1547810	1.0960680	1.9107560	C	-5.4170100	-0.5066880	0.5483050
C	6.6781700	0.8894690	0.4035400	C	-5.4553180	0.8056290	0.0478650
H	7.3455950	0.3306260	1.0538290	H	-4.2779170	2.4263230	-0.5851390
C	7.0606770	1.1813420	-0.9070400	H	-4.2238000	-2.1629890	1.1379690
H	8.0248290	0.8505620	-1.2825250	H	-6.3441260	-1.0363510	0.7572900
C	-2.9708820	6.4183830	0.6193160	C	-1.7904280	-2.3299760	1.5074490
H	-3.2079060	7.3007540	1.2232110	O	-2.4280460	-2.4081350	2.5493670
H	-3.8285300	6.2243390	-0.0356590	Rh	-0.1970250	-1.0058300	-0.7273540
H	-2.1188200	6.6727580	-0.0214140	N	-1.8016430	-1.3012880	0.5944010
C	-6.7463050	1.2490960	0.5146270	C	1.0267560	-0.7191320	2.0476770
H	-6.6836790	2.2147470	1.0251380	O	0.2761850	0.2933020	2.2246920
H	-7.0457520	1.4478640	-0.5222660	O	1.1173580	-1.3393270	0.9450360
H	-7.5527620	0.6727750	0.9786610	C	1.8757120	-1.1796960	3.2488890
H	-1.0993040	-1.2757540	1.5468710	C	2.8993310	-0.0645430	3.5609460
C	-0.9725460	-4.9797900	1.5110950	H	2.3930520	0.8843210	3.7569710
H	-1.9743230	-5.4138320	1.4883230	H	3.4823890	-0.3348510	4.4481540
H	-0.4234790	-5.2919380	0.6196970	H	3.6005620	0.0785880	2.7314130
H	-0.4413450	-5.2787350	2.4129030	C	2.6111360	-2.4923940	2.9407710
O	-1.0496490	-3.5438930	1.5767970	H	1.9095070	-3.2971900	2.7063980
TS23'				H	3.2873400	-2.3805660	2.0889130
C	-4.2384760	1.4164350	-0.2024390	H	3.2026880	-2.7963820	3.8112690
C	-2.9667280	0.8096300	0.0075920	C	0.9307630	-1.3589810	4.4578260
				H	0.4402190	-0.4161850	4.7091160

H	0.1456650	-2.0931550	4.2511270	H	-1.9635650	0.6631460	-3.3960820
H	1.5019870	-1.7013290	5.3276710	H	-2.3436010	-0.7649720	-4.3683460
C	-0.9951990	-2.4703060	-2.1881030	F	0.6323220	2.5954440	-1.6891670
C	0.3405140	-2.8533490	-1.8842150	F	0.6219480	3.1481810	0.4529500
C	1.2150560	-1.7704140	-2.3015870	C	-1.7517900	1.6120150	-0.2252900
C	0.4189580	-0.7481150	-2.8870660	C	-0.4560470	1.0912480	-0.1497750
C	-0.9717300	-1.1346090	-2.7513860	C	2.1347810	1.5169840	-0.2371930
C	0.8209850	-4.1608480	-1.3320260	H	2.2662790	0.6405300	-0.8721200
H	-0.0060150	-4.7614520	-0.9528690	H	2.2505060	1.1844010	0.7947580
H	1.3344180	-4.7398540	-2.1110100	C	4.6090240	2.0329370	-0.4097720
H	1.5264800	-4.0053470	-0.5108540	C	-1.9853890	3.1010540	-0.4826480
C	2.7119780	-1.8308460	-2.2216240	H	-2.7775070	3.2235370	-1.2284870
H	3.0390970	-2.1590400	-1.2307950	H	-1.1037740	3.5535880	-0.9207380
H	3.1032780	-2.5486070	-2.9541770	C	3.2062850	2.5803220	-0.5594140
H	3.1768050	-0.8644830	-2.4256480	H	3.0557160	2.9454080	-1.5797730
C	0.9192400	0.4234250	-3.6767540	H	3.0627860	3.4359680	0.1075460
H	0.2425170	1.2751890	-3.6247230	C	0.7144260	2.0445130	-0.3994640
H	1.9013900	0.7604370	-3.3410830	C	-2.3543650	3.8928770	0.7925170
H	1.0135970	0.1262170	-4.7299160	H	-3.2453740	3.4619450	1.2632750
C	-2.2273040	-3.2989540	-1.9840240	H	-1.5354670	3.7863510	1.5116030
H	-2.0984320	-4.0000910	-1.1585140	C	5.3047050	1.5201160	-1.5132340
H	-3.0963160	-2.6755900	-1.7626580	H	4.8424090	1.5569420	-2.4975820
H	-2.4470230	-3.8716880	-2.8942170	C	6.5850360	0.9810010	-1.3708750
C	-2.1454030	-0.4127720	-3.3471130	H	7.1084220	0.5947370	-2.2413640
H	-3.0520120	-0.5667730	-2.7577210	C	-2.5920680	5.3805830	0.5037300

H	-1.6943410	5.8051130	0.0348050	C	-2.7792520	0.5871250	1.0714220
H	-3.4003540	5.4862410	-0.2338860	C	-2.5936220	-0.7556730	1.5229290
C	5.2379260	2.0001680	0.8433720	C	-3.4723380	-1.2178910	2.5376860
H	4.7206830	2.4072280	1.7090820	C	-4.5484780	-0.4552080	2.9607900
C	6.5174070	1.4628110	0.9915770	C	-4.8269440	0.8108710	2.4214150
H	6.9878740	1.4519340	1.9709410	H	-4.1021170	2.2942660	1.0901890
C	7.1950250	0.9481360	-0.1158710	H	-3.3149320	-2.1998930	2.9514030
H	8.1924400	0.5331170	-0.0027690	H	-5.2089410	-0.8712690	3.7190290
C	-2.9413440	6.1828900	1.7613860	C	-1.4060590	-2.8273210	1.3064930
H	-3.1035520	7.2407760	1.5293430	O	-1.8194310	-3.3781940	2.3184760
H	-2.1367500	6.1234760	2.5028100	Rh	-0.6243310	-0.7512880	-0.8117500
H	-3.8536050	5.8013720	2.2339710	N	-1.6666290	-1.5557120	0.8532650
C	-6.7665570	1.5136160	-0.1947850	C	1.6927340	-1.4576410	1.1597010
H	-7.4137480	0.9441140	-0.8726480	O	1.0723400	-1.1135360	2.1682490
H	-7.3264100	1.6525100	0.7381850	O	1.2807860	-1.3263390	-0.0711240
H	-6.6108660	2.5021210	-0.6366070	C	3.0963580	-2.1249180	1.3199290
H	-0.2264610	0.6164710	1.0491860	C	3.8316410	-1.4442940	2.4906820
C	-0.8683340	-4.4255340	2.0616870	H	3.2146230	-1.4586060	3.3908590
H	-0.4809510	-4.0913200	3.0274540	H	4.7742730	-1.9649660	2.6954700
H	-1.8505940	-4.8777730	2.2228620	H	4.0738210	-0.4021260	2.2587140
H	-0.1835880	-5.1486730	1.6153390	C	3.9557080	-2.0404040	0.0481520
O	-0.9466030	-3.3432930	1.1293200	H	3.4812380	-2.5491460	-0.7952290
				H	4.1477150	-1.0027210	-0.2419070
24'				H	4.9270510	-2.5170380	0.2255070
C	-3.9308740	1.2997540	1.4817530	C	2.8517250	-3.6074730	1.6772820

H	2.2194960	-3.6928600	2.5658530	H	-4.0597470	-0.6428560	-1.7372300
H	2.3658190	-4.1390750	0.8534930	H	-3.5600490	0.8115280	-2.6019830
H	3.8054340	-4.1070370	1.8837460	H	-3.9667440	-0.6512060	-3.5035180
C	-1.6613290	-2.1054180	-2.2958720	F	0.5551570	2.6083960	-1.0879200
C	-0.2528190	-2.1956520	-2.4758330	F	0.4695130	3.1482920	1.0515680
C	0.2355250	-0.8777780	-2.8640770	C	-1.7667620	1.2941770	0.2752290
C	-0.8817550	-0.0082260	-2.9591280	C	-0.3940060	1.0472350	0.4981590
C	-2.0576090	-0.7377240	-2.5259990	C	2.1355940	1.6474020	0.3749100
C	0.6177430	-3.4074900	-2.3874780	H	2.3508490	0.8406990	-0.3273610
H	0.0364360	-4.3104990	-2.1991550	H	2.2350830	1.2274780	1.3795390
H	1.1703080	-3.5436020	-3.3247190	C	4.5611160	2.4020140	0.3432870
H	1.3416320	-3.2840020	-1.5766470	C	-2.2621030	2.4552950	-0.5807270
C	1.6577690	-0.5718160	-3.2223880	H	-3.2774390	2.2249650	-0.9155880
H	2.3327620	-0.9487610	-2.4491660	H	-1.6366070	2.5423030	-1.4638680
H	1.9304150	-1.0483910	-4.1729410	C	3.1163320	2.8231170	0.1824090
H	1.8210050	0.5031520	-3.3269940	H	2.9671810	3.2535010	-0.8132750
C	-0.8582470	1.3494250	-3.5959120	H	2.8746530	3.6074750	0.9058750
H	-1.7957340	1.8876210	-3.4532420	C	0.6879780	2.0683340	0.1924940
H	-0.0448290	1.9692380	-3.2175800	C	-2.2743990	3.8534940	0.0968600
H	-0.7150640	1.2278270	-4.6772800	H	-2.6713100	3.7909160	1.1160200
C	-2.6164690	-3.2106500	-1.9665790	H	-1.2500890	4.2140080	0.1927640
H	-2.0954890	-4.1312940	-1.7076170	C	5.3258720	2.0133140	-0.7652570
H	-3.2552920	-2.9389490	-1.1216420	H	4.8783250	2.0402450	-1.7564980
H	-3.2673660	-3.4086310	-2.8274410	C	6.6532180	1.6065530	-0.6166350
C	-3.4839640	-0.2762830	-2.5912800	H	7.2296270	1.3142720	-1.4901820

C	-3.1018020	4.8596010	-0.7141030
H	-2.7163620	4.9011080	-1.7425330
H	-4.1396320	4.5061890	-0.7926920
C	5.1648580	2.3753950	1.6086080
H	4.5905230	2.6818010	2.4798160
C	6.4914000	1.9694520	1.7625560
H	6.9407830	1.9592690	2.7516710
C	7.2403890	1.5828450	0.6494770
H	8.2737010	1.2695140	0.7676350
C	-3.0856180	6.2661030	-0.1067120
H	-3.6829260	6.9650120	-0.7013030
H	-2.0651410	6.6609820	-0.0520350
H	-3.4923210	6.2619340	0.9108380
C	-6.0263760	1.6110950	2.8694910
H	-6.9612620	1.0614580	2.7066800
H	-5.9768450	1.8456640	3.9396860
H	-6.0997950	2.5585350	2.3272890
H	-0.1373360	0.4706710	1.3859700
C	-0.4080860	-4.8899320	0.8085050
H	0.0395710	-4.9578970	1.8012390
H	-1.3521310	-5.4434670	0.8146320
H	0.2681230	-5.3050970	0.0595470
O	-0.6171930	-3.5256030	0.4276240

C	-3.6275170	0.8720420	-1.6707450
C	-2.7393640	1.1078800	-0.6170120
C	-3.1991620	0.8738210	0.7024100
C	-4.5020670	0.4015760	0.9160820
C	-5.3424840	0.1537670	-0.1682590
C	-4.9238130	0.3773300	-1.4830300
H	-3.2995200	1.1115770	-2.6789130
H	-4.8510950	0.2629490	1.9301640
H	-6.3520140	-0.2032580	0.0220260
C	-2.5312180	1.0763000	3.1022940
O	-3.5381870	0.6789310	3.6660690
Rh	0.1813740	-0.8542870	-1.1655440
N	-2.3178240	1.1783510	1.7571800
C	1.9055490	-2.0129840	1.0589340
O	1.2811190	-0.9070230	0.6906860
O	1.7827010	-3.0980920	0.4951670
C	2.8595390	-1.8748330	2.2760480
C	2.5478140	-0.6475400	3.1484580
H	1.5307340	-0.6862260	3.5519440
H	3.2399030	-0.6149840	3.9978380
H	2.6570940	0.2848870	2.5912310
C	4.2877290	-1.7515850	1.6940940
H	4.5298700	-2.6230070	1.0778920
H	4.3977880	-0.8491000	1.0846630
H	5.0203830	-1.6928000	2.5065210

C	2.7621250	-3.1559190	3.1267420	C	-0.5480620	0.6032280	-4.0877940
H	1.7685560	-3.2538370	3.5779400	H	-1.6339370	0.6738010	-4.0178390
H	2.9449490	-4.0417080	2.5155790	H	-0.1220060	1.5366050	-3.7180170
H	3.4985890	-3.1260130	3.9374590	H	-0.2884190	0.5037770	-5.1501290
C	-0.7298390	-1.7535050	-2.9437310	F	1.1673050	2.6790960	-2.1101600
C	0.2342940	-2.7478850	-2.4710720	F	0.7646760	3.2479910	-0.0049270
C	1.5110040	-2.1654670	-2.5300070	C	-1.4273500	1.8111020	-0.8421250
C	1.3704140	-0.7904170	-2.9944270	C	-0.2082860	1.2053070	-0.8079900
C	-0.0194090	-0.5792520	-3.3331120	C	2.3708890	1.6255120	-0.3634510
C	-0.1024710	-4.1437510	-2.0427970	H	2.6305520	0.7254890	-0.9183110
H	-0.0384220	-4.8399520	-2.8894350	H	2.2663290	1.3147160	0.6766190
H	0.5796220	-4.4780070	-1.2592730	C	4.8057720	2.2002740	0.0437430
H	-1.1206170	-4.1956910	-1.6496990	C	-1.6779230	3.3052630	-1.1232860
C	2.8263580	-2.8253630	-2.2565640	H	-2.4539670	3.3332180	-1.9022790
H	2.7059580	-3.7458590	-1.6890170	H	-0.7940160	3.7758700	-1.5496990
H	3.3181300	-3.0535560	-3.2121480	C	3.4807690	2.6893060	-0.4996430
H	3.4967930	-2.1726970	-1.6916950	H	3.5901690	2.9676780	-1.5524640
C	2.5110180	0.0685160	-3.4572120	H	3.1699080	3.5919890	0.0348090
H	2.2715690	1.1297400	-3.3915530	C	1.0102200	2.1359940	-0.8137180
H	3.4190450	-0.1176450	-2.8787790	C	-2.1760310	4.1506200	0.0634570
H	2.7408800	-0.1637050	-4.5064450	H	-3.0827470	3.7042670	0.4902140
C	-2.1902210	-2.0362700	-3.1188020	H	-1.4141080	4.1421150	0.8514150
H	-2.3251160	-2.8492170	-3.8433230	C	5.7478060	1.5838990	-0.7918360
H	-2.6441850	-2.3452980	-2.1737150	H	5.5349860	1.4900930	-1.8546640
H	-2.7330210	-1.1631880	-3.4799960	C	6.9577610	1.1063550	-0.2839860

H	7.6757930	0.6366940	-0.9508900	C	-1.5425940	-2.0982750	1.2731830
C	-2.4729410	5.6017010	-0.3376100	O	-0.7679010	-1.5453390	2.1861480
H	-1.5680230	6.0497270	-0.7701470	C	-2.4988260	-3.1659990	1.8038460
H	-3.2284240	5.6101880	-1.1356440	C	-3.0489150	-2.7662870	3.1883570
C	5.1141510	2.3311540	1.4056740	H	-3.7379140	-3.5427650	3.5366940
H	4.4006340	2.8162070	2.0679560	H	-2.2438710	-2.6719210	3.9206370
C	6.3225090	1.8575130	1.9183420	H	-3.5870540	-1.8158410	3.1585510
H	6.5427860	1.9743640	2.9759280	C	-3.6496680	-3.3917760	0.8102050
C	7.2488410	1.2407940	1.0746300	H	-3.2772130	-3.7309010	-0.1598470
H	8.1912810	0.8741770	1.4712380	H	-4.3233590	-4.1601030	1.2030980
C	-2.9587590	6.4612090	0.8339280	H	-4.2245500	-2.4758530	0.6515780
H	-3.1613580	7.4907450	0.5199560	C	-1.6582980	-4.4632130	1.9392260
H	-2.2102220	6.4985780	1.6336670	H	-2.2985040	-5.2677670	2.3159070
H	-3.8816380	6.0571800	1.2657650	H	-1.2448050	-4.7749260	0.9756050
C	-5.8316710	0.0992440	-2.6581590	H	-0.8286270	-4.3274100	2.6380610
H	-5.7044100	-0.9243480	-3.0349020	H	-0.0395060	-1.0477510	1.7094470
H	-6.8852430	0.2118850	-2.3843260				
H	-5.6282320	0.7784500	-3.4926160	TS26			
H	-1.4053080	1.5156900	1.4749080	C	-3.4114450	-1.2197400	-1.2968900
C	-1.4964880	1.4301570	5.1852330	C	-2.9064370	-0.1489630	-0.5476020
H	-1.6594140	0.4019530	5.5184670	C	-3.6094660	0.2250580	0.6202750
H	-0.5377680	1.7998600	5.5493620	C	-4.7567460	-0.4852850	1.0003980
H	-2.3121930	2.0555940	5.5572530	C	-5.2217950	-1.5488920	0.2348120
O	-1.4141820	1.4957390	3.7565860	C	-4.5521290	-1.9405990	-0.9296350
O	-1.4602360	-1.8131320	0.0702510	H	-2.9123180	-1.4735560	-2.2249200

H	-5.2988210	-0.1657770	1.8817930	C	1.7695010	-1.5330550	-2.6138900
H	-6.1225030	-2.0733360	0.5437190	C	0.3846820	-1.8538190	-2.9027900
C	-3.9773470	2.2546370	1.9780560	C	1.2845480	-4.6550540	-0.5311810
O	-5.1904620	2.3192170	1.8946020	H	1.7335330	-5.4935570	-1.0797980
Rh	0.6668110	-1.4293410	-0.7277550	H	1.8853120	-4.4370430	0.3531090
N	-3.1627980	1.3211070	1.3959240	H	0.2912370	-4.9638750	-0.1980620
C	2.6147210	-1.4136790	1.5632470	C	3.6996550	-2.6944820	-1.2924360
O	1.9728430	-0.6488390	0.7219290	H	3.7684350	-3.2093830	-0.3350990
O	2.5285350	-2.6442540	1.6299950	H	4.2536920	-3.2671350	-2.0483220
C	3.5888260	-0.6407640	2.5012730	H	4.1853510	-1.7214290	-1.1929680
C	2.9108570	0.6092200	3.0931340	C	2.6063590	-0.5213420	-3.3401890
H	2.0151110	0.3473800	3.6655710	H	2.0341900	0.3725630	-3.5850780
H	3.6029080	1.1248100	3.7690750	H	3.4701650	-0.2168630	-2.7440350
H	2.6143410	1.3084860	2.3098480	H	2.9887760	-0.9523460	-4.2755330
C	4.8112280	-0.2110880	1.6594350	C	-1.2541940	-3.7853450	-2.1850750
H	5.3172540	-1.0825320	1.2280730	H	-1.0527120	-4.8276990	-2.4579070
H	4.5220010	0.4624670	0.8487360	H	-1.7460770	-3.7845040	-1.2083900
H	5.5364520	0.3160210	2.2893130	H	-1.9527080	-3.3808660	-2.9183510
C	4.0513490	-1.5692890	3.6364390	C	-0.4493660	-1.1339090	-3.9187650
H	3.2099890	-1.8847750	4.2607450	H	-1.5077530	-1.3847390	-3.8354520
H	4.5216250	-2.4720760	3.2407800	H	-0.3433110	-0.0529990	-3.8191730
H	4.7731540	-1.0466720	4.2746200	H	-0.1193880	-1.4161470	-4.9271440
C	0.0326200	-3.0148860	-2.1540600	F	0.5338600	1.7628350	-2.6481560
C	1.2032940	-3.4417010	-1.4057860	F	-0.2594910	2.9909670	-0.9861720
C	2.2755980	-2.5556450	-1.7311750	C	-1.8087010	0.7195990	-1.1144430

C	-0.4806660	0.6261390	-0.7752350	H	5.6206010	4.4455530	2.1096000
C	1.7949580	1.9462780	-0.6603080	C	6.5365900	3.4869320	0.4086530
H	2.3780830	1.0522600	-0.8780800	H	7.5443160	3.5522560	0.8088160
H	1.7022920	1.9794810	0.4277760	C	-4.7979300	4.8194380	-2.1032060
C	3.9215890	3.3252810	-0.6325070	H	-5.1896390	5.4507980	-2.9078040
C	-2.4050480	1.7110750	-2.1192620	H	-4.2561740	5.4678220	-1.4051870
H	-2.9994800	1.1006060	-2.8161640	H	-5.6518310	4.3955470	-1.5630670
H	-1.6212320	2.1869610	-2.7037120	C	-5.0481700	-3.0989980	-1.7631150
C	2.5146670	3.2096450	-1.1775500	H	-4.6289750	-4.0526190	-1.4170860
H	2.5435070	3.1820860	-2.2714720	H	-6.1374550	-3.1887360	-1.7113260
H	1.9308840	4.0922390	-0.8991850	H	-4.7718320	-2.9847710	-2.8161190
C	0.4001640	1.7876720	-1.2396560	H	-2.1723500	1.3879850	1.5900960
C	-3.3298690	2.8045240	-1.5473930	C	-3.9450480	4.1826480	3.3230430
H	-4.1656050	2.3548560	-1.0005560	H	-4.6626320	3.7727410	4.0387140
H	-2.7618540	3.4043670	-0.8283240	H	-3.1984390	4.7880000	3.8377880
C	5.0165090	2.8309810	-1.3550660	H	-4.4862280	4.7876950	2.5908710
H	4.8505580	2.3911220	-2.3362420	O	-3.2111970	3.1354860	2.6779330
C	6.3126560	2.9088000	-0.8419810	O	-0.4940390	-2.0808840	0.9270370
H	7.1474970	2.5245040	-1.4218710	C	-0.7814460	-1.2961480	1.8701150
C	-3.8863600	3.7160730	-2.6497040	O	-0.6216670	-0.0221990	1.7751020
H	-3.0530090	4.1691690	-3.2037460	C	-1.2898420	-1.8882710	3.1929060
H	-4.4423870	3.1083770	-3.3773650	C	-2.0484290	-0.8381280	4.0215340
C	4.1627470	3.9066860	0.6205060	H	-2.3465600	-1.2792960	4.9784760
H	3.3275330	4.3042770	1.1926020	H	-1.4252380	0.0356380	4.2259350
C	5.4560690	3.9873730	1.1381960	H	-2.9519980	-0.4982850	3.5090640

C	-2.2002600	-3.0966060	2.8979310
H	-1.6628680	-3.8668310	2.3406020
H	-2.5462120	-3.5300830	3.8421570
H	-3.0791510	-2.7992010	2.3176610
C	-0.0394750	-2.3623090	3.9756240
H	-0.3618340	-2.8762180	4.8876790
H	0.5743960	-3.0417480	3.3800920
H	0.5837580	-1.5130070	4.2721920
H	-0.4008180	0.2318110	0.6256350

P1

C	3.7908090	-1.2759160	-0.6146540
C	2.6601810	-0.4638890	-0.4510930
C	2.8492010	0.9126320	-0.1861330
C	4.1526290	1.4249910	-0.0983170
C	5.2471970	0.5866920	-0.2777540
C	5.0935370	-0.7791030	-0.5443150
H	3.6398720	-2.3322550	-0.8233280
H	4.2881110	2.4758840	0.1162000
H	6.2459930	1.0101540	-0.2055190
C	1.6488110	3.0550660	0.3034660
O	2.5755160	3.8276320	0.4611720
N	1.7110790	1.7195530	0.0063140
F	-1.1803050	-0.9674630	-3.1580020
F	-1.0103690	-2.5946490	-1.6822940

C	1.3005150	-1.0937910	-0.5431610
C	0.4717930	-0.7252470	-1.5376330
C	-2.0331290	-0.5756310	-0.9940440
H	-1.9622450	0.5102190	-1.1228240
H	-1.8345880	-0.7833790	0.0628920
C	-4.5264690	-0.3935860	-0.5694110
C	0.9812000	-2.1334980	0.5141250
H	1.7895670	-2.8772040	0.5153550
H	0.0663900	-2.6691970	0.2579150
C	-3.4421600	-1.0654120	-1.3832740
H	-3.5950710	-0.8711700	-2.4491470
H	-3.4854680	-2.1505520	-1.2475950
C	-0.9258630	-1.2191770	-1.8223310
C	0.8684330	-1.5425260	1.9338550
H	1.7802310	-0.9810160	2.1723930
H	0.0437440	-0.8165560	1.9615620
C	-5.1042340	0.8088670	-0.9986570
H	-4.7900190	1.2432960	-1.9448670
C	-6.0802400	1.4486220	-0.2341440
H	-6.5199440	2.3771230	-0.5873790
C	0.6351700	-2.6174380	3.0025810
H	-0.2678210	-3.1901880	2.7513070
H	1.4661710	-3.3350810	2.9766500
C	-4.9548350	-0.9403190	0.6475470
H	-4.5236140	-1.8776030	0.9916270

C	-5.9304490	-0.3043110	1.4159000	H	-3.9618120	0.1044420	1.9057580
H	-6.2525880	-0.7474360	2.3540080	C	-4.6158630	-0.5411000	-0.0627120
C	-6.4959910	0.8940410	0.9773450	H	-4.6484040	-0.1291940	-1.0784760
H	-7.2584000	1.3886090	1.5720290	H	-3.9524240	-1.4135450	-0.1020300
C	0.5002330	-2.0407890	4.4148320	C	-6.0211990	-0.9723370	0.3709450
H	0.3385020	-2.8313420	5.1545790	H	-6.6730010	-0.0895690	0.4175890
H	-0.3446920	-1.3460890	4.4807320	H	-5.9784640	-1.3739730	1.3924150
H	1.4022970	-1.4914360	4.7063640	C	-6.6384530	-2.0159340	-0.5644910
C	6.2890670	-1.6740870	-0.7684670	H	-7.6402090	-2.3048710	-0.2316050
H	6.7114790	-1.5346960	-1.7713560	H	-6.7254630	-1.6301000	-1.5862030
H	7.0882220	-1.4608540	-0.0509260	H	-6.0262800	-2.9237170	-0.6048680
H	6.0225140	-2.7303610	-0.6704090	C	-0.2318180	1.6996050	-0.2893430
H	0.8182550	1.2574070	-0.0919150	C	0.8799330	0.6952520	-0.0215480
C	0.1125810	4.7912620	0.7135680	H	0.8712640	0.4546010	1.0502380
H	0.5314600	5.4386470	-0.0609140	H	0.6174840	-0.2449130	-0.5257980
H	-0.9702120	4.9070350	0.7615180	C	2.2652100	1.1895920	-0.4648990
H	0.5666950	5.0504890	1.6731400	H	2.4854700	2.1301690	0.0500340
O	0.3362090	3.4101430	0.4003050	H	2.2287590	1.4303470	-1.5321140
H	0.8019390	0.0227730	-2.2544380	C	3.3517070	0.1722520	-0.1907210
				C	4.0333570	0.1609240	1.0337760
2°				C	3.6809780	-0.8019970	-1.1427230
C	-2.6669870	0.9364420	0.4839390	C	5.0124810	-0.7962450	1.3017630
C	-1.5624350	1.2865430	0.1236210	H	3.7979810	0.9149910	1.7813470
C	-4.0052140	0.5136120	0.8873300	C	4.6592880	-1.7614350	-0.8798770
H	-4.6644250	1.3904430	0.9337890	H	3.1690460	-0.8033140	-2.1023060

C	5.3282030	-1.7623230	0.3451590	H	1.4652050	-5.3583230	0.2975210
H	5.5325500	-0.7839710	2.2555510	H	2.2954600	-5.8685320	1.7763520
H	4.9027710	-2.5047610	-1.6338670	H	0.5194140	-5.8086650	1.7274250
H	6.0928500	-2.5058080	0.5504250	C	1.4978360	-3.8287050	3.4422110
O	-0.0303520	2.7832060	-0.8151500	H	1.4278950	-2.8011040	3.8092960
90				H	0.6530690	-4.3920110	3.8482340
				H	2.4268550	-4.2796510	3.8082990
				C	2.7290830	-3.1446310	1.3458250
C	-3.1505250	2.1243290	0.5991620	H	2.7065480	-3.0696290	0.2547970
C	-2.2982190	1.0295260	0.7827050	H	2.8180960	-2.1356820	1.7559810
C	-1.9261450	0.6918100	2.0900830	H	3.6218520	-3.7114180	1.6330420
C	-2.4023070	1.4146540	3.1876880	C	-3.5655950	-0.5523560	-1.6073260
C	-3.2642800	2.4885550	2.9872950	C	-3.0196410	-1.7960760	-1.1427700
C	-3.6513430	2.8568410	1.6892800	C	-1.8398820	-2.0912300	-1.9351130
H	-3.4423490	2.4386250	-0.4006020	C	-1.6398770	-1.0053380	-2.8325010
H	-2.0680420	1.1243660	4.1798400	C	-2.6827750	-0.0240820	-2.6060560
H	-3.6362490	3.0541640	3.8383650	C	-3.6378100	-2.7153190	-0.1317320
C	-0.9465720	-0.4156680	2.2631980	H	-4.1440680	-3.5482060	-0.6373800
O	-0.3799770	-0.6990310	3.3190770	H	-2.8794780	-3.1270230	0.5389260
Rh	-1.5018790	-0.2083290	-0.6885250	H	-4.3814140	-2.1937110	0.4751370
N	-0.7858820	-1.0588260	1.0624850	C	-1.0526900	-3.3675430	-1.8885590
C	0.1668620	-3.1677540	1.4971740	H	-1.1505090	-3.8503390	-0.9152650
O	-0.9215250	-3.6946820	1.5792400	H	-1.4214270	-4.0672420	-2.6505130
O	0.3762850	-1.8850970	1.0902150	H	0.0067430	-3.1819640	-2.0761190
C	1.4803410	-3.8579410	1.8926880	C	-0.6034290	-0.9204950	-3.9136940
C	1.4331940	-5.3136540	1.3919020				

H	-0.2415970	0.1030050	-4.0465780	H	-0.2498730	3.1425510	1.3439660
H	0.2550070	-1.5545980	-3.6927500	H	1.3437450	3.2912500	0.6129960
H	-1.0372690	-1.2386950	-4.8708310	C	6.1080330	1.5391560	-1.6605270
C	-4.8969940	0.0085200	-1.2058880	H	5.6613960	1.7171570	-2.6364240
H	-5.6924140	-0.5303250	-1.7368590	C	7.2184870	2.2848400	-1.2619620
H	-5.0793660	-0.0954420	-0.1347560	H	7.6292220	3.0398070	-1.9268200
H	-4.9907600	1.0655840	-1.4598420	C	0.1616110	5.1057280	0.5262480
C	-2.9067080	1.2070590	-3.4378450	H	0.6896220	5.5355510	-0.3364160
H	-3.4852170	1.9606200	-2.8978350	H	-0.8954890	5.3796920	0.4082700
H	-1.9598270	1.6645740	-3.7364450	C	6.1625630	0.3335680	0.4225160
H	-3.4581520	0.9658820	-4.3560940	H	5.7580750	-0.4319440	1.0807990
C	-0.1233800	1.4966930	-0.8595620	C	7.2725990	1.0768750	0.8258200
C	0.5298600	0.4242240	-0.9709510	H	7.7252360	0.8876080	1.7952160
C	3.0358440	0.4314760	-0.7675030	C	7.8041950	2.0561970	-0.0156230
H	3.0106800	0.4899460	0.3293940	H	8.6706600	2.6326940	0.2954880
H	2.9713550	1.4705550	-1.1157900	C	0.7066000	5.7198450	1.8196490
C	5.5630300	0.5542860	-0.8253720	H	0.5984980	6.8092560	1.8192740
C	-0.2572170	2.9685630	-0.8120520	H	1.7701020	5.4903590	1.9497830
H	-1.3030390	3.2621480	-0.9370850	H	0.1743630	5.3306100	2.6944480
H	0.3006600	3.3800250	-1.6659530	C	-4.6063420	4.0080380	1.4695730
C	4.3384160	-0.2290870	-1.2477860	H	-5.6451290	3.7025700	1.6486570
H	4.3821510	-1.2488860	-0.8541150	H	-4.3959570	4.8389600	2.1508660
H	4.3082340	-0.3218870	-2.3388100	H	-4.5503400	4.3884490	0.4448070
C	1.7787280	-0.3088440	-1.2080860	O	1.8207360	-1.4119890	-1.7317990
C	0.2910140	3.5783180	0.4976320				

TS10^o				H	2.5981330	-4.4870340	3.2958820
C	-2.4951610	2.5747530	0.6687960	C	2.3304160	-3.7389350	0.6876090
C	-1.6486260	1.4508700	0.7602900	H	2.0017730	-3.7796880	-0.3552670
C	-1.2220230	1.0469110	2.0414030	H	2.6954130	-2.7288040	0.8858010
C	-1.5734630	1.7811590	3.1766080	H	3.1671400	-4.4359160	0.8084650
C	-2.3990700	2.8940650	3.0581310	C	-3.8716180	-0.3305510	-1.1151340
C	-2.8893540	3.2938600	1.7998590	C	-3.3978610	-1.6118330	-0.7319380
H	-2.8437280	2.9087070	-0.3054040	C	-2.3536950	-2.0058620	-1.6768840
H	-1.1998720	1.4481560	4.1405010	C	-2.2279240	-0.9673790	-2.6515110
H	-2.6799440	3.4578860	3.9444280	C	-3.1128480	0.1008720	-2.2730190
C	-0.4171260	-0.2035870	2.1503070	C	-3.9127160	-2.4682970	0.3856510
O	0.3757660	-0.4402320	3.0630980	H	-4.5055370	-3.2986940	-0.0196300
Rh	-1.6433900	-0.2065370	-0.6085630	H	-3.0933490	-2.8855350	0.9758240
N	-0.7315570	-1.0209210	1.0982580	H	-4.5569980	-1.8985470	1.0589820
C	-0.0447250	-3.2426420	1.5174690	C	-1.6747750	-3.3433560	-1.7150690
O	-1.1525340	-3.5661550	1.8883870	H	-1.6445480	-3.7945350	-0.7220250
O	0.2670730	-2.0400810	0.9681730	H	-2.2199600	-4.0297090	-2.3770520
C	1.2029900	-4.1274400	1.6610310	H	-0.6511600	-3.2561810	-2.0875630
C	0.7901270	-5.5942590	1.4442520	C	-1.3767610	-1.0123650	-3.8864170
H	0.4897840	-5.7732010	0.4057360	H	-1.1032550	-0.0085340	-4.2218800
H	1.6333580	-6.2558380	1.6686010	H	-0.4536020	-1.5648920	-3.7110170
H	-0.0484510	-5.8614040	2.0905820	H	-1.9304540	-1.4931340	-4.7039310
C	1.6785770	-3.9174090	3.1215430	C	-5.0053790	0.4265560	-0.4893460
H	1.8702540	-2.8587440	3.3174460	H	-5.9316390	0.2611680	-1.0546940
H	0.9184300	-4.2612160	3.8289700	H	-5.1820010	0.1081640	0.5399690

H	-4.8166940	1.5025450	-0.4726770	C	1.0666640	5.1635900	0.0540400
C	-3.3710680	1.3471070	-3.0709660	H	1.6946330	5.2237180	-0.8455780
H	-3.7300190	2.1647590	-2.4408740	H	0.1303360	5.6834000	-0.1922590
H	-2.4711100	1.6883460	-3.5886260	C	5.9253110	-0.3437120	0.1316740
H	-4.1391950	1.1649020	-3.8341900	H	5.4429600	-1.1666180	0.6544030
C	-0.2031890	1.5188570	-0.5607710	C	7.1089590	0.1958690	0.6363360
C	0.3041950	0.3814590	-0.9168760	H	7.5402510	-0.2080360	1.5481480
C	2.8228720	0.2540680	-0.9183240	C	7.7406060	1.2477900	-0.0303330
H	2.8337250	0.1063800	0.1697450	H	8.6639850	1.6665290	0.3596160
H	2.8464680	1.3430200	-1.0628340	C	1.7635660	5.8849010	1.2121400
C	5.3494090	0.1557390	-1.0451520	H	1.9667860	6.9319090	0.9650270
C	0.0825560	2.9732320	-0.8144470	H	2.7191950	5.4081120	1.4564410
H	-0.8396690	3.4994380	-1.0804460	H	1.1458770	5.8686160	2.1169780
H	0.7385980	3.0212530	-1.6934770	C	-3.8173840	4.4811110	1.6843140
C	4.0467140	-0.4076650	-1.5712020	H	-4.7686730	4.2918920	2.1954610
H	3.9971530	-1.4866560	-1.3940120	H	-3.3805030	5.3749610	2.1434620
H	3.9879060	-0.2738220	-2.6563840	H	-4.0419310	4.7162920	0.6399350
C	1.4922530	-0.2756070	-1.4455850	O	1.4377290	-1.2031100	-2.2479930
C	0.7601550	3.6936140	0.3677230				
H	0.1166020	3.6304390	1.2512620	11°			
H	1.6896220	3.1683770	0.6206350	C	-3.2483090	2.4119610	0.2395340
C	5.9954950	1.2101790	-1.7048700	C	-2.0230540	1.7527040	0.4880660
H	5.5683490	1.6042420	-2.6245710	C	-1.9460130	0.8797330	1.6050340
C	7.1801270	1.7532680	-1.2045110	C	-3.0797050	0.7025760	2.4231820
H	7.6673850	2.5671740	-1.7346220	C	-4.2673790	1.3612990	2.1497180

C	-4.3680040	2.2374160	1.0484220	C	-2.5159540	-2.7354280	-0.5486360
H	-3.3074710	3.0913420	-0.6072130	C	-1.3375880	-2.6774680	-1.3963190
H	-2.9981760	0.0557790	3.2918510	C	-1.5955770	-1.7465330	-2.4852080
H	-5.1273530	1.2174360	2.7994900	C	-2.8486440	-1.1236390	-2.2225500
C	-0.6254520	0.2515710	2.0282900	C	-2.6837080	-3.6453580	0.6317340
O	0.0302710	0.6765930	2.9762960	H	-2.8042360	-4.6852960	0.3025580
Rh	-1.4671260	-0.7020170	-0.5574420	H	-1.8141730	-3.5925170	1.2927200
N	-0.3811120	-0.8081830	1.2227510	H	-3.5675810	-3.3806700	1.2167630
C	1.1220560	-2.4423180	2.0189550	C	-0.1591950	-3.5968190	-1.2900290
O	0.2190590	-3.2185640	2.2489340	H	0.0138230	-3.8935490	-0.2541500
O	0.9730590	-1.2574560	1.3672660	H	-0.3392150	-4.5065660	-1.8788590
C	2.5759840	-2.6322660	2.4747270	H	0.7505190	-3.1285140	-1.6737200
C	2.8174830	-4.1242700	2.7555070	C	-0.7555030	-1.5761070	-3.7119890
H	2.7405170	-4.7194590	1.8392700	H	-0.6959580	-0.5333510	-4.0267800
H	3.8221050	-4.2656740	3.1672750	H	0.2663200	-1.9261240	-3.5517180
H	2.0880590	-4.5134820	3.4688480	H	-1.1851470	-2.1703320	-4.5294940
C	2.7172190	-1.8102640	3.7817500	C	-4.7525000	-1.3969250	-0.4620590
H	2.4397450	-0.7656100	3.6193710	H	-5.5452050	-1.6230740	-1.1856910
H	2.0701140	-2.2143490	4.5666380	H	-4.9635560	-1.9472870	0.4560640
H	3.7532030	-1.8563330	4.1349370	H	-4.8104370	-0.3278200	-0.2338010
C	3.5799190	-2.1174160	1.4256660	C	-3.5534760	-0.1319520	-3.1023890
H	3.4641750	-2.6400400	0.4696530	H	-4.1635590	0.5601830	-2.5158990
H	3.4665880	-1.0470510	1.2471940	H	-2.8380850	0.4579560	-3.6798600
H	4.6009210	-2.2952560	1.7793020	H	-4.2201530	-0.6413280	-3.8112780
C	-3.4160480	-1.7591000	-1.0336940	C	-0.8274130	2.0234590	-0.3855890

C	-0.3146110	0.9510980	-1.0087060	H	7.1666210	-1.4605080	-0.8845380
C	2.2250350	0.8489030	-1.3075930	C	7.2518270	0.6434840	-0.4199760
H	2.2476430	-0.0725990	-0.7124200	H	8.2224530	0.5831210	0.0639850
H	2.3320580	1.6544610	-0.5680990	C	1.1892550	6.0552980	2.0305840
C	4.7351030	0.8018730	-1.6814160	H	1.5355690	7.0874420	1.9118420
C	-0.3339850	3.4545410	-0.4986650	H	2.0264030	5.4640870	2.4181290
H	-1.1438640	4.0973230	-0.8747370	H	0.4041670	6.0521210	2.7951180
H	0.4582530	3.5032580	-1.2548330	C	-5.6531180	2.9851470	0.7818780
C	3.3710440	0.8871950	-2.3315850	H	-6.5158170	2.3097940	0.7763570
H	3.2405000	0.0661770	-3.0443480	H	-5.8396900	3.7348200	1.5601050
H	3.2885400	1.8090100	-2.9173990	H	-5.6230440	3.5052290	-0.1792750
C	0.8408010	0.9736250	-1.9333620	O	0.6978300	1.0678410	-3.1497970
C	0.1787720	4.0342960	0.8336760				
H	-0.6206140	3.9880560	1.5847050	12°			
H	0.9852080	3.3966640	1.2181010	C	3.0942370	2.8776050	0.0761580
C	5.3468770	1.9453480	-1.1474370	C	2.0649840	2.0126450	-0.3435100
H	4.8430150	2.9059690	-1.2290190	C	2.2251390	1.3579250	-1.5793910
C	6.5915310	1.8698030	-0.5218120	C	3.3750160	1.5806130	-2.3477080
H	7.0482310	2.7693080	-0.1180390	C	4.3838910	2.4270390	-1.8998050
C	0.6736810	5.4807160	0.7071700	C	4.2548450	3.0918890	-0.6720590
H	1.4706340	5.5276670	-0.0480040	H	2.9887490	3.3972050	1.0248250
H	-0.1414380	6.1114590	0.3256330	H	3.4640220	1.0918210	-3.3139960
C	5.4118020	-0.4209190	-1.5754880	H	5.2696240	2.5841550	-2.5107680
H	4.9594840	-1.3174680	-1.9935600	C	1.1348610	0.5076310	-2.1879370
C	6.6579470	-0.5025430	-0.9509090	O	0.4514680	0.9130020	-3.1229060

Rh	1.0565920	-1.2333190	0.3959950	H	4.5400090	-3.4563010	-0.5805120
N	1.1039050	-0.7519250	-1.6388620	H	3.0287530	-4.1588250	-1.1707160
C	-0.9172450	-1.9602680	-1.5921990	C	1.0308740	-4.5978070	0.8378360
O	0.0379970	-1.4977210	-2.3551690	H	1.3269170	-5.0077230	-0.1303530
O	-0.8819410	-1.8961730	-0.3473930	H	1.2763540	-5.3417850	1.6059010
C	-2.0883230	-2.5607480	-2.3687750	H	-0.0570900	-4.4787000	0.8372540
C	-1.5506630	-3.5160670	-3.4566110	C	0.3369350	-2.7125930	3.2870680
H	-0.9871200	-4.3459500	-3.0163700	H	-0.0659060	-1.7964320	3.7221430
H	-2.3934190	-3.9399440	-4.0116040	H	-0.4990990	-3.2815010	2.8705820
H	-0.9001780	-2.9927730	-4.1601490	H	0.7782700	-3.3159570	4.0918700
C	-2.8369500	-1.3769140	-3.0330380	C	4.2970480	-0.5969880	0.7077560
H	-3.2687300	-0.7101050	-2.2801400	H	4.1942430	0.4250360	1.0742450
H	-2.1647330	-0.7918790	-3.6652820	H	5.2052500	-1.0275930	1.1515930
H	-3.6558400	-1.7668390	-3.6462680	H	4.4449710	-0.5432730	-0.3727370
C	-3.0239940	-3.3142400	-1.4102420	C	2.3829340	-0.2476070	3.2834140
H	-2.5097570	-4.1441310	-0.9155710	H	2.8707970	0.6480100	2.8937770
H	-3.4236560	-2.6537420	-0.6370820	H	1.3936320	0.0372850	3.6460140
H	-3.8653180	-3.7247690	-1.9771750	H	2.9810630	-0.6179160	4.1265430
C	3.1065320	-1.4388640	1.0573210	C	0.8316190	1.8567880	0.4879880
C	2.7878080	-2.7163210	0.4176970	C	0.3051460	0.6543120	0.8083540
C	1.7215080	-3.2978300	1.1261180	C	-2.2708310	0.7171330	0.9749200
C	1.3610100	-2.4062750	2.2336080	H	-2.3677590	-0.1297330	0.2855710
C	2.2780460	-1.3115450	2.2317140	H	-2.2461440	1.6083250	0.3360330
C	3.4879770	-3.2390590	-0.8013080	C	-4.7922330	0.7839090	1.2267850
H	3.4597250	-2.5015190	-1.6095640	C	0.2108750	3.1687000	0.9709810

H	0.9515330	3.7345600	1.5533270	H	-0.6220200	6.5474400	-1.4836620
H	-0.6026290	2.9607580	1.6740720	C	5.3347280	4.0311370	-0.1865880
C	-3.4616460	0.7572500	1.9465750	H	5.1474220	4.3622610	0.8387020
H	-3.4045430	-0.1133760	2.6067960	H	6.3213370	3.5550740	-0.2119050
H	-3.3659610	1.6360650	2.5943340	H	5.3953370	4.9258470	-0.8179670
C	-0.9175830	0.5645860	1.6641580	O	-0.8578170	0.3327420	2.8703040
C	-0.3082000	4.0699470	-0.1646870				
H	0.5107570	4.2865540	-0.8618010	TS13^o			
H	-1.0606040	3.5215150	-0.7476450	C	2.7011420	3.3776650	-0.0215710
C	-5.3381100	1.9898830	0.7641340	C	1.8495900	2.3272250	-0.4086520
H	-4.8078360	2.9208540	0.9521020	C	2.0850640	1.7372110	-1.6680540
C	-6.5516620	2.0131480	0.0757740	C	3.1417910	2.1719190	-2.4799310
H	-6.9579700	2.9597260	-0.2701330	C	3.9670070	3.2095840	-2.0648090
C	-0.9089390	5.3877150	0.3414040	C	3.7598210	3.8238990	-0.8196830
H	-1.7279300	5.1705710	1.0415030	H	2.5422250	3.8615710	0.9376530
H	-0.1513060	5.9310390	0.9232360	H	3.2970000	1.6971320	-3.4443320
C	-5.5020050	-0.4004540	0.9826830	H	4.7768300	3.5474490	-2.7064070
H	-5.1024590	-1.3440650	1.3483070	C	1.2159820	0.5941450	-2.1569840
C	-6.7168830	-0.3831070	0.2947500	O	0.3864570	0.6506250	-3.0509830
H	-7.2535680	-1.3123510	0.1229090	Rh	1.2591730	-1.1150690	0.1961590
C	-7.2457540	0.8250480	-0.1625390	N	1.6958380	-0.4918460	-1.4906800
H	-8.1926900	0.8418120	-0.6945570	C	-0.6466730	-2.6221730	-1.3540670
C	-1.4264950	6.2851230	-0.7872680	O	0.2736980	-2.7385950	-2.1590190
H	-1.8478820	7.2178460	-0.3975310	O	-0.5883430	-1.9385180	-0.2291680
H	-2.2092210	5.7814170	-1.3657550	C	-2.0313390	-3.2696480	-1.6415630

C	-1.8138740	-4.5380610	-2.4866510	C	0.5043600	-2.8399340	3.0409840
H	-1.2387780	-5.2893580	-1.9342780	H	0.0400930	-1.9880030	3.5389100
H	-2.7807620	-4.9809060	-2.7503550	H	-0.2842200	-3.3857860	2.5167030
H	-1.2683400	-4.3060890	-3.4028980	H	0.9224560	-3.5092620	3.8046000
C	-2.8418510	-2.2397190	-2.4624940	C	4.3939010	-0.2127970	0.8617410
H	-3.0604880	-1.3394030	-1.8809770	H	4.0854100	0.7948810	1.1472710
H	-2.2942540	-1.9406990	-3.3606270	H	5.2786410	-0.4744120	1.4575940
H	-3.7973860	-2.6801500	-2.7692940	H	4.6919230	-0.1854590	-0.1882850
C	-2.7816530	-3.6249980	-0.3471960	C	2.2980380	-0.1899680	3.2868430
H	-2.2269910	-4.3592530	0.2479950	H	2.6807230	0.7755950	2.9494930
H	-2.9467270	-2.7452840	0.2777630	H	1.2725860	-0.0460710	3.6289030
H	-3.7549250	-4.0655970	-0.5922500	H	2.9157150	-0.5180690	4.1332360
C	3.3025500	-1.2169280	1.0904020	C	0.6843130	1.9291230	0.4376230
C	3.1621770	-2.4695430	0.3789590	C	0.2915430	0.6555560	0.6719700
C	2.0820720	-3.1722460	0.9652500	C	-2.2861540	0.5426810	0.7432350
C	1.5755760	-2.3923870	2.0916170	H	-2.3047520	-0.2525630	-0.0107190
C	2.3578920	-1.2120760	2.1916280	H	-2.2812110	1.4791140	0.1740240
C	3.9822940	-2.8726590	-0.8079950	C	-4.8144320	0.6449100	0.9243290
H	3.9085890	-2.1181100	-1.5988570	C	-0.0849300	3.1106140	1.0427140
H	5.0388580	-2.9788600	-0.5352400	H	0.5942200	3.6917340	1.6818950
H	3.6420280	-3.8219170	-1.2249100	H	-0.8582000	2.7435080	1.7235960
C	1.5625340	-4.5183270	0.5617870	C	-3.5104770	0.4587530	1.6703870
H	1.7505910	-4.7220510	-0.4932970	H	-3.5001590	-0.5073210	2.1843110
H	2.0401370	-5.3057170	1.1591760	H	-3.4159070	1.2194910	2.4538330
H	0.4853270	-4.5892000	0.7306010	C	-0.9582380	0.3911710	1.4679650

C	-0.7202260	4.0587660	0.0091080			
H	0.0588700	4.4570600	-0.6522550	14^o		
H	-1.4016080	3.4892450	-0.6368890	C	2.7206270	3.3836560 0.1184770
C	-5.3079540	1.9293460	0.6537090	C	1.8858890	2.3545020 -0.3559340
H	-4.7584650	2.7973950	1.0118750	C	2.1585430	1.8426420 -1.6408980
C	-6.4934370	2.1092550	-0.0594480	C	3.2183960	2.3508800 -2.4039790
H	-6.8591160	3.1136670	-0.2549690	C	4.0269220	3.3644960 -1.9042090
C	-1.4813160	5.2213190	0.6594570	C	3.7927860	3.8890720 -0.6236930
H	-2.2616450	4.8208590	1.3217140	H	2.5336570	3.8068110 1.1010010
H	-0.7963280	5.7853350	1.3078490	H	3.3927090	1.9459890 -3.3965890
C	-5.5483750	-0.4569840	0.4642620	H	4.8429880	3.7542150 -2.5074110
H	-5.1880370	-1.4614690	0.6727900	C	1.3518950	0.7045610 -2.2042910
C	-6.7352870	-0.2827620	-0.2497670	O	0.6223820	0.7597800 -3.1880200
H	-7.2895940	-1.1513480	-0.5948310	Rh	1.2165080	-1.1293040 0.0620030
C	-7.2116870	1.0019160	-0.5154190	N	1.7020120	-0.4522430 -1.5727240
H	-8.1362110	1.1394590	-1.0688760	C	-0.7199420	-2.9147630 -1.0638200
C	-2.1163560	6.1698750	-0.3622570	O	0.2347070	-3.3055220 -1.7267860
H	-2.6521310	6.9879700	0.1303690	O	-0.6529300	-1.9596350 -0.1498010
H	-2.8312400	5.6406620	-1.0022520	C	-2.1424740	-3.4974270 -1.2696890
H	-1.3568360	6.6142800	-1.0153380	C	-2.9011540	-3.6153590 0.0645040
C	4.6474680	4.9581100	-0.3656320	H	-2.9984610	-2.6472530 0.5594810
H	4.5187450	5.1681490	0.6996990	H	-3.9043530	-4.0201700 -0.1115600
H	5.7046130	4.7341540	-0.5428530	H	-2.3888140	-4.2947080 0.7557050
H	4.4184230	5.8800140	-0.9142860	C	-2.0191850	-4.8839560 -1.9257330
O	-0.9141220	0.0456960	2.6442020	H	-1.4687120	-4.8247300 -2.8663910

H	-1.4893860	-5.5863180	-1.2734930	H	4.6392280	-0.1481910	-0.4133800
H	-3.0165880	-5.2919260	-2.1237430	H	4.0408130	0.8436530	0.9181070
C	-2.8944310	-2.5436350	-2.2268840	C	2.2843700	-0.1149090	3.0868870
H	-3.0310570	-1.5520130	-1.7869500	H	2.5942200	0.8595480	2.7046360
H	-2.3500890	-2.4258920	-3.1687980	H	1.2688320	-0.0193010	3.4724270
H	-3.8865890	-2.9501050	-2.4537160	H	2.9570350	-0.3823390	3.9126420
C	3.2896080	-1.1815870	0.9059840	C	0.6898770	1.9158950	0.4253950
C	3.1993330	-2.4720100	0.2581010	C	0.2720980	0.6370930	0.5734600
C	2.1746940	-3.2008520	0.8993660	C	-2.3141940	0.5937370	0.6051690
C	1.6334940	-2.3869350	1.9820520	H	-2.3538270	-0.1588920	-0.1904690
C	2.3558890	-1.1662440	2.0208690	H	-2.2729630	1.5583560	0.0874320
C	4.0114320	-2.8826000	-0.9298560	C	-4.8403370	0.7689120	0.7677380
H	5.0763840	-2.9479610	-0.6767630	C	-0.0893850	3.0713160	1.0682760
H	3.6913390	-3.8508860	-1.3176890	H	0.5745760	3.6114750	1.7570870
H	3.8999300	-2.1476810	-1.7354050	H	-0.8869400	2.6798270	1.7055300
C	1.7609020	-4.6115920	0.6171940	C	-3.5508600	0.5042490	1.5154440
H	1.9306160	-4.8842090	-0.4238890	H	-3.5769490	-0.4853040	1.9819190
H	2.3283150	-5.2972890	1.2609660	H	-3.4403790	1.2226140	2.3359580
H	0.7017000	-4.7655630	0.8328980	C	-1.0005650	0.3580860	1.3342390
C	0.5828440	-2.8383780	2.9509250	C	-0.6831290	4.0778000	0.0651590
H	0.1433720	-1.9914150	3.4775020	H	0.1210300	4.5069380	-0.5447040
H	-0.2284060	-3.3602770	2.4364780	H	-1.3424530	3.5477660	-0.6351320
H	1.0134720	-3.5304590	3.6866470	C	-5.3009350	2.0791220	0.5743030
C	4.3579770	-0.1630040	0.6413800	H	-4.7362940	2.9094930	0.9931900
H	5.2550380	-0.4063780	1.2267250	C	-6.4737030	2.3319720	-0.1380310

H	-6.8140470	3.3551090	-0.2726580	C	4.4181070	3.0484980	-1.6559620
C	-1.4639940	5.2079970	0.7485480	C	4.1564630	3.5283780	-0.3636760
H	-2.2708220	4.7768940	1.3576580	H	2.7901700	3.4823380	1.2712650
H	-0.8024570	5.7324470	1.4520200	H	3.7383860	1.7512810	-3.2450580
C	-5.5934420	-0.2840670	0.2304370	H	5.2947630	3.3961660	-2.1972250
H	-5.2585720	-1.3078730	0.3778570	C	1.6631340	0.5829750	-2.3167110
C	-6.7675440	-0.0367850	-0.4830090	O	1.6214730	0.5177760	-3.5549880
H	-7.3374910	-0.8683330	-0.8885440	Rh	1.0463420	-1.2509370	0.1102270
C	-7.2115680	1.2730410	-0.6708710	N	1.1651820	-0.3124000	-1.4862730
H	-8.1262920	1.4669880	-1.2237160	C	-1.0564610	-2.8761130	-0.9628680
C	-2.0558210	6.2131840	-0.2446510	O	-0.1303930	-3.3836690	-1.5944830
H	-2.6092290	7.0056600	0.2697960	O	-0.9129620	-1.9087470	-0.0805400
H	-2.7454790	5.7220080	-0.9402180	C	-2.5232070	-3.3301850	-1.1806220
H	-1.2697490	6.6888680	-0.8418720	C	-3.2996290	-3.3631230	0.1486510
C	4.6641490	4.9938740	-0.0745000	H	-3.3093160	-2.3845100	0.6321040
H	5.7276080	4.7570020	-0.1867030	H	-4.3349890	-3.6745380	-0.0313820
H	4.4879560	5.9362660	-0.6071720	H	-2.8568730	-4.0790300	0.8507370
H	4.4674210	5.1718770	0.9862460	C	-2.5222020	-4.7299600	-1.8193460
O	-0.9783020	-0.0523520	2.4887090	H	-1.9677640	-4.7326320	-2.7596210
TS15^o				H	-2.0580500	-5.4680890	-1.1569090
				H	-3.5516860	-5.0500380	-2.0150580
C	3.0001480	3.0864720	0.2823900	C	-3.1785710	-2.3231390	-2.1540190
C	2.1015680	2.1560310	-0.2850140	H	-3.2381000	-1.3205950	-1.7215900
C	2.4208280	1.6649280	-1.5700590	H	-2.6133590	-2.2589160	-3.0890340
C	3.5609140	2.1295210	-2.2436770	H	-4.1979500	-2.6462750	-2.3934180

C	3.2414620	-1.5794010	0.5087890	C	0.8330800	1.8490410	0.4581670
C	2.7369890	-2.8718180	0.1111580	C	0.2845930	0.6339290	0.6690220
C	1.7297610	-3.2548090	1.0466510	C	-2.2991590	0.7699420	0.6644490
C	1.6119200	-2.2222730	2.0490600	H	-2.3812410	-0.0288500	-0.0813180
C	2.5721100	-1.1979170	1.7276030	H	-2.1829270	1.6950380	0.0887550
C	3.1669040	-3.6720420	-1.0786040	C	-4.8001220	1.1661620	0.7780090
H	3.7221980	-4.5631110	-0.7595790	C	0.1341100	3.1006060	1.0122370
H	2.2921210	-3.9967430	-1.6488060	H	0.8148250	3.6377950	1.6845100
H	3.8122540	-3.0915980	-1.7401560	H	-0.7116030	2.8142890	1.6434310
C	0.9957140	-4.5602930	1.0584430	C	-3.5482010	0.8287960	1.5601160
H	0.9507930	-4.9991210	0.0625320	H	-3.6650930	-0.1314330	2.0718690
H	1.5028350	-5.2614540	1.7342290	H	-3.3872200	1.5741130	2.3475690
H	-0.0274210	-4.4376050	1.4210320	C	-1.0125790	0.4920710	1.4216510
C	0.7916560	-2.3037910	3.3006930	C	-0.3479870	4.0722630	-0.0811880
H	0.4097380	-1.3236220	3.5881530	H	0.5041590	4.3807060	-0.6986520
H	-0.0692370	-2.9617540	3.1643040	H	-1.0355750	3.5459870	-0.7568800
H	1.3967830	-2.7087270	4.1227600	C	-5.1282600	2.4994170	0.4923800
C	4.3936740	-0.8640500	-0.1323760	H	-4.4894200	3.2972260	0.8655890
H	5.3374040	-1.3403690	0.1622430	C	-6.2627680	2.8170290	-0.2549630
H	4.3302940	-0.8950020	-1.2221440	H	-6.4994580	3.8571550	-0.4620600
H	4.4370930	0.1834520	0.1680070	C	-1.0414120	5.3163180	0.4891910
C	2.9209800	-0.0356890	2.6057970	H	-1.8899910	5.0065470	1.1150750
H	3.2683370	0.8222830	2.0283320	H	-0.3478550	5.8422440	1.1598570
H	2.0648100	0.2755560	3.2059270	C	-5.6472870	0.1582030	0.2980090
H	3.7275890	-0.3325010	3.2895700	H	-5.4153840	-0.8811440	0.5167500

C	-6.7841690	0.4704520	-0.4497260	O	2.4785690	2.0558470	-1.0174150
H	-7.4284480	-0.3269120	-0.8100640	Rh	2.1725280	-0.5937470	0.1881560
C	-7.0953780	1.8017380	-0.7302520	N	0.7813360	1.0334760	0.1233530
H	-7.9804160	2.0466350	-1.3104970	C	0.9796760	-1.5173450	-1.8838760
C	-1.5319240	6.2788770	-0.5972470	O	1.9790070	-0.7419790	-1.9822120
H	-2.0203250	7.1573350	-0.1628930	O	0.6090630	-1.8597370	-0.7074950
H	-2.2532820	5.7903750	-1.2618050	C	0.2200870	-1.9748380	-3.1293510
H	-0.7003440	6.6321020	-1.2173620	C	-0.5172210	-3.2980090	-2.8588940
C	5.0897830	4.5159620	0.2963510	H	-1.2358590	-3.2025690	-2.0416600
H	6.1142620	4.1292890	0.3403710	H	-1.0614860	-3.6068980	-3.7578180
H	5.1282300	5.4577570	-0.2635360	H	0.1846440	-4.0974960	-2.5988470
H	4.7742230	4.7484340	1.3171180	C	1.2098200	-2.1423250	-4.2982830
O	-1.0165040	0.1685670	2.6027100	H	1.7568760	-1.2157790	-4.4843030
17^o				H	1.9403050	-2.9314430	-4.0892470
				H	0.6665190	-2.4190820	-5.2081010
C	-1.4444480	4.6513180	-0.0630680	C	-0.7985400	-0.8592730	-3.4703250
C	-0.7593170	3.4101310	-0.0181320	H	-1.5152380	-0.7113230	-2.6565490
C	0.5288450	3.3477880	-0.6014290	H	-0.2901740	0.0908470	-3.6574610
C	1.0781620	4.4831870	-1.2248320	H	-1.3598860	-1.1348590	-4.3696780
C	0.3778590	5.6734390	-1.2686050	C	3.9340140	0.2121190	1.1658730
C	-0.9001220	5.7725190	-0.6740000	C	4.3100380	-0.9075450	0.3314560
H	-2.4226740	4.7390200	0.3975420	C	3.6270940	-2.0775660	0.7969500
H	2.0664990	4.3873290	-1.6614390	C	2.8188110	-1.6797420	1.9396400
H	0.8112640	6.5441470	-1.7549530	C	3.0241180	-0.2791810	2.1748190
C	1.3336210	2.1192420	-0.5326050	C	5.2259730	-0.8063060	-0.8490360

H	6.2645850	-0.7042410	-0.5103500	C	-2.6762470	2.2600780	1.2427620
H	5.1620310	-1.6874750	-1.4896870	H	-2.7442870	3.1485010	1.8860090
H	4.9758530	0.0707680	-1.4513550	H	-2.8033120	1.4156080	1.9290920
C	3.7488200	-3.4708280	0.2540960	C	-2.6929530	-2.0159450	1.6826100
H	4.0691010	-3.4637820	-0.7901550	H	-1.8928350	-2.6347710	2.0995430
H	4.4848540	-4.0497900	0.8262930	H	-3.1608100	-1.5040200	2.5315480
H	2.7943780	-4.0002500	0.3056810	C	-0.9748550	-0.1388560	1.3808230
C	1.9725380	-2.5968560	2.7683080	C	-3.8614960	2.2799720	0.2537050
H	1.1095060	-2.0720960	3.1798800	H	-3.7530950	3.1244020	-0.4371870
H	1.6077250	-3.4412960	2.1785420	H	-3.8281520	1.3816000	-0.3769760
H	2.5656440	-3.0011970	3.5993260	C	-5.0660180	-2.5264810	0.9401290
C	4.5283600	1.5848960	1.0980190	H	-5.3942700	-1.6299390	1.4615990
H	5.4521790	1.6171930	1.6923200	C	-5.9981530	-3.3070480	0.2540570
H	4.7540470	1.8681790	0.0708740	H	-7.0445610	-3.0142590	0.2443750
H	3.8433420	2.3362840	1.4926580	C	-5.2241680	2.3620020	0.9529830
C	2.4621440	0.5198260	3.3109860	H	-5.3279040	1.5159750	1.6470940
H	2.4726250	1.5873460	3.0822180	H	-5.2577030	3.2665040	1.5760490
H	1.4320180	0.2321250	3.5209590	C	-3.3148090	-4.0489510	0.3025080
H	3.0702070	0.3637210	4.2116890	H	-2.2686750	-4.3460250	0.3253050
C	-1.2987810	2.2213510	0.6048270	C	-4.2425250	-4.8322340	-0.3857290
C	-0.4919520	1.1019110	0.6463940	H	-3.9145770	-5.7337340	-0.8961630
C	-2.0681130	-0.9725510	0.7417850	C	-5.5888850	-4.4629590	-0.4130470
H	-1.5801390	-1.4702370	-0.1057440	H	-6.3130800	-5.0729880	-0.9453940
H	-2.8304160	-0.3206580	0.3063990	C	-6.4045360	2.3688230	-0.0235850
C	-3.7110220	-2.8828840	0.9734730	H	-7.3618420	2.4308170	0.5044830

H	-6.4188440	1.4582700	-0.6333910	C	2.1093950	-2.0957600	3.0625490
H	-6.3467740	3.2222690	-0.7087640	C	2.7041860	-3.5152940	2.9369330
C	-1.6502410	7.0831080	-0.7094150	H	3.2737360	-3.6282520	2.0071600
H	-1.0783960	7.8812120	-0.2213430	H	3.3864610	-3.7107020	3.7716380
H	-1.8329450	7.4075550	-1.7407540	H	1.9122340	-4.2678540	2.9493060
H	-2.6179190	7.0078690	-0.2056480	C	1.3321860	-1.9794990	4.3920780
O	-0.4710040	-0.4630000	2.4472530	H	0.8759950	-0.9901990	4.4988630
TS18^o				H	0.5337740	-2.7228110	4.4386480
C	-4.1372540	1.1767770	-0.7242870	H	2.0128730	-2.1360350	5.2366600
C	-2.9941100	0.7362560	-0.0328560	C	3.2339610	-1.0519000	3.0177150
C	-3.0834210	-0.5427790	0.5612330	H	3.7748510	-1.0806790	2.0678810
C	-4.2201290	-1.3563770	0.4172230	H	2.8422030	-0.0394910	3.1504230
C	-5.3261380	-0.8801680	-0.2676090	H	3.9484810	-1.2454180	3.8260460
C	-5.2938270	0.3993050	-0.8533000	C	-0.7929910	-1.6805850	-2.4947910
H	-4.1154860	2.1489510	-1.2065240	C	0.0313330	-2.7492110	-1.9397160
H	-4.2210400	-2.3460430	0.8635930	C	1.3495950	-2.2554460	-1.8300270
H	-6.2144180	-1.4982850	-0.3652430	C	1.3764770	-0.8771470	-2.3121160
C	-2.0177690	-0.9539560	1.6625440	C	0.0568610	-0.5622750	-2.7912220
O	-2.0327850	-0.7215790	2.8475310	C	-0.4801100	-4.1070300	-1.5603560
Rh	-0.0062510	-0.8997610	-0.6013920	H	-0.7396670	-4.6876370	-2.4545110
N	-1.4399340	-1.5771370	0.6790320	H	0.2621840	-4.6721960	-0.9941480
C	1.0856370	-1.9135490	1.9117850	H	-1.3753020	-4.0283530	-0.9371460
O	0.1189410	-2.6984880	1.8637830	C	2.5503050	-2.9760450	-1.2975490
O	1.3021680	-0.9598650	1.0669170	H	2.2782540	-3.9148520	-0.8113860
				H	3.2497470	-3.2040310	-2.1114090

H	3.0811510	-2.3575280	-0.5685180	C	0.6545140	1.9882970	-0.1996930
C	2.6113080	-0.0488450	-2.5068830	C	-2.1134240	3.4254650	1.8384860
H	2.3824460	1.0173570	-2.4833450	H	-1.2292510	3.0429810	2.3618130
H	3.3537980	-0.2428380	-1.7289930	H	-2.0678030	4.5211050	1.9192420
H	3.0777800	-0.2762080	-3.4752430	C	4.7688790	1.8350060	0.6963400
C	-2.2409950	-1.8229980	-2.8591250	H	4.6062320	1.4640150	1.7054000
H	-2.3422090	-2.3121070	-3.8370170	C	5.8945020	1.4180660	-0.0163810
H	-2.7766760	-2.4304410	-2.1260950	H	6.5971820	0.7261600	0.4406040
H	-2.7393940	-0.8532990	-2.9156650	C	-3.3661950	2.9314220	2.5813710
C	-0.3317460	0.6799280	-3.5359380	H	-3.4265860	1.8384440	2.5292770
H	-1.4141180	0.8259670	-3.5314070	H	-3.2352980	3.1660870	3.6455530
H	0.1325710	1.5649150	-3.0963790	C	4.0935330	3.2107980	-1.1583150
H	-0.0104020	0.5949190	-4.5824840	H	3.3827740	3.8963780	-1.6090820
C	-1.7689600	1.5741400	0.0486960	C	5.2211650	2.8019200	-1.8731120
C	-0.5243280	1.0669380	-0.1507200	H	5.3939400	3.1893130	-2.8737920
C	1.5057280	2.1452320	1.0499380	C	6.1252810	1.9013160	-1.3064460
H	1.8859430	1.1519430	1.3122660	H	7.0048930	1.5852060	-1.8604210
H	0.8296110	2.4162420	1.8713600	C	-4.6801700	3.5580350	2.1009500
C	3.8484410	2.7330930	0.1358450	H	-5.5225300	3.2188670	2.7130810
C	-1.9898800	3.0649230	0.3367030	H	-4.9062010	3.2932530	1.0629890
H	-2.8800850	3.4275780	-0.1883360	H	-4.6433270	4.6522840	2.1641430
H	-1.1566870	3.6336130	-0.0832940	C	-6.4941480	0.9240600	-1.6018220
C	2.6363520	3.1854260	0.9283100	H	-6.2339530	1.7759130	-2.2355720
H	2.2325470	4.1006650	0.4845350	H	-6.9413340	0.1498600	-2.2336200
H	2.9587750	3.4411170	1.9451850	H	-7.2713630	1.2571270	-0.9027430

O	0.9303360	2.5985490	-1.2335410	H	0.1706820	-2.8549030	2.8148930
				H	-0.9889350	-2.2342030	4.0037240
19^o				H	-0.5792190	-3.9573230	3.9865420
C	0.8510100	3.8883550	-0.0955300	C	-1.5453120	-4.5437110	1.4520850
C	0.4046840	2.5883170	0.2122260	H	-2.3562840	-4.7680630	0.7493180
C	-0.8112480	2.5114560	0.9200800	H	-0.6434950	-4.3312800	0.8729670
C	-1.5073560	3.6524340	1.3209270	H	-1.3683110	-5.4449580	2.0502490
C	-1.0171880	4.9182970	1.0108590	C	-2.5620520	1.1565880	-1.9711820
C	0.1708720	5.0505860	0.2829900	C	-3.5636470	0.2668810	-1.3757120
H	1.7731620	3.9999130	-0.6552570	C	-3.2157400	-1.0556710	-1.7016940
H	-2.4425780	3.5431640	1.8635870	C	-1.9697740	-1.0282000	-2.4671790
H	-1.5679860	5.8003770	1.3257620	C	-1.6315880	0.3586650	-2.7027850
C	-1.7486480	0.8927200	2.3322330	C	-4.7507530	0.7019440	-0.5684950
O	-2.0768940	0.5951080	3.4101850	H	-5.6355840	0.8241460	-1.2066000
Rh	-1.4573720	-0.1363890	-0.5714350	H	-4.9789930	-0.0299590	0.2088310
N	-1.3719590	1.2117540	1.1971310	H	-4.5680640	1.6619870	-0.0782620
C	-2.1438330	-2.0866780	1.5142340	C	-3.9783160	-2.2969160	-1.3524760
O	-3.1884080	-1.4292360	1.6144010	H	-4.6550570	-2.5628270	-2.1753130
O	-1.1488970	-1.7729880	0.7320410	H	-3.3068970	-3.1445000	-1.1954670
C	-1.9151010	-3.3606080	2.3696270	H	-4.5650700	-2.1626820	-0.4437460
C	-3.1918120	-3.6901470	3.1589270	C	-1.3289600	-2.2132670	-3.1252840
H	-4.0334650	-3.8827450	2.4873140	H	-0.2550360	-2.0633240	-3.2470070
H	-3.0321430	-4.5821200	3.7756380	H	-1.4793830	-3.1218730	-2.5369520
H	-3.4762650	-2.8607460	3.8105630	H	-1.7695020	-2.3837990	-4.1171300
C	-0.7547070	-3.0818920	3.3507060	C	-2.6444190	2.6540830	-1.9942200

H	-3.2707850	2.9833390	-2.8339350	C	6.0308070	-1.3493950	-1.9395810
H	-3.0866600	3.0516160	-1.0786480	H	6.3486730	-0.9298990	-2.8905120
H	-1.6594510	3.1102540	-2.1100930	C	3.2370900	2.6686300	2.0949820
C	-0.5459480	0.8513870	-3.6126850	H	3.5286940	3.5843220	1.5621250
H	-0.2563610	1.8768890	-3.3729190	H	2.1773440	2.7899190	2.3468840
H	0.3417620	0.2207470	-3.5368160	C	5.2042360	-2.4389040	0.4830350
H	-0.9037210	0.8378890	-4.6509930	H	4.8892210	-2.8718550	1.4302250
C	1.1876370	1.3809780	-0.1774950	C	6.4917030	-1.9143460	0.3593250
C	0.5889970	0.2121900	-0.5149390	H	7.1695600	-1.9398660	1.2084350
C	1.8848990	-1.9407960	0.0784360	C	6.9098880	-1.3662950	-0.8549110
H	0.9778540	-2.4309860	0.4549750	H	7.9130780	-0.9614940	-0.9559880
H	2.2833580	-1.3796470	0.9310210	C	4.0547810	2.5492730	3.3858490
C	4.3092210	-2.4245330	-0.5967030	H	3.9119500	3.4209540	4.0331910
C	2.7148040	1.5166370	-0.2041880	H	5.1262980	2.4653740	3.1706490
H	3.0135120	2.4428090	-0.7112040	H	3.7643770	1.6602310	3.9577360
H	3.1246500	0.7156110	-0.8245010	C	0.7250240	6.4145560	-0.0570930
C	2.9047300	-2.9736940	-0.4363590	H	-0.0742650	7.1271210	-0.2833840
H	2.9281450	-3.8105540	0.2712300	H	1.2994060	6.8276950	0.7814770
H	2.5473700	-3.3669640	-1.3926630	H	1.3945280	6.3710060	-0.9208360
C	1.3888570	-0.9589910	-0.9748650	O	1.5878220	-1.1666380	-2.1735210
C	3.4251750	1.4590800	1.1694890				
H	3.1051790	0.5529370	1.7001890	27 [Cp*(RhOAc)₂]			
H	4.4991530	1.3302690	0.9773220	Rh	0.0412780	0.2090320	-0.0875670
C	4.7429180	-1.8734050	-1.8117280	O	-1.8552200	-0.3381970	-0.6737680
H	4.0564350	-1.8503890	-2.6522280	O	-1.0257510	1.6865200	1.0935880

C	-2.5451730	-1.2289750	-0.0121110	H	1.4575700	-2.6701290	2.6197990
O	-2.1416680	-1.9042910	0.9376950	H	0.7027670	-1.1712130	3.1822660
C	-1.1540730	2.4325300	0.0684000	H	-0.2452490	-2.3071790	2.2167420
O	-0.5641260	2.0858410	-1.0056030	C	0.4268150	-3.0345770	-0.6000060
C	-3.9789730	-1.3603760	-0.5169130	H	0.1088800	-3.0555110	-1.6447110
H	-4.5779440	-0.5444160	-0.0977150	H	1.1591100	-3.8397080	-0.4564170
H	-4.0221080	-1.2764310	-1.6055230	H	-0.4440140	-3.2291220	0.0274560
H	-4.4051990	-2.3095290	-0.1880800	C	1.6165900	-0.7682600	-1.1603690
C	-2.0136420	3.6661580	0.1153380	C	1.7176120	-0.9102850	-2.6497030
H	-3.0369620	3.3873100	-0.1579450	H	0.9156180	-1.5369790	-3.0452940
H	-2.0298190	4.0830630	1.1241270	H	1.6551230	0.0616470	-3.1455510
H	-1.6575650	4.4076650	-0.6023410	H	2.6745140	-1.3692030	-2.9309380
C	2.1819460	0.3253250	-0.3770990				
C	1.0500300	-1.7196940	-0.2429440	1a'			
C	1.9127320	0.0645830	0.9977250	C	2.1133210	-1.2580560	0.1378720
C	1.1842710	-1.1952330	1.0879000	C	0.7297310	-1.0863700	0.1320430
C	2.9054080	1.5068390	-0.9503930	C	0.1767560	0.1944930	0.0015970
H	3.9448950	1.2429160	-1.1830160	C	1.0372800	1.2961380	-0.1025060
H	2.4315460	1.8505900	-1.8731760	C	2.4151310	1.1156950	-0.1014100
H	2.9197580	2.3465420	-0.2526430	C	2.9789960	-0.1642570	0.0176690
C	2.2959500	0.9139490	2.1724840	H	2.5269840	-2.2572140	0.2464630
H	1.4679580	1.0001850	2.8805650	H	0.0863690	-1.9512120	0.2629220
H	3.1474470	0.4684050	2.7016760	H	0.6003000	2.2855500	-0.1848990
H	2.5814310	1.9225370	1.8668320	H	3.0683380	1.9799110	-0.1929730
C	0.7486480	-1.8764600	2.3492070	C	-1.2970650	0.4663930	-0.0230460

O	-1.7794760	1.5547190	0.2455830	C	6.5870130	-2.2066930	0.5484320
N	-2.0839240	-0.6464780	-0.3157450	H	7.5820520	-2.5179310	0.2153400
H	-1.7071850	-1.3124000	-0.9803730	H	6.6884770	-1.7903790	1.5567970
O	-3.4206140	-0.3824070	-0.6526210	H	5.9647560	-3.1054160	0.6231710
C	-4.2357900	-0.4138440	0.5220850	C	0.2159290	1.5768620	0.2335270
H	-5.2548900	-0.2578710	0.1609530	F	-0.1079560	2.7559260	-0.4087500
H	-4.1635320	-1.3837800	1.0279760	F	0.2346530	1.8750260	1.5821800
H	-3.9601580	0.3918110	1.2083680	C	-0.8783320	0.5483620	-0.0318890
C	4.4771830	-0.3466910	0.0421750	H	-0.8742160	0.3211600	-1.1027040
H	4.9633540	0.2457050	-0.7397210	H	-0.6067650	-0.3728360	0.4933770
H	4.8983820	-0.0209750	1.0010460	C	-2.2715510	1.0338920	0.4129790
H	4.7569680	-1.3936870	-0.1021200	H	-2.5055400	1.9606790	-0.1196960
				H	-2.2326430	1.2794670	1.4787120
2a				C	-3.3438900	-0.0022790	0.1552870
C	2.6411070	0.7694650	-0.5476350	C	-4.0275080	-0.0398350	-1.0673520
C	1.5537990	1.1523060	-0.1838000	C	-3.6551140	-0.9680330	1.1216770
C	3.9656000	0.3050160	-0.9551710	C	-4.9933720	-1.0147130	-1.3191980
H	4.6360110	1.1701080	-1.0461040	H	-3.8040410	0.7066450	-1.8260190
H	3.8998380	-0.1363720	-1.9587570	C	-4.6201440	-1.9448890	0.8746730
C	4.5774300	-0.7218020	0.0217280	H	-3.1396210	-0.9490610	2.0790950
H	4.6272530	-0.2756220	1.0223050	C	-5.2923030	-1.9718210	-0.3483070
H	3.9048570	-1.5846620	0.1005680	H	-5.5157830	-1.0235410	-2.2716920
C	5.9720520	-1.1854930	-0.4128970	H	-4.8505200	-2.6816160	1.6391320
H	6.6345300	-0.3132100	-0.4949460	H	-6.0464650	-2.7291960	-0.5411870
H	5.9132370	-1.6188570	-1.4205900				

HOAc				C	2.0591950	-1.8259440	0.9336640
O	-0.7802390	-1.0452700	0.0000040	H	2.9758240	-1.3952000	0.5263320
C	-0.0920720	0.1252250	0.0000080	H	2.2737710	-2.1925230	1.9453950
O	-0.6429770	1.2027890	0.0000020	H	1.7977000	-2.6868960	0.3133990
C	1.3965520	-0.1114860	0.0000080	C	-1.0631880	-2.5156420	0.9154040
H	1.6816910	-0.6937570	0.8810450	H	-2.0395490	-2.5242600	0.4265560
H	1.6817080	-0.6933400	-0.8813160	H	-0.4123890	-3.2095270	0.3785670
H	1.9166030	0.8453260	0.0001820	H	-1.1907180	-2.8971640	1.9366540
H	-1.7211550	-0.8008120	-0.0000560	C	-0.5877510	2.6271720	0.9961500
				H	-1.5239370	2.8296010	0.4714130
HF				H	-0.6947850	2.9812860	2.0297250
F	0.0000000	0.0000000	0.0925400	H	0.2003760	3.2148270	0.5205040
H	0.0000000	0.0000000	-0.8328590	C	-2.7155270	0.2329150	1.0498750
				H	-3.0365180	1.1496240	0.5502180
Cp*RhF₂				H	-3.2049400	-0.6005730	0.5415050
Rh	-0.0062450	0.0142200	-0.7692710	H	-3.0803900	0.2634820	2.0841660
C	-0.2633010	1.1644770	0.9840670	F	-1.3610260	0.0463720	-2.1474080
C	1.0826980	0.5968650	0.9966010	F	1.3004830	0.0479110	-2.1909080
C	0.9492300	-0.8188700	0.9628780				
C	-0.4823710	-1.1346660	0.9487690	28			
C	-1.2234720	0.0902250	1.0169670	N	-0.2620230	0.4511250	1.6153810
C	2.3584430	1.3839830	1.0106270	C	-2.6844590	-0.1156700	1.1220130
H	2.6083440	1.6968350	2.0321530	C	-3.6208970	-1.1666460	1.1156390
H	3.1922800	0.7966400	0.6219360	H	-3.3764100	-2.0818720	1.6437010
H	2.2771200	2.2822890	0.3934960	C	-4.8380850	-1.0288910	0.4612550

H	-5.5431850	-1.8566060	0.4601080	H	-0.2906920	-4.1788980	0.0668690
C	-5.1775020	0.1701080	-0.1875500	H	-0.3272070	-2.9888340	1.3766650
C	-4.2522890	1.2199580	-0.1538480	C	-1.4450790	-1.3972780	-2.2633530
H	-4.4990020	2.1637920	-0.6333370	H	-1.5807670	-2.1107330	-3.0865600
C	-3.0204210	1.0886540	0.4877850	H	-2.2125370	-1.5944920	-1.5127400
H	-2.3422400	1.9329040	0.5099460	H	-1.6176770	-0.3922220	-2.6558260
C	2.2593010	-1.3144660	-1.4908410	C	1.1430350	-0.1210500	-3.5459150
C	1.7778700	-2.0984310	-0.3759780	H	0.8980390	-0.7529820	-4.4083690
C	0.3501800	-2.2489500	-0.5392060	H	0.4071980	0.6847200	-3.4831960
C	-0.0637410	-1.5079980	-1.6903070	H	2.1211740	0.3300590	-3.7213910
C	1.1307900	-0.9345430	-2.2895660	C	3.6967840	-1.0154810	-1.7855630
O	-0.4737580	2.9266630	0.5581150	H	4.1494730	-1.8754600	-2.2965890
O	0.0258440	1.6370420	-1.2247530	H	3.8010470	-0.1466740	-2.4390570
C	-0.1964020	2.7714550	-0.6490770	H	4.2450590	-0.8216970	-0.8629990
C	-0.1173620	3.9813660	-1.5656150	C	2.6333010	-2.8235050	0.6195520
H	0.9376500	4.1946980	-1.7683710	H	3.0378030	-3.7420310	0.1731060
H	-0.6020670	3.7734110	-2.5232850	H	3.4603670	-2.1894750	0.9420870
H	-0.5713760	4.8515120	-1.0896370	H	2.0568610	-3.1124870	1.5014940
Rh	0.8739480	-0.0922720	-0.3202500	O	3.8824410	0.0870060	1.1738580
C	-1.4266450	-0.3546710	1.8940740	O	2.1997560	1.3531590	0.3409720
O	-1.3601560	-1.2461010	2.7233200	C	3.3553290	1.1741680	0.9105960
O	0.4947580	0.6651170	2.8035600	C	4.0410830	2.4888420	1.2683180
H	-0.4495260	1.4406010	1.2856080	H	4.0990960	3.1390100	0.3905270
C	-0.5109830	-3.1315970	0.3097910	H	3.4441150	3.0136210	2.0207310
H	-1.5723800	-2.9620710	0.1256740	H	5.0409350	2.2973760	1.6599680

C	1.3832590	-0.4012460	3.1629540
H	2.0488910	-0.6515490	2.3350290
H	1.9791870	0.0253170	3.9735580
H	0.8315190	-1.2715540	3.5218150
C	-6.5166930	0.3293160	-0.8645810
H	-7.2983610	0.5681780	-0.1326090
H	-6.5006330	1.1367260	-1.6017770
H	-6.8211680	-0.5916880	-1.3716170

TS29

N	-0.1627000	0.7597170	1.4744980
C	-2.5819690	0.2009000	1.1270820
C	-3.5631070	-0.7678750	1.4021990
H	-3.3606410	-1.4973520	2.1788030
C	-4.7722340	-0.7790510	0.7153820
H	-5.5100110	-1.5454130	0.9416680
C	-5.0641800	0.1962060	-0.2517270
C	-4.0999060	1.1799930	-0.4973040
H	-4.3095570	1.9637150	-1.2214600
C	-2.8781640	1.1870910	0.1779650
H	-2.1810800	1.9896460	-0.0115440
C	2.0302490	-1.6753180	-1.3336960
C	1.5668470	-2.2011650	-0.0625200
C	0.1247120	-2.2768930	-0.1219000
C	-0.3078250	-1.7256150	-1.3665620

C	0.8850840	-1.3630470	-2.1225810
O	-0.1428110	2.9809670	0.2608140
O	0.1274030	1.5628530	-1.4609710
C	0.0625260	2.7237310	-0.9849870
C	0.2260600	3.9119850	-1.8968260
H	1.2889100	4.1774390	-1.9140440
H	-0.0803130	3.6583540	-2.9127660
H	-0.3349130	4.7695170	-1.5218480
Rh	0.8119230	-0.1718470	-0.3022210
C	-1.3377830	0.1646840	1.9801650
O	-1.4005990	-0.3627150	3.0866090
O	0.7139820	1.1117750	2.5458520
H	-0.1969310	1.9084420	0.8885290
C	-0.7321930	-2.9212660	0.9249400
H	-1.7930220	-2.7958520	0.7085060
H	-0.5162390	-3.9964440	0.9529300
H	-0.5443050	-2.5176400	1.9232700
C	-1.7077660	-1.6611740	-1.9002440
H	-1.9100090	-2.5342310	-2.5349400
H	-2.4497330	-1.6427780	-1.1010980
H	-1.8558790	-0.7668810	-2.5101370
C	0.8721410	-0.7890800	-3.5056360
H	0.6320730	-1.5701710	-4.2379710
H	0.1230250	0.0015900	-3.5916920
H	1.8411710	-0.3625190	-3.7707530

C	3.4640760	-1.5414260	-1.7474930	N	-0.1501940	0.7344260	1.4815090
H	3.8236840	-2.5000820	-2.1442160	C	-2.5688900	0.1995890	1.1352390
H	3.5859770	-0.7901640	-2.5311240	C	-3.5571320	-0.7616000	1.4104130
H	4.0833120	-1.2548680	-0.8969280	H	-3.3618720	-1.4895890	2.1903230
C	2.4329700	-2.8178810	0.9936910	C	-4.7646090	-0.7670750	0.7203410
H	2.7388130	-3.8252720	0.6795670	H	-5.5078350	-1.5281440	0.9468630
H	3.3222840	-2.2092460	1.1594530	C	-5.0484310	0.2078050	-0.2495800
H	1.8970290	-2.9146930	1.9404090	C	-4.0774850	1.1849880	-0.4949100
O	3.9177920	-0.0042620	1.0054870	H	-4.2807860	1.9689010	-1.2207520
O	2.2947470	1.2408240	0.0351260	C	-2.8572520	1.1852270	0.1834960
C	3.4560890	1.0651710	0.5956970	H	-2.1541220	1.9824080	-0.0063230
C	4.2440060	2.3645810	0.7330450	C	2.0081940	-1.6769020	-1.3537750
H	4.2587420	2.9088970	-0.2155990	C	1.5433530	-2.2079540	-0.0844400
H	3.7494040	3.0051020	1.4703900	C	0.1000220	-2.2742810	-0.1412680
H	5.2628530	2.1534860	1.0604740	C	-0.3301550	-1.7099530	-1.3800690
C	1.4484370	0.0373770	3.1431350	C	0.8644180	-1.3503190	-2.1365210
H	2.0681240	-0.4697800	2.4007530	O	-0.0912830	3.0083890	0.2777210
H	2.1068280	0.5352840	3.8601740	O	0.1298170	1.5888500	-1.4510530
H	0.7863690	-0.6543710	3.6662810	C	0.0940590	2.7466760	-0.9769690
C	-6.3946710	0.2076740	-0.9650640	C	0.2680250	3.9402420	-1.8775970
H	-6.3439390	0.7721700	-1.9004540	H	1.3319750	4.2017040	-1.8858640
H	-6.7344240	-0.8067380	-1.1968980	H	-0.0341960	3.6946920	-2.8964910
H	-7.1697700	0.6728090	-0.3431570	H	-0.2911500	4.7976620	-1.4994630
				Rh	0.8040560	-0.1750590	-0.3008950
				C	-1.3279120	0.1634430	1.9949680

O	-1.4089650	-0.3358250	3.1145430	C	3.4560060	1.0370980	0.6031720
O	0.7394500	1.0765350	2.5457780	C	4.2507920	2.3301330	0.7592600
H	-0.1570200	2.0856950	0.8231420	H	4.2651450	2.8911130	-0.1796080
C	-0.7583230	-2.9215710	0.9028730	H	3.7617460	2.9595280	1.5098470
H	-1.8188150	-2.7930590	0.6869440	H	5.2696260	2.1087100	1.0798670
H	-0.5444310	-3.9972370	0.9268460	C	1.4494280	-0.0098190	3.1508760
H	-0.5697180	-2.5223790	1.9029400	H	2.0588880	-0.5335690	2.4116280
C	-1.7302290	-1.6311030	-1.9111490	H	2.1177200	0.4764080	3.8668060
H	-1.9352700	-2.4921490	-2.5611980	H	0.7710440	-0.6841560	3.6759620
H	-2.4715370	-1.6246530	-1.1112940	C	-6.3775120	0.2259150	-0.9656300
H	-1.8763010	-0.7257490	-2.5049950	H	-7.1527600	0.6909540	-0.3438380
C	0.8520240	-0.7657790	-3.5152040	H	-6.3231680	0.7934850	-1.8989770
H	0.6107310	-1.5408090	-4.2536040	H	-6.7197890	-0.7866670	-1.2019480
H	0.1038480	0.0263360	-3.5959250				
H	1.8217490	-0.3388280	-3.7772520	31			
C	3.4424670	-1.5491330	-1.7682910	N	0.0223770	-1.6409560	-0.0712890
H	3.7969700	-2.5078640	-2.1693680	C	2.4306870	-1.1919930	0.0331500
H	3.5677320	-0.7951470	-2.5488110	C	3.5184640	-1.0872720	0.9135770
H	4.0640140	-1.2697510	-0.9169610	H	3.4444860	-1.5542890	1.8909920
C	2.4076760	-2.8408910	0.9635440	C	4.6783320	-0.4199040	0.5307740
H	2.7099750	-3.8449440	0.6354740	H	5.5060810	-0.3367070	1.2314040
H	3.2991580	-2.2374560	1.1367470	C	4.8097680	0.1231640	-0.7585640
H	1.8717130	-2.9485650	1.9090330	C	3.7329530	-0.0133660	-1.6432700
O	3.9086610	-0.0391440	1.0044790	H	3.8209770	0.3776680	-2.6544180
O	2.2991150	1.2251140	0.0369450	C	2.5544050	-0.6544320	-1.2553400

H	1.7369450	-0.7705530	-1.9595260	H	-3.9788690	1.4319170	0.0413670
C	-1.9402260	2.0204730	0.3475800	C	-2.5463170	0.6999450	2.5172120
C	-1.5759220	1.2689660	1.5296160	H	-2.9607880	1.5036400	3.1406450
C	-0.1217610	1.2777130	1.6483470	H	-3.3658070	0.1996100	1.9960430
C	0.3917260	1.9527250	0.5105150	H	-2.0645950	-0.0234060	3.1783170
C	-0.7386430	2.3842080	-0.3158280	O	-3.7571730	-0.9394920	-0.1559080
Rh	-0.8119190	0.1923190	-0.1257250	O	-2.0625790	-0.5122580	-1.5821680
C	1.2563230	-2.0462640	0.4260360	C	-3.2397880	-0.9849350	-1.2778390
O	1.4445620	-3.0775420	1.0677260	C	-3.9482560	-1.6400540	-2.4542710
O	-0.8451020	-2.7450690	-0.2357400	H	-3.8102140	-1.0573060	-3.3686270
C	0.6571390	0.7443290	2.8136040	H	-3.5011150	-2.6256020	-2.6224040
H	1.6971850	0.5512980	2.5459050	H	-5.0100290	-1.7626330	-2.2358580
H	0.6481260	1.4689920	3.6377080	C	-1.5400360	-3.0951420	0.9698840
H	0.2303220	-0.1890750	3.1884180	H	-2.1828600	-2.2706570	1.2956760
C	1.8193360	2.3159550	0.2483320	H	-2.1698590	-3.9437980	0.6907730
H	2.0044540	3.3347450	0.6152750	H	-0.8338110	-3.3956960	1.7471430
H	2.5149240	1.6426740	0.7498080	C	6.0941290	0.7929770	-1.1862850
H	2.0531440	2.3003610	-0.8173150	H	6.8569890	0.0494800	-1.4488610
C	-0.6213000	3.1503510	-1.5984150	H	5.9431020	1.4294810	-2.0628390
H	-0.5294050	4.2258220	-1.3979320	H	6.5113360	1.4108310	-0.3844360
H	0.2602870	2.8439920	-2.1671610				
H	-1.4976260	2.9998520	-2.2317730	32			
C	-3.3445970	2.3103820	-0.0908690	Rh	-1.0129480	-0.1271350	0.1657150
H	-3.7573810	3.1366940	0.5015730	N	0.0521260	1.6429120	-0.1306360
H	-3.3824510	2.6029000	-1.1422230	C	-0.3382800	-1.8602480	-0.9397370

C	-1.4861600	-2.2579520	-0.1265120	C	-3.0256590	0.3977260	-2.3357570
C	-2.5995710	-1.4747620	-0.5249490	H	-2.4555210	1.2835030	-2.6224990
C	-2.1609940	-0.5700770	-1.5862710	H	-3.4281830	-0.0691670	-3.2445220
C	-0.7854860	-0.8685550	-1.8781450	H	-3.8697350	0.7295470	-1.7266960
O	-2.1445830	1.0340720	1.6220430	C	-3.9908340	-1.5199920	0.0312130
O	-0.4009780	-0.1113460	2.2724880	H	-4.3843790	-0.5125560	0.1893310
C	-1.3360460	0.7103360	2.5483030	H	-4.6619500	-2.0371700	-0.6659530
C	-1.4537120	1.3106710	3.9234510	H	-4.0276350	-2.0473100	0.9865620
O	-0.9154980	2.5131810	-0.7304940	C	-1.4484100	-3.3163750	0.9346900
C	1.2635460	1.7678930	-0.7800710	H	-2.3118760	-3.2534020	1.6001320
C	2.3899970	0.8940100	-0.2840330	H	-1.4460300	-4.3148840	0.4794940
C	2.4664490	0.3511150	1.0058760	H	-0.5474040	-3.2272450	1.5471920
C	3.4543010	0.6663610	-1.1702050	C	1.0131940	-2.5071960	-0.8912120
C	3.5702810	-0.4158270	1.3832570	H	1.2802420	-2.7867770	0.1304670
H	1.6648520	0.5203640	1.7138820	H	1.0198780	-3.4199970	-1.5018300
C	4.5459510	-0.1102740	-0.7901840	H	1.7939490	-1.8414330	-1.2623330
H	3.4098430	1.1258010	-2.1524010	C	-0.8832320	3.7901090	-0.1033970
C	4.6257230	-0.6643790	0.4963450	H	0.0782980	4.2856140	-0.2756400
H	3.6129850	-0.8236330	2.3910000	H	-1.6808820	4.3697950	-0.5778290
H	5.3557330	-0.2803970	-1.4965110	H	-1.0823900	3.7041910	0.9712640
O	1.4783510	2.5734230	-1.6913750	C	5.8316950	-1.4676240	0.9233520
C	0.0187640	-0.2494550	-2.9809390	H	6.2525670	-2.0355500	0.0875470
H	-0.1306160	0.8310770	-3.0384550	H	6.6279500	-0.8145800	1.3029550
H	1.0867060	-0.4264940	-2.8468580	H	5.5822320	-2.1724210	1.7223970
H	-0.2795240	-0.6907230	-3.9405080	H	-0.8236180	2.2055990	3.9703900

H	-2.4851130	1.6049570	4.1259010
H	-1.1000510	0.6063050	4.6790750

TS33

Rh	-0.5662270	-0.2267220	0.0869890
N	-0.4139650	1.6859500	-0.6403140
C	-0.1226490	-1.8322030	-1.3295080
C	-0.4457410	-2.4577660	-0.0510680
C	-1.7742590	-2.0880530	0.2861340
C	-2.3022090	-1.2382310	-0.7708760
C	-1.2909330	-1.1324550	-1.7869450
O	-1.4841690	0.6370650	1.8071940
O	0.4869670	1.3363890	2.6087420
C	-0.7746440	1.2295830	2.6771110
C	-1.4738750	1.8601050	3.8617550
O	-1.5345720	2.2396810	-1.2922540
C	0.7930020	2.0756890	-1.1591400
C	1.8938690	1.2491910	-0.5547360
C	1.5710020	0.3151250	0.4554720
C	3.1961460	1.3583010	-1.0413480
C	2.6060060	-0.5016750	0.9508550
H	0.8719510	0.7647520	1.4960910
C	4.1972750	0.5340070	-0.5294550
H	3.3981210	2.0832140	-1.8245660
C	3.9213970	-0.4053160	0.4791260

H	2.3919020	-1.1965530	1.7613020
H	5.2124560	0.6205520	-0.9110450
O	0.9847060	2.9737120	-1.9800020
C	-1.4460280	-0.4114870	-3.0921830
H	-2.0017340	0.5188330	-2.9624240
H	-0.4790300	-0.1597850	-3.5317190
H	-1.9864570	-1.0466550	-3.8058360
C	-3.6902960	-0.6743230	-0.8418280
H	-3.6893800	0.2930480	-1.3496440
H	-4.3642260	-1.3475290	-1.3883230
H	-4.1054800	-0.5246270	0.1577570
C	-2.5388450	-2.4849240	1.5130040
H	-3.0027230	-1.6129990	1.9824600
H	-3.3357160	-3.1925100	1.2528740
H	-1.8944210	-2.9637490	2.2532230
C	0.4396860	-3.4122610	0.6959200
H	0.2135480	-3.4229220	1.7650300
H	0.3054200	-4.4343700	0.3179400
H	1.4936850	-3.1533400	0.5795870
C	1.1400830	-2.0554920	-2.1092670
H	2.0118100	-2.0989020	-1.4530670
H	1.0845400	-3.0011740	-2.6641080
H	1.3121240	-1.2547360	-2.8314070
C	-1.8877160	3.4869590	-0.6935690
H	-1.0836240	4.2169570	-0.8275840

H	-2.7836070	3.8242060	-1.2232020
H	-2.1126530	3.3587990	0.3719870
C	5.0267940	-1.2544090	1.0636230
H	5.7074030	-1.6181400	0.2866120
H	5.6306460	-0.6810380	1.7778800
H	4.6270300	-2.1216800	1.5975830
H	-1.4342850	2.9487430	3.7528510
H	-2.5152400	1.5418520	3.9161840
H	-0.9459160	1.6036440	4.7833440

34

Rh	0.4651170	-0.0404920	0.0068140
N	0.1073560	1.8708460	0.0839810
C	1.5320840	-1.4960740	1.1963180
C	1.0362100	-2.1917510	0.0442540
C	1.5850250	-1.5424420	-1.1047820
C	2.5576840	-0.5411270	-0.6526140
C	2.5291530	-0.5158630	0.7541060
O	1.1251140	2.8217100	0.2696100
C	-1.1971630	2.3643240	0.2299730
C	-2.1639730	1.2344640	0.1193140
C	-1.6114800	-0.0544440	-0.0185570
C	-3.5369540	1.4544030	0.1440850
C	-2.5044660	-1.1209670	-0.1427950
C	-4.4063390	0.3668430	0.0239300

H	-3.9079340	2.4691610	0.2601290
C	-3.9024790	-0.9287330	-0.1264920
H	-2.1380590	-2.1378530	-0.2572810
H	-5.4816700	0.5260150	0.0456250
O	-1.4825420	3.5409920	0.4034590
C	3.3440270	0.3530650	1.6648760
H	3.6813530	1.2584350	1.1569010
H	2.7663250	0.6662900	2.5382390
H	4.2285920	-0.1868470	2.0266160
C	3.4181940	0.2890090	-1.5578870
H	3.7431940	1.2088180	-1.0670850
H	4.3152290	-0.2675180	-1.8589190
H	2.8843340	0.5676850	-2.4703730
C	1.3530450	-1.9214260	-2.5369230
H	1.3791910	-1.0452790	-3.1899420
H	2.1297370	-2.6168780	-2.8826520
H	0.3843460	-2.4073700	-2.6709760
C	0.1696470	-3.4163740	0.0547020
H	-0.4084910	-3.5127920	-0.8672300
H	0.7895990	-4.3174170	0.1484970
H	-0.5326000	-3.4119510	0.8916090
C	1.2291890	-1.8285490	2.6262230
H	0.2347500	-2.2677320	2.7307130
H	1.9599240	-2.5501880	3.0159960
H	1.2708800	-0.9391960	3.2596800

C	1.2607760	3.6710110	-0.8754620	H	-0.1638900	-2.9226860	-1.0918810
H	0.3611690	4.2734800	-1.0217900	H	-1.1005870	-1.7344880	-1.9833820
H	2.1110820	4.3211560	-0.6533710	C	-0.3392340	0.9355410	-2.4825780
H	1.4731860	3.0780020	-1.7748600	H	-0.3050080	1.9920130	-2.2094320
C	-4.8322340	-2.1101860	-0.2840330	H	-0.4276560	0.8706550	-3.5748740
H	-5.8685160	-1.8361710	-0.0664750	H	-1.2475970	0.5135670	-2.0476030
H	-4.8035930	-2.5063200	-1.3069780	C	2.5860700	2.2089520	-2.0599640
H	-4.5540120	-2.9320160	0.3854800	H	3.0351980	2.3142140	-3.0561340
				H	1.7182160	2.8703260	-2.0145070
28'				H	3.3058300	2.5362380	-1.3087000
Rh	1.5015120	-0.1090300	0.0194120	C	4.5446270	-0.1106320	-1.1134630
O	3.5107310	2.1444920	1.0015800	H	5.1166610	-0.0218350	-2.0462560
O	-0.0259620	-0.8329210	1.4418580	H	4.7051670	0.7820490	-0.5054880
C	2.3745410	2.3185160	1.4469660	H	4.9313720	-0.9715060	-0.5636850
O	1.3219790	1.5931920	1.1700930	C	2.3300440	-1.5172650	-1.4021300
C	0.8897730	-1.1608920	2.2736910	C	2.8844540	-2.8696130	-1.0691680
O	2.0964580	-1.0389270	1.9089670	H	3.5949780	-2.8154380	-0.2407200
C	2.0784310	3.4431960	2.4340880	H	2.0902790	-3.5648510	-0.7884660
C	0.5344840	-1.6392070	3.6548720	H	3.4095180	-3.2903380	-1.9360860
C	0.9884930	-1.2244380	-1.7801880	C	-2.9988930	2.3320460	0.7019110
C	3.0856560	-0.2690090	-1.4125690	C	-2.7946630	0.9532610	0.7139640
C	0.8869650	0.2118100	-2.0135410	C	-3.5623280	0.1181420	-0.1145190
C	2.1981950	0.7792990	-1.8356760	C	-4.5311180	0.6999570	-0.9444620
C	-0.1249460	-2.2181580	-1.9252530	C	-4.7312950	2.0770680	-0.9454090
H	0.0114800	-2.7942220	-2.8492900	C	-3.9709940	2.9185090	-0.1205990

H	-2.3845110	2.9613060	1.3408350	Rh	0.6879400	-0.2249130	-0.2400610
H	-2.0194000	0.5531880	1.3581580	O	3.6276620	-0.7066730	1.1637960
H	-5.1132570	0.0459470	-1.5848380	O	-0.3517680	-0.0735950	2.7726200
H	-5.4882640	2.5085810	-1.5958840	C	3.0761670	0.3367380	1.5171180
C	-3.4091640	-1.3756680	-0.2054490	O	1.9288040	0.7931170	1.0881070
O	-4.0227210	-2.0411460	-1.0338090	C	0.1112720	-1.2305670	2.5274250
N	-2.5989300	-1.9591490	0.7518250	O	0.4039280	-1.6298640	1.3546650
H	-1.7834460	-1.4600640	1.1114070	C	3.7171110	1.2583900	2.5531450
O	-2.2150340	-3.2883260	0.4965110	C	0.3295960	-2.1851010	3.6748400
C	-3.1882700	-4.1939550	1.0209890	C	-0.1975220	-0.4524120	-2.2683930
C	-4.2065250	4.4097540	-0.0997060	C	1.7979070	-1.4936330	-1.6398650
H	-4.6711270	4.7553320	-1.0277960	C	0.8552920	0.5509000	-2.2565620
H	-4.8743910	4.6909040	0.7243340	C	2.0873120	-0.1155310	-1.9176360
H	-3.2716880	4.9613360	0.0405430	C	-1.5899600	-0.2431260	-2.7816010
H	-3.3288630	-4.0408100	2.0977940	H	-1.5905860	-0.3715320	-3.8724100
H	-4.1409670	-4.0830380	0.4959580	H	-2.3010810	-0.9584220	-2.3658420
H	-2.7782760	-5.1906700	0.8390040	H	-1.9590210	0.7603310	-2.5659280
H	1.3707310	-2.1806680	4.0991560	C	0.7095150	1.9696370	-2.7210580
H	0.3079800	-0.7687540	4.2799760	H	1.4711340	2.6154580	-2.2783950
H	-0.3554790	-2.2719040	3.6220450	H	0.8141280	2.0280940	-3.8124970
H	1.1260510	3.9268620	2.2020190	H	-0.2675700	2.3769430	-2.4539120
H	1.9969500	3.0217560	3.4419370	C	3.4461860	0.5122760	-1.8744310
H	2.8890290	4.1732050	2.4231110	H	3.9484760	0.3646710	-2.8394550
				H	3.3841800	1.5871860	-1.6918100
TS29'				H	4.0550750	0.0618190	-1.0897830

C	2.7964190	-2.5566520	-1.2965060	C	-0.4429400	5.0616850	0.5817060
H	3.3322370	-2.8816210	-2.1983020	H	0.6472450	4.9859960	0.6204540
H	3.5117060	-2.1806330	-0.5638320	H	-0.7108460	5.7282070	-0.2452750
H	2.3055930	-3.4324590	-0.8664970	H	-0.7722060	5.5500670	1.5071560
C	0.3752770	-1.6921350	-1.8614960	H	-3.9345850	-2.9528170	2.0327050
C	-0.3320960	-3.0082690	-1.7425100	H	-5.0439900	-2.1264470	0.8848210
H	0.0552210	-3.5842120	-0.8985270	H	-4.5487340	-3.8215330	0.5909010
H	-1.4070950	-2.8883960	-1.5991110	H	1.4062190	-2.2591690	3.8601030
H	-0.1710220	-3.6010570	-2.6521420	H	-0.1709080	-1.8289670	4.5753000
C	-0.3629630	2.5282160	0.6752480	H	-0.0267420	-3.1814800	3.4034910
C	-0.9176490	1.2330310	0.5733690	H	3.0631100	1.3468840	3.4262510
C	-2.2958210	1.1548860	0.2204410	H	4.6872260	0.8633530	2.8572150
C	-3.0246720	2.3244160	-0.0362020	H	3.8394870	2.2640690	2.1389420
C	-2.4291820	3.5784820	0.0567980				
C	-1.0844030	3.7026540	0.4296340	30'			
H	0.6788590	2.6037910	0.9714920	Rh	0.6376280	-0.2337170	-0.2105750
H	-0.5285970	0.4934450	1.6655750	O	3.3457650	-0.6165800	1.5224610
H	-4.0697760	2.2231630	-0.3090840	O	0.4979240	0.8331470	3.0583940
H	-3.0190890	4.4691830	-0.1487900	C	3.0496710	0.5703160	1.4671550
C	-3.1058380	-0.1092050	0.0748090	O	1.9188930	1.0500740	0.9595030
O	-4.2147710	-0.1143660	-0.4501620	C	-0.0132660	-0.3565160	2.8968170
N	-2.5715550	-1.2584320	0.6264510	O	-0.0440270	-0.9554240	1.8032930
H	-1.5650570	-1.3580060	0.7108120	C	3.9627200	1.6579540	2.0156360
O	-3.1175600	-2.4690650	0.1708310	C	-0.5669510	-0.9856200	4.1445150
C	-4.2323100	-2.8517190	0.9825750	C	0.0952010	-0.7260250	-2.2746270

C	1.4898560	-2.1940280	-1.0834850	C	-0.7796600	1.2933380	-0.1423870
C	1.4196010	-0.1569000	-2.1957280	C	-2.1864500	1.1573580	-0.2335940
C	2.2899000	-1.1387060	-1.5407810	C	-2.9983410	2.2978810	-0.3933200
C	-1.0326500	-0.1934020	-3.1072900	C	-2.4578820	3.5744930	-0.4231860
H	-0.9298230	-0.5759990	-4.1317440	C	-1.0718600	3.7465940	-0.3115160
H	-2.0119420	-0.4908740	-2.7313810	H	0.8055590	2.7480400	-0.1171940
H	-1.0151580	0.8971460	-3.1557210	H	0.9785370	1.1020400	2.1970560
C	1.8918120	1.0736070	-2.9126380	H	-4.0692930	2.1540570	-0.5022200
H	2.7219770	1.5481000	-2.3829800	H	-3.1091160	4.4377440	-0.5388200
H	2.2401820	0.8257990	-3.9242680	C	-2.9702960	-0.1298330	-0.2479350
H	1.0899390	1.8091610	-3.0022740	O	-3.8474720	-0.3600640	-1.0771330
C	3.7794240	-1.0180990	-1.4432750	N	-2.7520660	-0.9675520	0.8272150
H	4.2331040	-1.3714340	-2.3791790	H	-1.8224020	-1.0009230	1.2362160
H	4.0921570	0.0197640	-1.3043280	O	-3.2747840	-2.2697290	0.7371330
H	4.1821140	-1.6002890	-0.6155170	C	-4.6241250	-2.2927510	1.2081550
C	1.9420960	-3.3898960	-0.2998500	C	-0.4614050	5.1288060	-0.3194440
H	2.2148060	-4.2182380	-0.9666870	H	-0.8837760	5.7496100	-1.1173240
H	2.8068590	-3.1430950	0.3194460	H	-0.6515850	5.6508830	0.6267440
H	1.1491730	-3.7489050	0.3614160	H	0.6226470	5.0864460	-0.4592720
C	0.1076200	-1.9311680	-1.5047200	H	-4.6865390	-1.9382800	2.2443100
C	-1.0173200	-2.9121540	-1.3669980	H	-5.2676810	-1.6893780	0.5623520
H	-1.0436380	-3.3657120	-0.3736940	H	-4.9254740	-3.3420650	1.1575160
H	-1.9918870	-2.4560280	-1.5416090	H	-1.2455640	-1.7997430	3.8911030
H	-0.8853670	-3.7230390	-2.0963470	H	0.2670860	-1.3877860	4.7300780
C	-0.2686420	2.6060630	-0.1860330	H	-1.0719520	-0.2337450	4.7544720

H	4.2189750	2.3657870	1.2210350
H	3.4439540	2.2257870	2.7948150
H	4.8706170	1.2160150	2.4273600

31'

Rh	-0.5056640	-0.2492510	0.0712100
O	0.2382250	2.1015030	2.3588850
C	0.0602720	0.9566580	2.8391910
O	-0.2492510	-0.0959410	2.1718350
C	0.2478280	0.7476810	4.3338510
C	-2.6398290	-0.6013700	-0.7183960
C	-1.2015670	-2.3079730	-0.0462070
C	-1.6026130	-0.7758870	-1.7391640
C	-0.7858150	-1.8934750	-1.3593700
C	-3.7538010	0.3993680	-0.8095400
H	-4.3156120	0.4619330	0.1253320
H	-3.3646010	1.3957990	-1.0335180
H	-4.4572550	0.1218610	-1.6047060
C	-1.5675320	-0.0373340	-3.0465070
H	-0.5802340	-0.0870020	-3.5115660
H	-2.2913600	-0.4653160	-3.7527250
H	-1.8176790	1.0172840	-2.9075920
C	0.2707610	-2.5444280	-2.2012660
H	-0.1644730	-3.3756000	-2.7709050
H	0.7064820	-1.8421680	-2.9150450

H	1.0849350	-2.9438620	-1.5931320
C	-0.6891660	-3.4815480	0.7368770
H	-0.6766320	-3.2650140	1.8086430
H	-1.3210060	-4.3665590	0.5819190
H	0.3275620	-3.7482650	0.4383130
C	-2.3879210	-1.5276910	0.3085760
C	-3.1309010	-1.6971410	1.5993650
H	-2.4553440	-1.5569320	2.4495010
H	-3.9465960	-0.9776000	1.6946870
H	-3.5578350	-2.7046680	1.6705940
C	2.4618070	-1.1242410	0.2095670
C	1.5215100	-0.1468560	-0.1371880
C	1.9963000	1.0290770	-0.7487800
C	3.3545850	1.2084840	-1.0489520
C	4.2636530	0.2182050	-0.7020890
C	3.8297890	-0.9545450	-0.0558190
H	2.1381640	-2.0384440	0.7028700
H	3.6740920	2.1204390	-1.5456220
H	5.3201300	0.3484270	-0.9226860
C	0.9952140	2.0626520	-1.0625990
O	1.0662520	2.9492380	-1.8886730
N	-0.1758410	1.8731400	-0.2134630
H	0.0363000	2.0782050	0.8282190
O	-1.2966780	2.6262600	-0.6370710
C	-1.2303300	3.9873560	-0.1781520

C	4.8316110	-2.0052140	0.3620340	C	-1.5793330	0.1255090	-2.9919000
H	5.5841530	-2.1733760	-0.4156410	H	-0.6211050	0.0967320	-3.5096840
H	5.3687490	-1.6970900	1.2677640	H	-2.3637300	-0.1924030	-3.6966580
H	4.3451910	-2.9607350	0.5783810	H	-1.7741630	1.1603890	-2.6940310
H	-2.1715900	4.4362810	-0.5034610	C	0.4661760	-2.3336450	-2.3883590
H	-1.1615050	4.0252060	0.9145880	H	0.4756150	-3.4684710	-2.3723500
H	-0.3894330	4.5110870	-0.6381660	H	0.2840720	-1.9839650	-3.4538790
H	-0.4425870	-0.0092060	4.7120340	H	1.4772950	-1.9519300	-2.0351420
H	1.2680920	0.3903850	4.5122550	C	-0.3402950	-3.5537860	0.4816800
H	0.1141600	1.6900950	4.8670930	H	-0.3648330	-3.4215180	1.5677510
TS33'				H	-0.8576990	-4.4938670	0.2373860
Rh	-0.4833310	-0.2682280	0.0804010	H	0.7010720	-3.6428490	0.1737580
O	0.0183610	2.0613860	2.4070560	C	-2.2441320	-1.7375320	0.2229180
C	-0.0748280	0.8827700	2.8827790	C	-2.9231010	-2.0384190	1.5319760
O	-0.2866880	-0.1957450	2.1647900	H	-2.2338410	-1.8557690	2.3591780
C	0.0753130	0.6416610	4.3776440	H	-3.8014240	-1.4024530	1.6692130
C	-2.5934660	-0.7507360	-0.7263070	H	-3.2440840	-3.0869920	1.5674100
C	-0.9984100	-2.3856100	-0.2061530	C	2.5118660	-1.0023890	0.2545460
C	-1.5657000	-0.7638490	-1.7783730	C	1.5292490	-0.0565780	-0.0699310
C	-0.6493770	-1.8449180	-1.4977170	C	1.9430400	1.1520620	-0.6658830
C	-3.7758000	0.1804850	-0.7027790	C	3.2866040	1.3949920	-0.9794270
H	-4.3245730	0.0895870	0.2445540	C	4.2432780	0.4422100	-0.6539980
H	-3.4379750	1.2154410	-0.8054500	C	3.8665440	-0.7600030	-0.0225880
H	-4.4666640	-0.0506240	-1.5193190	H	2.2287280	-1.9333500	0.7324210
				H	3.5595450	2.3249620	-1.4675670

H	5.2889710	0.6193340	-0.8822640	H	-3.0063980	1.7101600	-1.6512430
C	0.8928220	2.1333080	-0.9719310	H	-2.9722740	2.4943230	3.2471740
O	0.9244950	3.0768130	-1.7595810	H	-4.1514330	4.1015270	1.7198510
N	-0.2844570	1.8286600	-0.1303180	C	-1.6777360	0.2204030	2.5294880
H	-0.1252820	2.1033650	1.1096830	O	-1.4516290	0.3888370	3.7296200
O	-1.5080480	2.5000680	-0.6425920	Rh	-1.3162700	-0.7474080	-0.2676100
C	-1.5204850	3.9224370	-0.2123550	N	-1.4132850	-0.9079000	1.7965960
C	4.9263810	-1.7764310	0.3632160	C	-1.3034840	-2.5531330	3.4696800
H	5.6485640	-1.9134440	-0.4432640	O	-0.5977530	-1.8708250	2.4299460
H	5.4734460	-1.4354980	1.2536190	C	-2.9418610	-1.4944550	-1.6987450
H	4.4731760	-2.7443820	0.5936050	C	-2.7022290	-2.4646610	-0.6718790
H	-2.4898830	4.2962560	-0.5542520	C	-1.3544920	-2.9752710	-0.8331290
H	-1.4522130	3.9921810	0.8774540	C	-0.7580660	-2.2699510	-1.9129640
H	-0.7077640	4.4589020	-0.6997590	C	-1.7251030	-1.3240640	-2.4352070
H	-0.7641660	0.0487640	4.7433800	C	-3.7351440	-3.0057530	0.2720470
H	0.9955800	0.0750430	4.5583420	H	-4.3354790	-3.7813820	-0.2221500
H	0.1213860	1.5968070	4.9003210	H	-3.2705390	-3.4518300	1.1524560
35				H	-4.4156410	-2.2225710	0.6143590
C	-3.0114740	1.8582360	-0.5734490	C	-0.7586140	-4.1027780	-0.0415510
C	-2.3652290	0.9524690	0.2734170	H	-0.7782520	-3.8819310	1.0278330
C	-2.3767580	1.2021970	1.6509190	H	-1.3131610	-5.0327290	-0.2181310
C	-3.0094410	2.3322790	2.1733510	H	0.2827620	-4.2741300	-0.3187690
C	-3.6562520	3.2208840	1.3172900	C	0.6101480	-2.5003270	-2.4843650
C	-3.6746820	2.9902830	-0.0666070	H	1.0295960	-1.5784810	-2.8959480
				H	1.3016240	-2.8715330	-1.7274850

H	0.5652810	-3.2319700	-3.3012000	H	-0.4737520	3.2583660	0.3816200
C	-4.2769480	-0.8872600	-2.0123120	H	1.2759550	3.1748790	0.2239160
H	-4.8844880	-1.6066060	-2.5770060	C	6.4085310	-0.8281100	-0.7862160
H	-4.8267830	-0.6242060	-1.1060870	H	5.9886760	-1.7308490	-1.2246530
H	-4.1861900	0.0135060	-2.6216950	C	7.5879550	-0.2916640	-1.3048200
C	-1.5440850	-0.4805360	-3.6653920	H	8.0785770	-0.7766180	-2.1443220
H	-2.1788350	0.4092720	-3.6417050	C	0.3462790	4.6529000	-1.0597200
H	-0.5092100	-0.1468120	-3.7761120	H	1.1639280	4.6813780	-1.7935220
H	-1.8043070	-1.0446090	-4.5706750	H	-0.5850890	4.7579580	-1.6326870
F	1.8661610	-0.4847440	2.0276590	C	6.3265510	0.9282150	0.8583940
F	1.9021530	-2.0990460	0.5277700	H	5.8421200	1.4030320	1.7086430
C	0.2082930	0.8010290	-0.6478290	C	7.5058660	1.4683140	0.3434740
C	0.7236590	-0.1314040	0.0154860	H	7.9321880	2.3606180	0.7935520
C	3.2336190	-0.1840270	0.1295090	C	8.1401780	0.8602090	-0.7415020
H	3.2283420	0.9044460	0.2477010	H	9.0603550	1.2771320	-1.1407210
H	3.2709710	-0.3941820	-0.9443020	C	0.4836750	5.8318310	-0.0909220
C	5.7599450	-0.2264490	0.3009460	H	0.4754700	6.7885740	-0.6231400
C	0.1964020	2.1152480	-1.3272800	H	1.4203640	5.7729650	0.4746650
H	-0.7248510	2.2384780	-1.9037740	H	-0.3390390	5.8429080	0.6321950
H	1.0294500	2.1302040	-2.0449390	H	-0.6286360	-3.3494670	3.7974840
C	4.4620020	-0.7893290	0.8382750	H	-1.5200520	-1.8733380	4.2966630
H	4.3782700	-0.5907360	1.9108710	H	-2.2379890	-2.9918390	3.0951960
H	4.4408630	-1.8762590	0.7115110	C	-4.4095870	3.9299150	-0.9956180
C	1.9117570	-0.7222300	0.6806490	H	-4.0024200	3.8935580	-2.0113040
C	0.3450270	3.2970280	-0.3441570	H	-5.4743240	3.6717150	-1.0631550

H	-4.3524750	4.9655450	-0.6456660
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TS36

C	-2.6695790	2.1193220	0.1684840
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C	-1.6309260	1.2432790	0.5370860
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C	-0.9830440	1.4571180	1.7681830
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C	-1.3231240	2.5458000	2.5731030
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C	-2.3486080	3.4044950	2.1865670
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C	-3.0502130	3.1892250	0.9857940
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H	-3.1823460	1.9835910	-0.7811250
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H	-0.7781000	2.6905100	3.5015410
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H	-2.6182790	4.2466390	2.8195210
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C	0.0436220	0.4596610	2.1939290
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O	0.9768170	0.7125960	2.9621750
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Rh	-1.4460800	-0.8103950	-0.0796870
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N	-0.2686360	-0.7529340	1.6459980
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C	0.8095870	-2.2493500	3.1103380
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O	0.7497060	-1.7352910	1.7771190
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C	-3.6391570	-1.4484900	-0.0825490
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C	-2.8520880	-2.4193100	0.5903930
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C	-1.8864700	-2.9662040	-0.3567700
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C	-2.1167030	-2.3332120	-1.6199140
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C	-3.1567500	-1.3576350	-1.4455030
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C	-3.0387690	-2.8949330	2.0007620
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H	-3.8040140	-3.6812880	2.0384770
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H	-2.1137260	-3.3119210	2.4019720
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H	-3.3551150	-2.0865460	2.6641130
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C	-0.9394400	-4.0947550	-0.0683030
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H	-0.3469270	-3.8860550	0.8256030
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H	-1.4855180	-5.0343950	0.0853420
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H	-0.2395750	-4.2405100	-0.8925930
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C	-1.4333840	-2.6553470	-2.9173820
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H	-1.3867310	-1.7814720	-3.5723930
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H	-0.4117670	-3.0001420	-2.7574810
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H	-1.9836360	-3.4397700	-3.4528510
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C	-4.8083280	-0.7011650	0.4875190
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H	-4.7678700	-0.6719180	1.5788790
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H	-4.8425720	0.3325140	0.1341370
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H	-5.7523230	-1.1826880	0.2010120
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C	-3.7779730	-0.5361940	-2.5391220
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H	-4.2413970	0.3727510	-2.1476230
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H	-3.0429360	-0.2444410	-3.2934470
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H	-4.5643870	-1.1059890	-3.0518120
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C	-0.3235200	0.9833220	-0.9385780
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C	0.2829410	-0.1516710	-0.9342940
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C	2.7776190	-0.3702680	-0.6259210
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H	2.5893080	-0.6464590	0.4156740
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H	2.8711410	0.7203110	-0.6601420
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C	5.2926870	-0.5885700	-0.3901080
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C	-0.2857370	2.2746460	-1.7017380
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H	-1.2956850	2.5480210	-2.0255930	H	0.5131140	6.1530590	-0.1488580
H	0.2961780	2.0694140	-2.6096850	H	1.5365590	-3.0661950	3.0718430
C	4.0647730	-1.0344300	-1.1546740	H	1.1434280	-1.4773010	3.8073670
H	3.9529400	-2.1214260	-1.0836390	H	-0.1660500	-2.6408640	3.4254920
H	4.1800000	-0.7936760	-2.2163030	C	-4.1876200	4.1031820	0.5907140
C	1.5441570	-0.7498980	-1.4342160	H	-4.5485520	3.8828430	-0.4181730
C	0.3484530	3.4537300	-0.9409650	H	-5.0366470	4.0005870	1.2772180
H	-0.2178090	3.6510780	-0.0252040	H	-3.8821050	5.1550570	0.6160230
H	1.3613340	3.1719180	-0.6262000	F	1.4358730	-2.1282970	-1.4827480
C	6.1460460	0.3942920	-0.9081340	F	1.7256190	-0.3603240	-2.7607770
H	5.9331060	0.8238260	-1.8845210				
C	7.2653920	0.8233510	-0.1923300	37			
H	7.9164560	1.5845390	-0.6137250	C	1.4168940	1.8123580	2.2462060
C	0.4099080	4.7263260	-1.7956340	C	1.2719760	1.5608170	0.8618480
H	0.9625040	4.5190290	-2.7223780	C	2.4429940	1.4440560	0.0671400
H	-0.6079480	5.0039300	-2.1035320	C	3.7058180	1.5906110	0.6783610
C	5.5901300	-1.1329810	0.8673800	C	3.8150720	1.8318560	2.0375070
H	4.9395910	-1.8980340	1.2848110	C	2.6633990	1.9513480	2.8475140
C	6.7064310	-0.7068230	1.5868050	H	0.5183210	1.9217960	2.8489180
H	6.9196490	-1.1415740	2.5594500	H	4.5958930	1.5360580	0.0580110
C	7.5489980	0.2739110	1.0586160	H	4.7980770	1.9523970	2.4871880
H	8.4198160	0.6053470	1.6171170	C	2.3254840	1.3221610	-1.4501690
C	1.0616480	5.9039490	-1.0641470	O	2.5034180	2.2778910	-2.2047500
H	1.0871740	6.7999690	-1.6929450	Rh	1.2869020	-0.9147090	-0.0624920
H	2.0924240	5.6689280	-0.7764160	N	2.0484590	0.0310010	-1.7364260

C	2.6527430	-0.1971510	-3.9927110	H	-0.0761870	-1.7964480	3.2729040
O	1.5839760	-0.2438820	-3.0468280	H	1.2689920	-2.8304300	3.7711070
C	2.6311140	-2.3773230	1.1079450	F	-1.8303690	0.9180800	-2.0777620
C	2.5348390	-2.8194250	-0.2200610	F	-1.4865720	-1.2291370	-1.7412650
C	1.1150190	-2.9903500	-0.5297380	C	-0.0901010	1.5000390	0.2213250
C	0.3664870	-2.7874470	0.7010750	C	-0.3514910	0.3043110	-0.3322320
C	1.2802470	-2.3228400	1.6803500	C	-2.8930900	-0.0946850	-0.2273440
C	3.6487390	-3.0557300	-1.1941870	H	-3.0258370	0.8636980	0.2820270
H	3.8627930	-4.1284840	-1.2829730	H	-2.7383000	-0.8427680	0.5552680
H	3.3839920	-2.6858290	-2.1872910	C	-5.3954160	-0.5008880	-0.1890620
H	4.5691850	-2.5539410	-0.8879700	C	-0.9271740	2.7668500	0.2300960
C	0.5917550	-3.5678290	-1.8103670	H	-1.2152600	3.0138070	1.2641750
H	1.0524530	-3.0784660	-2.6719390	H	-1.8518810	2.5955150	-0.3253440
H	0.8149590	-4.6421320	-1.8634790	C	-4.1529300	-0.4346390	-1.0500090
H	-0.4859380	-3.4332660	-1.8977750	H	-4.2735500	0.3226000	-1.8310510
C	-1.0804970	-3.1224440	0.9005480	H	-3.9974590	-1.3914050	-1.5581670
H	-1.5121050	-2.5738690	1.7409870	C	-1.6208260	-0.0156440	-1.0737910
H	-1.6650130	-2.9010910	0.0073070	C	-0.2025580	3.9815280	-0.3836700
H	-1.1861880	-4.1938210	1.1165960	H	0.6998780	4.2072670	0.1994050
C	3.8746910	-2.0349800	1.8722520	H	0.1457000	3.7219440	-1.3900670
H	4.0576490	-2.7784110	2.6584680	C	-5.8222420	-1.7146180	0.3671440
H	4.7531570	-2.0113160	1.2241210	H	-5.2696340	-2.6251550	0.1456050
H	3.7920470	-1.0569510	2.3570950	C	-6.9490520	-1.7724770	1.1888850
C	0.9861720	-1.9960280	3.1155440	H	-7.2658600	-2.7251080	1.6048410
H	1.5433600	-1.1145600	3.4453710	C	-1.0923870	5.2295370	-0.4401740

H	-1.9930630	5.0049320	-1.0280440	C	-0.5941700	-3.5756700	2.6493570
H	-1.4440160	5.4749690	0.5722610	C	-0.6920430	-3.8108950	1.2694720
C	-6.1325010	0.6565070	0.0992410	H	-0.2369310	-3.0611880	-0.6875810
H	-5.8222920	1.6062270	-0.3308070	H	0.1635010	-2.2492570	4.1914020
C	-7.2595330	0.6044840	0.9203020	H	-1.0566820	-4.2713010	3.3456830
H	-7.8194260	1.5126120	1.1264920	C	1.4248520	-0.3705040	2.6824340
C	-7.6716880	-0.6114980	1.4692810	O	1.3820550	0.1084000	3.8180360
H	-8.5512390	-0.6546230	2.1053070	Rh	1.4875610	-0.2947130	-0.2764660
C	-0.3812970	6.4449080	-1.0436060	N	2.2084880	0.0822850	1.6426610
H	-1.0403650	7.3190990	-1.0776790	C	3.8967610	1.2670880	2.7778510
H	-0.0466990	6.2372770	-2.0658500	O	2.7903240	1.3611040	1.8756560
H	0.5040510	6.7171480	-0.4575880	C	2.6224200	-1.7121530	-1.6775050
H	2.2079640	-0.5033560	-4.9438150	C	3.5433290	-0.8459670	-1.0093610
H	3.0564960	0.8153070	-4.0764480	C	3.3167910	0.5148600	-1.4750440
H	3.4557140	-0.8964910	-3.7209590	C	2.2128070	0.4833410	-2.3546950
C	2.7972750	2.2559290	4.3210320	C	1.7509370	-0.8950430	-2.4636550
H	3.4611560	1.5405870	4.8196340	C	4.6843170	-1.2898150	-0.1427280
H	3.2260830	3.2525000	4.4796880	H	5.5024570	-1.6822330	-0.7610710
H	1.8282810	2.2267200	4.8265790	H	5.0778450	-0.4607360	0.4465480
				H	4.3798030	-2.0759800	0.5522360
35'				C	4.1733670	1.6945120	-1.1184050
C	-0.1113820	-2.8921840	0.3770680	H	4.2292060	1.8251100	-0.0351610
C	0.5830670	-1.7723610	0.8417690	H	5.1920670	1.5629440	-1.5038340
C	0.6782830	-1.5728150	2.2257700	H	3.7759810	2.6176750	-1.5459480
C	0.0844860	-2.4586960	3.1281410	C	1.6196590	1.6307210	-3.1176010

H	0.5274930	1.6034630	-3.0881980	C	-1.7442900	0.0459360	-1.2381300
H	1.9432100	2.5936970	-2.7170950	C	0.8824830	3.6773150	0.4146840
H	1.9229560	1.5868290	-4.1714560	H	1.9149070	3.3675230	0.2230480
C	2.6540860	-3.2106050	-1.6395470	H	0.4257140	3.9124330	-0.5560520
H	3.3366740	-3.5904300	-2.4113590	C	-6.1326180	-0.5489600	0.3631100
H	3.0034960	-3.5813740	-0.6734340	H	-5.6678730	-1.5207290	0.5141510
H	1.6704630	-3.6449560	-1.8265820	C	-7.2814610	-0.2128020	1.0801060
C	0.7488360	-1.3897260	-3.4675680	H	-7.7042980	-0.9225240	1.7857040
H	0.2980860	-2.3340020	-3.1560090	C	0.8798490	4.9278370	1.3022080
H	-0.0587140	-0.6743150	-3.6242220	H	-0.1567770	5.2204820	1.5184630
H	1.2421070	-1.5595740	-4.4343660	H	1.3368010	4.6804630	2.2690850
F	-1.7464450	0.7386850	-2.4514090	C	-6.1903680	1.5905200	-0.7403060
F	-1.7243710	-1.2815450	-1.5947590	H	-5.7709980	2.2952690	-1.4548940
C	0.0401860	1.2948410	0.2215690	C	-7.3401390	1.9308560	-0.0259740
C	-0.5210910	0.4305790	-0.4952650	H	-7.8090830	2.8977470	-0.1864200
C	-3.0392730	0.3496540	-0.4944100	C	-7.8888970	1.0296590	0.8879430
H	-3.0381710	1.4143780	-0.2391380	H	-8.7849080	1.2916840	1.4432440
H	-3.0177420	-0.2066680	0.4478480	C	1.6217740	6.1091100	0.6690600
C	-5.5700270	0.3475830	-0.5559170	H	1.6063180	6.9871940	1.3227220
C	0.1281250	2.5027170	1.0673620	H	1.1673500	6.3976450	-0.2858870
H	0.6089570	2.2468900	2.0160870	H	2.6710150	5.8587420	0.4742430
H	-0.9038230	2.8098750	1.2930310	H	4.3478230	2.2641600	2.7864460
C	-4.3024330	-0.0046680	-1.3047480	H	3.5538040	0.9978010	3.7791070
H	-4.2703710	0.5284440	-2.2600190	H	4.6312630	0.5327490	2.4247720
H	-4.2857920	-1.0750890	-1.5335440	C	-1.3990230	-5.0406660	0.7462460

H	-2.2181090	-5.3433960	1.4062740	C	4.8268220	1.2175470	-0.1918860
H	-1.8135040	-4.8712810	-0.2525790	H	5.6576900	1.5760180	-0.8136410
H	-0.7120960	-5.8939170	0.6733210	H	4.6779420	1.9397050	0.6124540
TS36'				H	5.1298550	0.2716850	0.2626760
C	1.1606000	-2.7806600	-0.4182710	C	2.6887650	3.4989800	-0.6554950
C	1.1704750	-1.6444290	0.4123350	H	2.8395880	3.4677430	0.4268750
C	1.5438150	-1.8032910	1.7639810	H	3.5279550	4.0470590	-1.1029980
C	1.8242380	-3.0678130	2.2775630	H	1.7807670	4.0758830	-0.8449400
C	1.7924630	-4.1831350	1.4427900	C	0.4970070	2.3562070	-2.8037550
C	1.4746100	-4.0493880	0.0811140	H	-0.4265320	1.7698320	-2.7866550
H	0.8454450	-2.6883650	-1.4518420	H	0.2973280	3.3070480	-2.3077530
H	2.0911670	-3.1507060	3.3272940	H	0.7270300	2.5720430	-3.8550750
H	2.0245570	-5.1668410	1.8438450	C	4.0259610	-1.3178230	-1.9897270
C	1.6954400	-0.5719110	2.5934850	H	4.4939450	-1.3526240	-2.9818290
O	1.5628620	-0.5353170	3.8201490	H	4.8226590	-1.3926580	-1.2461290
Rh	1.5930690	0.3478630	-0.2522010	H	3.3962140	-2.2066190	-1.8864940
N	2.0705250	0.4587350	1.7731280	C	1.3216390	-0.5909270	-3.5246220
C	3.1268730	1.9215280	3.2930580	H	1.5701680	-1.6468890	-3.3981830
O	2.0418010	1.7459030	2.3763940	H	0.2340410	-0.4967210	-3.4909640
C	3.2368240	-0.0533360	-1.8186470	H	1.6519790	-0.2955460	-4.5297160
C	3.5850870	1.0662070	-1.0202270	F	-1.3817060	-1.6271740	-1.6061390
C	2.5879100	2.1117440	-1.2227600	F	-1.5395200	-2.6206680	0.3507320
C	1.6346000	1.6143050	-2.1642390	C	-0.2685580	0.7102840	0.5520190
C	1.9934320	0.2595140	-2.4839470	C	-0.3825920	-0.5367610	0.2215730
				C	-2.8984340	-0.7392970	-0.0122790

H	-2.9209010	0.2242770	-0.5288330	H	-8.8347880	0.7917150	0.3394240
H	-3.0005030	-0.5383110	1.0588570	C	-2.3056680	5.3916830	0.2033840
C	-5.4067110	-0.9705720	-0.2700500	H	-2.8109270	6.1754820	0.7767550
C	-0.9275550	1.8601970	1.2218240	H	-2.9647390	5.1102880	-0.6260020
H	-0.2591310	2.1946500	2.0252600	H	-1.3982890	5.8300400	-0.2282090
H	-1.8476400	1.4981660	1.7005830	H	3.0855020	2.9737320	3.5904090
C	-4.0624360	-1.6290440	-0.4936820	H	3.0030740	1.2747230	4.1641490
H	-3.9237510	-1.8470540	-1.5573240	H	4.0879820	1.7130360	2.8068320
H	-4.0170250	-2.5842520	0.0379090	C	1.4196030	-5.2637320	-0.8172230
C	-1.5335300	-1.3821640	-0.2424310	H	0.4871500	-5.8220360	-0.6674650
C	-1.2652310	3.0586470	0.3180520	H	1.4665390	-4.9843160	-1.8739540
H	-0.3395490	3.4438730	-0.1225220	H	2.2454000	-5.9526030	-0.6110500
H	-1.8974190	2.7291020	-0.5175320				
C	-6.0695320	-1.0950490	0.9589920	37'			
H	-5.6238520	-1.6978180	1.7471210	C	-0.5873810	-2.4634250	-0.6837860
C	-7.2945910	-0.4644790	1.1795630	C	-0.3746940	-1.1980290	-0.0816120
H	-7.7948440	-0.5771710	2.1374170	C	0.0068850	-1.1571730	1.2892340
C	-1.9735770	4.1829840	1.0838350	C	0.1776900	-2.3709070	1.9922510
H	-2.8970780	3.7913230	1.5310080	C	-0.0307850	-3.5899070	1.3720660
H	-1.3399110	4.5012770	1.9223040	C	-0.4303740	-3.6530450	0.0176720
C	-6.0051530	-0.1978280	-1.2743290	H	-0.9144450	-2.4867340	-1.7180280
H	-5.5089070	-0.0982420	-2.2372600	H	0.4474380	-2.3306600	3.0437180
C	-7.2308180	0.4344180	-1.0586930	H	0.0900220	-4.5111700	1.9373720
H	-7.6811670	1.0244310	-1.8522040	C	0.0767260	0.1732210	2.0410800
C	-7.8792870	0.3034820	0.1705100	O	-0.8489530	0.6068400	2.7228520

Rh	1.9862450	-0.1448740	0.0468630	C	2.8417480	-2.5527630	-2.1551000
N	1.3122580	0.6816630	1.8186680	H	2.2513600	-3.2957800	-1.6125930
C	1.6706730	2.1823650	3.5833730	H	2.2326780	-2.1809110	-2.9820200
O	1.5039900	2.0456850	2.1711580	H	3.7100320	-3.0702930	-2.5846140
C	3.7912870	-1.6372870	0.1135030	F	-2.0442290	1.5421150	-2.0369950
C	4.2051370	-0.3951580	0.6082470	F	-2.0709700	-0.5964550	-2.5531990
C	3.9277950	0.6162360	-0.4195340	C	0.4778310	0.8946570	-0.8613420
C	3.4648560	-0.0788870	-1.6078280	C	-0.5977960	0.0850470	-0.8350990
C	3.2857350	-1.4399770	-1.2514900	C	-3.1556410	0.0764950	-0.5570730
C	4.7892580	-0.0835930	1.9528480	H	-3.0404040	0.7318630	0.3124780
H	5.8530840	0.1703460	1.8636190	H	-3.1214850	-0.9502210	-0.1803220
H	4.2810330	0.7691600	2.4110090	C	-5.6884030	0.0446190	-0.3789350
H	4.7024480	-0.9296440	2.6378540	C	0.5958620	2.2908720	-1.4197520
C	4.3631180	2.0490330	-0.3296560	H	0.1421530	2.3368070	-2.4167900
H	4.1310450	2.4673880	0.6529330	H	1.6530470	2.5486280	-1.5394630
H	5.4463290	2.1358250	-0.4905540	C	-4.4992590	0.3342560	-1.2685740
H	3.8670410	2.6683990	-1.0797690	H	-4.5249390	1.3763560	-1.6032330
C	3.2825700	0.5140260	-2.9739770	H	-4.5441310	-0.2893060	-2.1670900
H	2.4982080	0.0009760	-3.5357160	C	-1.9542140	0.2877770	-1.4707470
H	3.0195040	1.5722760	-2.9279480	C	-0.0575360	3.3648360	-0.5217970
H	4.2145440	0.4303680	-3.5480320	H	-1.1300440	3.1561420	-0.4515620
C	3.8414000	-2.9691160	0.8013320	H	0.3519940	3.2835970	0.4902360
H	4.5773160	-3.6266080	0.3212820	C	-6.3448800	-1.1920180	-0.4363390
H	4.1198540	-2.8692740	1.8526030	H	-6.0081290	-1.9404470	-1.1503020
H	2.8722100	-3.4772570	0.7612020	C	-7.4252980	-1.4717680	0.4020770

H	-7.9232920	-2.4355210	0.3378900	C	-1.2644040	1.9358690	1.3647570
C	0.1526190	4.7854430	-1.0605560	C	-2.1439210	2.7665820	2.0706800
H	1.2301240	4.9907720	-1.1377560	C	-2.7556170	3.8580450	1.4607680
H	-0.2447190	4.8536360	-2.0830790	C	-2.4755550	4.1725550	0.1236980
C	-6.1452080	0.9974340	0.5425880	H	-1.3300320	3.6134640	-1.5972170
H	-5.6511730	1.9647400	0.5987850	H	-2.3324790	2.5531270	3.1190970
C	-7.2238180	0.7225000	1.3835350	H	-3.4417610	4.4811190	2.0297710
H	-7.5631340	1.4756480	2.0893800	C	-0.5675890	0.8383970	2.1486140
C	-7.8682160	-0.5145790	1.3161950	O	0.1846340	1.1259890	3.0803180
H	-8.7101890	-0.7288630	1.9683170	Rh	-1.4477220	-1.1329580	-0.0454850
C	-0.5055710	5.8571190	-0.1852230	N	-0.9477050	-0.4299890	1.8052880
H	-0.3420220	6.8624660	-0.5882280	C	-0.5751710	-1.8278030	3.6574100
H	-0.1033640	5.8352260	0.8339500	O	-0.0927670	-1.4287550	2.3766190
H	-1.5875500	5.6981220	-0.1146530	C	-3.4560260	-0.6127210	-0.4849490
H	1.8952900	3.2400420	3.7486380	C	-3.5975580	-1.8125450	0.3425940
H	0.7535910	1.9087040	4.1123080	C	-2.9421830	-2.8565910	-0.3216560
H	2.5069610	1.5678480	3.9429610	C	-2.4543980	-2.3594980	-1.6214410
C	-0.7061380	-4.9880800	-0.6328020	C	-2.8359220	-1.0061190	-1.7484070
H	-0.8967190	-4.8797490	-1.7037130	C	-4.2806910	-1.8394140	1.6768210
H	0.1356850	-5.6780510	-0.5049380	H	-5.3631460	-1.7042480	1.5607650
H	-1.5834620	-5.4696550	-0.1846490	H	-4.1181380	-2.7873940	2.1947780
38				H	-3.9102130	-1.0380670	2.3229030
C	-1.5687000	3.3620700	-0.5664240	C	-2.7395540	-4.2643570	0.1540770
C	-0.9566630	2.2390630	0.0194160	H	-3.0036400	-4.3793800	1.2071770
				H	-3.3566820	-4.9608330	-0.4274890

H	-1.6973890	-4.5766090	0.0333890	H	3.1924080	-2.6682790	-0.6933210
C	-1.7698700	-3.2109110	-2.6497540	H	3.6878230	-1.5873340	-1.9908510
H	-1.2264040	-2.6016900	-3.3746240	C	1.1698700	-0.7839110	-1.1587460
H	-1.0510680	-3.8929680	-2.1885230	C	2.0233510	3.1304280	-0.4842080
H	-2.5012400	-3.8195020	-3.1977390	H	1.3800330	3.8063100	0.0922230
C	-4.1662540	0.6798130	-0.2286310	H	2.5148740	2.4832840	0.2536270
H	-3.6980080	1.5116850	-0.7560870	C	5.9356510	-0.7586900	-0.8592020
H	-5.2080460	0.6012480	-0.5702730	H	5.7864180	-0.3913970	-1.8721220
H	-4.1787120	0.9263610	0.8343150	C	7.1567390	-0.5428760	-0.2175260
C	-2.6645430	-0.1134120	-2.9403630	H	7.9501260	-0.0079980	-0.7325210
H	-2.3893990	0.8990630	-2.6361540	C	3.0807000	3.9470640	-1.2382690
H	-1.8837200	-0.4833720	-3.6080490	H	3.7231210	3.2667670	-1.8147180
H	-3.5998970	-0.0547260	-3.5116680	H	2.5823860	4.5903530	-1.9771070
F	0.7475200	-2.1236000	-0.8978840	C	5.1151560	-1.9213520	1.0824250
F	1.3530280	-0.7562860	-2.5324330	H	4.3221600	-2.4631860	1.5930300
C	0.0754900	1.4498170	-0.7226180	C	6.3329820	-1.7073390	1.7280780
C	0.0298120	0.1019060	-0.7189650	H	6.4819230	-2.0821890	2.7369640
C	2.5091810	-0.6316050	-0.4502080	C	7.3591170	-1.0167600	1.0793540
H	2.3197970	-0.7208560	0.6239340	H	8.3088480	-0.8517980	1.5802020
H	2.8815950	0.3803410	-0.6219670	C	3.9484410	4.8066600	-0.3133450
C	4.8979340	-1.4496820	-0.2201320	H	4.6934870	5.3769770	-0.8782290
C	1.1524610	2.2736530	-1.4229640	H	4.4840210	4.1869260	0.4143390
H	0.6592390	2.9458960	-2.1397250	H	3.3378100	5.5213580	0.2499580
H	1.7818040	1.6219820	-2.0346790	H	-0.5344910	-0.9877590	4.3568580
C	3.5649340	-1.6610750	-0.9056320	H	-1.5990660	-2.2184260	3.5916640

H	0.0983610	-2.6217990	3.9932090	C	-1.7721660	-2.7445480	-1.6158210
C	-3.1056230	5.3766300	-0.5376010	C	-2.6029700	-1.5839250	-1.5668520
H	-2.6456820	6.3081550	-0.1850700	C	-3.0352190	-2.8706790	1.9618570
H	-2.9892280	5.3447540	-1.6248040	H	-4.0701060	-3.2323140	2.0135940
H	-4.1757140	5.4434300	-0.3140040	H	-2.3922650	-3.6301830	2.4113080
TS39				H	-2.9625280	-1.9672990	2.5724280
C	-2.5674590	2.9243950	-0.5386670	C	-1.0151140	-4.5838980	0.0647470
C	-1.5931260	2.0512830	-0.0191420	H	-1.1852300	-4.8854420	1.1001610
C	-1.6930440	1.6414650	1.3269540	H	-1.2679990	-5.4303120	-0.5841820
C	-2.7394530	2.1515760	2.1089010	H	0.0527110	-4.3650330	-0.0574250
C	-3.7058720	2.9939490	1.5706210	C	-1.0456840	-3.3045850	-2.8025690
C	-3.6393640	3.3903770	0.2264780	H	-0.8977020	-2.5482340	-3.5765270
H	-2.4862290	3.2500350	-1.5729550	H	-0.0608530	-3.6798000	-2.5125760
H	-2.7680710	1.8909440	3.1626450	H	-1.6069720	-4.1358730	-3.2487660
H	-4.5109690	3.3636160	2.2015800	C	-4.1862660	-0.4914940	0.2145090
C	-0.6252370	0.8499040	2.0614940	H	-4.1085660	0.4682250	-0.2989550
O	-0.0650250	1.3904040	3.0226810	H	-5.1805320	-0.9091750	0.0031360
Rh	-0.9200930	-1.3526380	-0.1422170	H	-4.1284520	-0.2939980	1.2859210
N	-0.4318130	-0.4357010	1.6610570	C	-2.9298880	-0.6752230	-2.7140580
C	0.3372720	-1.5648890	3.5662060	H	-3.0521730	0.3575880	-2.3809800
O	0.6951490	-1.0187100	2.3023590	H	-2.1505330	-0.6955580	-3.4789270
C	-3.1205770	-1.4488790	-0.2263810	H	-3.8701940	-0.9894290	-3.1852410
C	-2.6523800	-2.5893850	0.5399390	F	1.0013220	-2.1079250	-0.3068700
C	-1.8153970	-3.3721590	-0.3018260	F	1.2375730	-0.8220080	-2.5297250
				C	-0.4168840	1.6654120	-0.8479960

C	-0.0101550	0.3873960	-0.9545740	H	6.1991760	-0.8151580	2.8332910
C	2.5140610	0.0449080	-0.7116600	C	7.2709940	-0.1118500	1.0982470
H	2.3352030	0.0693270	0.3663220	H	8.1843430	0.1017580	1.6462490
H	2.8179340	1.0672920	-0.9940970	C	2.3168980	5.9656800	-0.3472890
C	4.9046330	-0.6693990	-0.3206980	H	2.8202970	6.7720380	-0.8906940
C	0.3204100	2.7995220	-1.5498800	H	3.0609190	5.4786640	0.2927250
H	-0.3766830	3.3328110	-2.2111270	H	1.5670570	6.4216180	0.3087730
H	1.0919320	2.3832590	-2.2081480	H	-0.0176560	-0.7822690	4.2441690
C	3.6226490	-0.9603160	-1.0722740	H	-0.4216410	-2.3513600	3.4598310
H	3.2471580	-1.9554770	-0.8232620	H	1.2561900	-2.0056220	3.9643700
H	3.8099330	-0.9362590	-2.1506730	C	-4.6846550	4.3079150	-0.3638210
C	1.1952400	-0.1701910	-1.3702470	H	-4.7727780	5.2347180	0.2142970
C	0.9548010	3.8166190	-0.5810520	H	-4.4435990	4.5792740	-1.3954990
H	0.1785020	4.2281860	0.0746330	H	-5.6752240	3.8376270	-0.3658690
H	1.6619850	3.2958600	0.0774110				
C	6.0282260	-0.1515130	-0.9761650	40			
H	5.9839150	0.0320470	-2.0474810	C	-0.6974710	1.8990730	1.7350750
C	7.2043270	0.1245180	-0.2750330	C	0.2947160	1.7095730	0.7663480
H	8.0668630	0.5224890	-0.8027190	C	1.5365830	2.3566900	0.9094330
C	1.6729100	4.9610550	-1.3080870	C	1.7411560	3.2082870	1.9967170
H	2.4431020	4.5463250	-1.9734400	C	0.7455220	3.3897680	2.9555140
H	0.9575030	5.4815970	-1.9597510	C	-0.4888790	2.7355360	2.8411830
C	4.9841120	-0.9039490	1.0605860	H	-1.6554070	1.3987860	1.6145650
H	4.1197720	-1.3057110	1.5843680	H	2.6920010	3.7270820	2.0699250
C	6.1557560	-0.6268110	1.7641310	C	2.6164920	2.2170770	-0.1288580

O	3.3432470	3.1775240	-0.3959200	H	0.1156730	-4.2818300	-0.1457410
Rh	1.6135010	-0.7731040	-0.3150920	C	3.9819860	-2.9892540	-1.0361360
N	2.7250720	0.9820200	-0.7268810	H	3.5392650	-2.8265730	-2.0244880
C	4.6481550	0.7053410	-2.0395770	H	4.9688100	-2.5232010	-1.0215630
O	3.2840860	1.0956250	-2.0058410	H	4.1186830	-4.0687490	-0.9011820
C	1.7418480	-2.9267100	0.2740930	F	-1.3920620	-2.5175400	-0.6984020
C	1.2153170	-2.2053330	1.3943670	F	1.4684260	-1.0765910	-2.2787550
C	2.1962720	-1.2361230	1.8128800	C	0.0433620	0.8877830	-0.4598820
C	3.3751440	-1.4402020	1.0083840	C	-0.4851060	-0.3842710	-0.4062260
C	3.0850870	-2.4395630	0.0322210	C	-2.9869480	-0.7686950	-0.6392170
C	-0.0614560	-2.4899720	2.1258640	H	-3.3821610	-1.0373950	-1.6282430
H	0.1499350	-3.1591310	2.9702930	H	-3.0726780	0.3163230	-0.5446280
H	-0.5008920	-1.5764890	2.5323040	C	-5.3147220	-1.1195750	0.3240230
H	-0.7968120	-2.9709140	1.4829420	C	0.0584240	1.6147450	-1.8091320
C	2.1186320	-0.3734280	3.0378540	H	0.3500010	0.8991070	-2.5808450
H	1.1064920	0.0025230	3.2027950	H	0.8143700	2.4030510	-1.7941230
H	2.4178440	-0.9395690	3.9304160	C	-3.8469130	-1.4661690	0.4442460
H	2.7767220	0.4933100	2.9545460	H	-3.7091940	-2.5483590	0.3545120
C	4.6691550	-0.7178580	1.2143590	H	-3.4727420	-1.1768960	1.4337590
H	5.4420600	-1.0673960	0.5280510	C	-1.5387230	-1.1591470	-0.5823510
H	4.5489010	0.3586450	1.0610110	C	-1.3070270	2.2480760	-2.1383290
H	5.0250350	-0.8793940	2.2384120	H	-2.0611910	1.4613370	-2.2635080
C	1.1396300	-4.0873040	-0.4605290	H	-1.6421970	2.8793360	-1.3030500
H	1.1305110	-3.8972420	-1.5377960	C	-5.8500130	-0.0115290	0.9946340
H	1.7336300	-4.9925220	-0.2818240	H	-5.2069720	0.5855690	1.6376740

C	-7.1958320	0.3303300	0.8549660	C	-1.2041630	1.7179280	1.7234920
H	-7.5926090	1.1905990	1.3868600	C	-0.0787520	1.6273790	0.8950030
C	-1.2500670	3.0942430	-3.4181280	C	1.1396240	2.1775670	1.3167640
H	-0.5016590	3.8872920	-3.2915500	C	1.2094570	2.8491580	2.5395680
H	-0.8931570	2.4676330	-4.2459310	C	0.0815750	2.9508060	3.3480530
C	-6.1649780	-1.8792820	-0.4914220	C	-1.1424160	2.3869210	2.9527820
H	-5.7684450	-2.7465460	-1.0145850	H	-2.1439160	1.2766390	1.4019550
C	-7.5112300	-1.5412510	-0.6347600	H	2.1583870	3.2894310	2.8299270
H	-8.1547260	-2.1451230	-1.2685000	C	2.3199290	2.1017720	0.4048260
C	-8.0311190	-0.4339820	0.0382660	O	3.2549330	2.9044030	0.4815410
H	-9.0794570	-0.1712450	-0.0698040	Rh	1.5945800	-0.9404850	-0.2974400
C	-2.6005440	3.7160690	-3.7869480	N	2.1855560	1.1278370	-0.5555500
H	-2.5262090	4.3167560	-4.6993830	C	4.0923490	0.9070770	-1.9356430
H	-2.9680010	4.3704150	-2.9878450	O	2.8043170	1.4868860	-1.7537920
H	-3.3604930	2.9448680	-3.9583290	C	1.8346680	-3.0771930	0.0892110
H	5.2537070	1.3451550	-1.3879390	C	1.2825740	-2.4789070	1.2696680
H	4.7723380	-0.3478040	-1.7628010	C	2.2134340	-1.4971080	1.7585110
H	4.9595770	0.8381240	-3.0789500	C	3.3955200	-1.5571750	0.9209940
H	0.9247100	4.0500160	3.8005730	C	3.1599010	-2.5084770	-0.1106200
C	-1.5854120	2.9605010	3.8558050	C	0.0028440	-2.8701750	1.9469110
H	-2.2055400	3.8231980	3.5815470	H	0.1984830	-3.6835230	2.6577950
H	-2.2495310	2.0938420	3.9294470	H	-0.4240760	-2.0364940	2.5085170
H	-1.1754310	3.1602870	4.8503440	H	-0.7396870	-3.2149010	1.2282710
				C	2.0983480	-0.7376770	3.0480450
				H	1.0636780	-0.4622950	3.2649140
TS41							

H	2.4652650	-1.3458870	3.8861210	C	-3.8564540	-1.4693050	0.1190440
H	2.6842000	0.1833540	3.0270500	H	-3.7267870	-2.5543810	0.0520190
C	4.6367860	-0.7496140	1.1551910	H	-3.5277720	-1.1703920	1.1216440
H	5.3483330	-0.8512840	0.3342000	C	-1.4871650	-1.1786070	-0.7740000
H	4.4115840	0.3147430	1.2696750	C	0.0109890	3.2365130	-1.7201530
H	5.1340180	-1.0858070	2.0734970	H	-0.5712390	3.7420620	-0.9383120
C	1.2696890	-4.2012090	-0.7279090	H	1.0677320	3.3938520	-1.4864970
H	1.3431580	-3.9768470	-1.7956160	C	-5.8742210	-0.0068340	0.5865050
H	1.8243910	-5.1290580	-0.5363290	H	-5.2632620	0.5688500	1.2786940
H	0.2193340	-4.3769390	-0.4979990	C	-7.2067430	0.3526870	0.3792660
C	4.0739750	-2.9131910	-1.2276890	H	-7.6248130	1.2051650	0.9074590
H	3.5820310	-2.7623110	-2.1941920	C	-0.2959660	3.8827450	-3.0788900
H	5.0025200	-2.3388550	-1.2239560	H	0.2840590	3.3693850	-3.8568540
H	4.3347330	-3.9749690	-1.1421780	H	-1.3542970	3.7258410	-3.3313140
F	-1.3230420	-2.5342320	-0.9212800	C	-6.1218780	-1.8380120	-0.9561240
F	1.5237560	-1.0042000	-2.2995120	H	-5.7046310	-2.6978260	-1.4754130
C	-0.1730990	0.9530220	-0.4374130	C	-7.4545400	-1.4824970	-1.1672890
C	-0.4461820	-0.4137780	-0.4837460	H	-8.0670630	-2.0655960	-1.8493340
C	-2.9308670	-0.8014680	-0.9296170	C	-8.0015460	-0.3846820	-0.4999960
H	-3.2636570	-1.1020960	-1.9321040	H	-9.0396930	-0.1087820	-0.6608480
H	-3.0312480	0.2866910	-0.8740130	C	0.0207090	5.3810740	-3.1095190
C	-5.3116880	-1.1056110	-0.0771160	H	-0.1997280	5.8157450	-4.0900900
C	-0.3050840	1.7385810	-1.7304320	H	1.0789260	5.5633750	-2.8925740
H	-1.3540070	1.5876050	-2.0378030	H	-0.5682290	5.9269720	-2.3632730
H	0.2992080	1.2139720	-2.4789750	H	4.8021140	1.3137650	-1.2076070

H	4.0417320	-0.1829660	-1.8705580	C	2.7701640	-0.9799350	1.4221790
H	4.3914820	1.1904990	-2.9477500	C	3.5468790	-0.8052060	0.2041620
H	0.1445150	3.4732720	4.2995160	C	3.7213530	-2.1198820	-0.4146990
C	-2.3719380	2.5267850	3.8190910	C	1.4939760	-2.9864550	2.5020430
H	-3.1173350	1.7603510	3.5873540	H	0.8923530	-2.2540750	3.0444020
H	-2.1228460	2.4475900	4.8819050	H	0.8154580	-3.7280330	2.0722530
H	-2.8490390	3.5036300	3.6712500	H	2.1332230	-3.5035200	3.2299890
				C	2.5917770	0.0290090	2.5145560
42				H	1.6305380	-0.0811310	3.0192970
C	-0.5869950	1.7739080	2.1232540	H	3.3831050	-0.1013720	3.2652310
C	0.0985840	1.9933200	0.9331480	H	2.6535070	1.0511450	2.1415980
C	1.1405410	2.9181470	0.8801560	C	4.2912310	0.4278010	-0.2075720
C	1.5135730	3.6561320	2.0017800	H	4.4048080	0.4764840	-1.2925280
C	0.8171760	3.4420460	3.1903580	H	3.7894330	1.3406390	0.1141660
C	-0.2359860	2.5092740	3.2667510	H	5.2971060	0.4210900	0.2348650
H	-1.3919810	1.0444200	2.1718050	C	2.7442340	-4.4957450	0.0120360
H	2.3212640	4.3791350	1.9363150	H	3.0589310	-4.7409750	-1.0039440
C	1.6727180	2.9797250	-0.5037270	H	3.3144880	-5.1235300	0.7084770
O	2.5200930	3.7269060	-0.9687020	H	1.6902730	-4.7734600	0.1085210
Rh	1.6137990	-1.4051300	-0.3823890	C	4.4565660	-2.3651950	-1.6995970
N	1.0201700	1.9537600	-1.1811660	H	5.4072280	-1.8237120	-1.7159570
C	1.9548230	1.4398070	-3.2723470	H	4.6712990	-3.4272480	-1.8374450
O	0.8825600	2.0892290	-2.5606870	H	3.8497450	-2.0299840	-2.5487830
C	2.9532340	-3.0426490	0.3178320	F	-0.6020540	-2.3594170	-0.4421160
C	2.3295970	-2.3320630	1.4426790	F	1.3938210	-1.4616500	-2.3506180

C	-0.0754300	-0.1346810	-0.4111550	H	-7.0032300	-4.1604150	-0.9302200
C	-2.5633940	-1.0881900	-0.6837820	C	-7.5253690	-2.2062500	-0.1823250
H	-2.7592110	-1.7117430	-1.5660380	H	-8.5886060	-2.3272920	-0.3688300
H	-2.9889340	-0.1084310	-0.8940350	C	-2.9479960	5.4549800	-2.0291170
C	-4.7688050	-1.8955760	0.3089040	H	-3.9196360	5.7519740	-2.4377940
C	-1.4666620	1.9617770	-1.0514450	H	-2.1746570	5.7912440	-2.7286180
H	-2.2843980	1.6712320	-0.3842800	H	-2.8012480	5.9997070	-1.0893890
H	-1.6326850	1.4686520	-2.0139940	H	2.9092670	1.9089320	-3.0146380
C	-3.2843420	-1.7169750	0.5383560	H	1.9484440	0.3659780	-3.0712630
H	-2.8205740	-2.6839800	0.7560960	H	1.7295770	1.6315740	-4.3247030
H	-3.1163360	-1.0773960	1.4136380	H	1.0849890	4.0068390	4.0799240
C	-1.0809600	-0.9988330	-0.5075780	C	-0.9987880	2.3295530	4.5589050
C	-1.5189340	3.4834990	-1.2465890	H	-1.4844500	1.3504980	4.6063260
H	-1.3389000	3.9944220	-0.2921790	H	-0.3425710	2.4274020	5.4292590
H	-0.7228980	3.7942600	-1.9311890	H	-1.7844720	3.0887290	4.6605080
C	-5.6744370	-0.8722770	0.6210870	C	-0.1485430	1.3873320	-0.4475100
H	-5.3051170	0.0501730	1.0641440				
C	-7.0404870	-1.0233770	0.3787520	49			
H	-7.7262410	-0.2194960	0.6320000	C	-2.2653640	2.1208260	-2.0618790
C	-2.8724130	3.9405730	-1.8101540	C	-1.9524390	1.5562490	-0.8121320
H	-3.0611060	3.4247880	-2.7614230	C	-2.9971560	0.9971740	-0.0471570
H	-3.6778390	3.6288070	-1.1302770	C	-4.3084370	1.0474250	-0.5412370
C	-5.2698390	-3.0780420	-0.2532290	C	-4.5901660	1.5874020	-1.7916540
H	-4.5823600	-3.8849860	-0.4967510	C	-3.5641710	2.1325090	-2.5777760
C	-6.6348590	-3.2342670	-0.4976360	H	-1.4661810	2.5644120	-2.6515870

H	-5.1118960	0.6690390	0.0842170	C	-2.4524610	-1.6244890	-2.3787490
H	-5.6151420	1.6034080	-2.1552130	H	-2.6384450	-2.3055460	-3.2212600
C	-2.8157310	0.4759360	1.3648410	H	-3.3973870	-1.4695610	-1.8555370
O	-3.4245090	1.0034400	2.2980500	H	-2.1397790	-0.6609110	-2.7834390
Rh	-0.5714200	-1.3933560	0.2840130	C	0.6987020	-1.3748740	-2.7922740
N	-2.0587240	-0.6546270	1.4631100	H	0.2356050	-0.3934850	-2.9193320
C	-2.7403060	-1.7617480	3.4239550	H	1.7609450	-1.2196650	-2.5906710
O	-1.7143910	-0.9859310	2.8077820	H	0.6166790	-1.9114670	-3.7462590
C	-1.4112710	-2.2119530	-1.4764340	F	1.3929300	1.5782950	1.8984490
C	-1.6696410	-3.2525990	-0.4761570	F	1.3512280	-0.6256620	1.7410140
C	-0.4320160	-3.6840030	0.0135460	C	-0.5602780	1.6442170	-0.2684140
C	0.6328350	-2.9933650	-0.7356090	C	0.0657330	0.5425050	0.1867800
C	0.0304200	-2.1553020	-1.6995680	C	2.6624080	0.5914710	0.1699550
C	-3.0411510	-3.6891360	-0.0594140	H	2.6549840	1.4811120	-0.4683480
H	-3.5464820	-4.2056490	-0.8845940	H	2.6584030	-0.2730160	-0.4991240
H	-3.0067530	-4.3731260	0.7913010	C	5.1941240	0.5556390	0.2247250
H	-3.6536230	-2.8289830	0.2257670	C	0.0056670	3.0595530	-0.1909950
C	-0.1672940	-4.6844860	1.0995290	H	-0.1182250	3.5464070	-1.1680830
H	0.5709970	-4.3078330	1.8145700	H	1.0794700	3.0389220	0.0101850
H	-1.0745890	-4.9275590	1.6559690	C	3.9274620	0.5838490	1.0525520
H	0.2312280	-5.6171570	0.6802280	H	3.9126990	1.4714370	1.6927230
C	2.0939020	-3.2850600	-0.5582330	H	3.8947750	-0.2860480	1.7157870
H	2.7201160	-2.5615830	-1.0839530	C	1.3589380	0.5752700	0.9565630
H	2.3803230	-3.2754360	0.4975310	C	-0.6807500	3.9279950	0.8819490
H	2.3357350	-4.2802390	-0.9535790	H	-1.7638560	3.9372800	0.7083440

H	-0.5280560	3.4584720	1.8604980				
C	5.8447340	-0.6539060	-0.0543210	TS39'			
H	5.4521340	-1.5783330	0.3637940	C	3.2395730	1.3632160	1.8868360
C	6.9942840	-0.6859470	-0.8459280	C	2.5382600	1.0033080	0.7200750
H	7.4872580	-1.6337700	-1.0443320	C	3.1457830	0.1188110	-0.1947230
C	-0.1536440	5.3679380	0.9095500	C	4.4336160	-0.3601810	0.0911660
H	0.9326980	5.3547750	1.0760910	C	5.0920990	-0.0250780	1.2692940
H	-0.3044440	5.8311420	-0.0759570	C	4.5009070	0.8505600	2.1927720
C	5.7295260	1.7365870	-0.3091520	H	2.7766920	2.0534640	2.5876550
H	5.2451000	2.6865700	-0.0944930	H	4.9250880	-0.9798880	-0.6525240
C	6.8775430	1.7100030	-1.1015980	H	6.0851620	-0.4237800	1.4640130
H	7.2789840	2.6371460	-1.5013390	C	2.6201810	-0.1846640	-1.5867950
C	7.5138470	0.4970520	-1.3738870	O	3.3536830	0.0931160	-2.5444260
H	8.4101720	0.4753030	-1.9870610	Rh	-0.0074260	-1.2220460	-0.2418790
C	-0.8232600	6.2284880	1.9860180	N	1.4227980	-0.8134570	-1.6767740
H	-0.4297390	7.2506800	1.9853370	C	1.5437110	-2.0175930	-3.6806590
H	-0.6602870	5.8078640	2.9845130	O	0.9584900	-0.9097040	-3.0071560
H	-1.9059780	6.2868800	1.8276870	C	0.7182160	-2.1965610	1.6082660
H	-2.3725910	-1.9851230	4.4295800	C	0.9572390	-3.0855360	0.5066320
H	-3.6665180	-1.1839890	3.4876040	C	-0.3040220	-3.4061730	-0.0972130
H	-2.9109910	-2.7007760	2.8809660	C	-1.3396400	-2.7509690	0.6812340
C	-3.8647160	2.7414570	-3.9278690	C	-0.7210160	-2.0159330	1.7270530
H	-4.4150280	2.0438250	-4.5693840	C	2.2926220	-3.6261530	0.0932360
H	-4.4845410	3.6406630	-3.8287560	H	2.4942120	-4.5668290	0.6219990
H	-2.9482510	3.0275060	-4.4517540	H	2.3297550	-3.8261340	-0.9791320

H	3.0973170	-2.9278320	0.3291620	C	1.1317900	3.1369860	0.5574440
C	-0.5672140	-4.3351470	-1.2448720	H	1.5429830	3.4640000	1.5212020
H	-1.2621660	-3.8880600	-1.9623400	H	0.0832560	3.4557200	0.5469110
H	0.3515850	-4.5840060	-1.7793050	C	-3.6082880	1.2547250	-0.8745350
H	-1.0108100	-5.2755200	-0.8913460	H	-3.5266830	2.1080150	-1.5554650
C	-2.7989890	-2.8334730	0.3504110	H	-3.5017020	0.3491610	-1.4730830
H	-3.4110920	-2.2774120	1.0637740	C	-1.0640400	1.3001610	-0.4815660
H	-2.9706600	-2.4157770	-0.6476070	C	1.8956740	3.8532100	-0.5759890
H	-3.1382300	-3.8756130	0.3542240	H	2.9394940	3.5171520	-0.5805110
C	1.7234030	-1.7601750	2.6313120	H	1.4691400	3.5455900	-1.5384930
H	1.7425920	-2.4722300	3.4680390	C	-5.6739370	0.1082690	0.0428110
H	2.7298120	-1.7046960	2.2143990	H	-5.2880000	-0.8297580	-0.3483830
H	1.4824520	-0.7761080	3.0383230	C	-6.8940380	0.1290010	0.7217930
C	-1.3956270	-1.2665950	2.8386200	H	-7.4495870	-0.7942750	0.8619630
H	-0.9069200	-0.3074760	3.0315820	C	1.8456370	5.3813340	-0.4503000
H	-2.4484540	-1.0734710	2.6205010	H	0.7975400	5.7114670	-0.4318710
H	-1.3562780	-1.8473670	3.7691430	H	2.2762410	5.6813080	0.5152180
F	-1.0109800	1.9288820	-1.6500020	C	-5.4684990	2.4890710	0.3324030
F	-1.4830430	-0.7173100	-1.5754510	H	-4.9233240	3.4168670	0.1712900
C	1.2137540	1.6204530	0.4403750	C	-6.6864300	2.5150560	1.0124220
C	0.1360240	0.8948510	0.0797710	H	-7.0796200	3.4585680	1.3808070
C	-2.4290590	1.2956780	0.1208560	C	-7.4031070	1.3327960	1.2110550
H	-2.4788560	2.2319950	0.7031450	H	-8.3536550	1.3516390	1.7363720
H	-2.4885260	0.4863000	0.8480280	C	2.5857680	6.0956690	-1.5857960
C	-4.9419220	1.2860170	-0.1599330	H	2.5338070	7.1837510	-1.4741420

H	2.1561750	5.8383260	-2.5601840	C	-0.9024990	-2.6851490	0.6596240
H	3.6437070	5.8117940	-1.6078600	C	-0.3806450	-1.9515560	1.7602720
H	1.0922830	-2.0221170	-4.6768890	C	1.0706860	-2.0088060	1.6954320
H	2.6278890	-1.8946880	-3.7658810	C	1.4227720	-2.8388170	0.5881740
H	1.3033960	-2.9628430	-3.1751880	C	0.2108640	-3.2168990	-0.0959600
C	5.2164110	1.2324350	3.4674380	C	-1.1409510	-1.3727560	2.9154410
H	5.3796010	0.3602870	4.1117080	H	-0.9538360	-1.9794050	3.8103110
H	6.2020250	1.6629380	3.2569150	H	-0.8275610	-0.3500360	3.1373610
H	4.6467170	1.9681220	4.0421470	H	-2.2165650	-1.3675700	2.7376330
				C	2.0012890	-1.4979690	2.7539810
40'				H	1.6119740	-0.5918580	3.2224550
C	2.5839210	1.8146170	1.7694770	H	2.1349420	-2.2518110	3.5416850
C	2.3180050	1.1560560	0.5646790	H	2.9848750	-1.2584850	2.3453890
C	3.3509970	0.4735850	-0.1044970	C	2.8098420	-3.2898320	0.2495400
C	4.6348270	0.4792070	0.4430540	H	2.9139030	-3.5264340	-0.8093820
C	4.8883590	1.1291320	1.6519540	H	3.5515100	-2.5274260	0.4952110
C	3.8690940	1.8095600	2.3315820	H	3.0504480	-4.1914430	0.8281090
H	1.7779380	2.3522820	2.2635230	C	-2.3354860	-2.8961410	0.2758740
H	5.4302100	-0.0211600	-0.1008840	H	-2.5369600	-2.4079090	-0.6843950
C	3.1163680	-0.1743200	-1.4449390	H	-2.5483220	-3.9652530	0.1642810
O	3.9887550	-0.1046980	-2.3189360	H	-3.0255970	-2.4932850	1.0193990
Rh	0.3613280	-1.0121100	-0.1958910	C	0.0584460	-4.1492640	-1.2622880
N	1.9180810	-0.8143800	-1.5976180	H	-0.4752820	-3.6685720	-2.0876440
C	2.2039510	-2.1437450	-3.5268890	H	1.0260100	-4.4896170	-1.6338420
O	1.5631240	-1.0110730	-2.9425800	H	-0.5126470	-5.0379520	-0.9659210

F	-1.3805450	2.7618460	1.3197040	C	-6.0566180	1.4459210	0.9118830
F	-0.9588410	-0.6296230	-1.6393930	H	-5.8107450	2.2526890	1.5990090
C	0.9737960	1.2363430	-0.0820090	C	-7.3291070	0.8734620	0.9442930
C	-0.2149460	0.9393680	0.5371660	H	-8.0660070	1.2345680	1.6565850
C	-2.7477400	0.8583320	0.9668780	C	-7.6573080	-0.1544390	0.0581820
H	-3.1609450	0.9267690	1.9819380	H	-8.6489200	-0.5975930	0.0783940
H	-2.6935450	-0.1926500	0.6874740	C	0.6582390	5.8316200	-2.2315620
C	-5.0908820	1.0034310	-0.0028410	H	0.6426300	6.3791150	-3.1797300
C	0.8942840	2.0000520	-1.4070130	H	1.5086070	6.2023890	-1.6476050
H	0.0296000	1.6382720	-1.9676350	H	-0.2556200	6.0882460	-1.6834950
H	1.7824480	1.8020960	-2.0119980	H	3.2852640	-1.9925530	-3.5746590
C	-3.6993580	1.5959460	-0.0128350	H	1.9689760	-3.0636650	-2.9797570
H	-3.7346250	2.6548630	0.2622350	H	1.7873020	-2.2141930	-4.5354080
H	-3.2702200	1.5313760	-1.0179140	H	5.8930180	1.1185190	2.0676420
C	-1.3759000	1.4402480	0.9259080	C	4.1524950	2.5548830	3.6147040
C	0.7865800	3.5185490	-1.1533210	H	4.4188010	3.5998330	3.4123170
H	-0.1165880	3.7303080	-0.5700400	H	3.2798720	2.5663550	4.2750360
H	1.6378300	3.8508270	-0.5431320	H	4.9879660	2.1070570	4.1609990
C	-5.4337640	-0.0279160	-0.8887750				
H	-4.6983850	-0.3721780	-1.6124240	TS41'			
C	-6.7054890	-0.6026830	-0.8599620	C	2.4349490	1.6044910	2.1716970
H	-6.9551950	-1.3953600	-1.5600320	C	2.2816330	1.0313580	0.9034110
C	0.7613960	4.3204440	-2.4614350	C	3.2958330	0.2240940	0.3686040
H	1.6673290	4.0972200	-3.0402050	C	4.4751590	0.0373860	1.0927430
H	-0.0838790	3.9825860	-3.0757590	C	4.6299180	0.6237950	2.3466750

C	3.6129450	1.4133570	2.9067820	H	2.4090170	-4.6232610	0.0916260
H	1.6365200	2.2232260	2.5739550	C	-2.8389630	-2.5176410	0.3699310
H	5.2613640	-0.5654400	0.6485500	H	-3.1392510	-2.0626170	-0.5787490
C	3.1294130	-0.3524030	-1.0028770	H	-3.2323070	-3.5418690	0.3855510
O	4.1085800	-0.6202500	-1.7080270	H	-3.3225010	-1.9698250	1.1803780
Rh	0.1003320	-1.0436220	-0.2437310	C	-0.9362720	-3.8596780	-1.6891030
N	1.8198490	-0.4541870	-1.3976960	H	-1.5195190	-3.1625650	-2.2991370
C	1.6038200	-1.5854140	-3.4567120	H	-0.1090050	-4.2330960	-2.2953540
O	1.6735640	-0.3340970	-2.7799760	H	-1.5819280	-4.7127310	-1.4449980
C	-1.3458780	-2.5396490	0.5139850	F	-1.1372650	2.8464420	1.3893180
C	-0.5538050	-2.0912800	1.6145470	F	-1.0280050	-0.3742330	-1.7612870
C	0.8247700	-2.4232090	1.3469620	C	1.0602170	1.3273080	0.1034700
C	0.8640960	-3.1462320	0.0966890	C	-0.1974460	0.9208230	0.5257290
C	-0.4578110	-3.1939430	-0.4336660	C	-2.7218250	1.1403030	0.9364070
C	-1.0508710	-1.4760040	2.8886490	H	-3.1297680	1.2033000	1.9548070
H	-1.1423660	-2.2497540	3.6617380	H	-2.7810970	0.1049090	0.6052860
H	-0.3614650	-0.7142490	3.2590010	C	-5.0260170	1.5852250	-0.0393190
H	-2.0302650	-1.0118310	2.7630130	C	1.0974060	2.3160340	-1.0538750
C	1.9574470	-2.2928840	2.3219440	H	0.4933320	3.1626370	-0.6896960
H	1.9013380	-1.3605810	2.8887840	H	0.5264720	1.8745750	-1.8776870
H	1.9382350	-3.1233740	3.0409350	C	-3.5804480	2.0279360	-0.0040230
H	2.9251180	-2.3114170	1.8187460	H	-3.5082180	3.0677410	0.3307490
C	2.0973980	-3.7537140	-0.5003590	H	-3.1468400	1.9751180	-1.0079870
H	1.9267790	-4.0899010	-1.5241830	C	-1.2924740	1.5556630	0.9232310
H	2.9310900	-3.0474260	-0.5211930	C	2.4538180	2.8276900	-1.5471030

H	3.0382220	3.2223910	-0.7056120	H	2.8364690	2.3050890	4.7219100
H	3.0343190	2.0089690	-1.9824910	H	4.3631430	1.4310800	4.9376390
C	-5.4592940	0.6406850	-0.9809600				
H	-4.7507980	0.2572060	-1.7118060	42'			
C	-6.7842800	0.2020510	-0.9973360	C	2.2274050	2.3349120	1.6849520
H	-7.1031210	-0.5241270	-1.7402510	C	2.2788660	1.2523960	0.8060890
C	2.2838610	3.9292510	-2.6037240	C	3.1879870	0.2183900	1.0246170
H	1.6985260	3.5326490	-3.4436460	C	4.0854340	0.2450740	2.0993220
H	1.6942520	4.7550550	-2.1813610	C	4.0460840	1.3359110	2.9555060
C	-5.9561670	2.0798710	0.8853140	C	3.1220190	2.3881640	2.7604270
H	-5.6394550	2.8203090	1.6166830	H	1.4959220	3.1219480	1.5371460
C	-7.2818630	1.6433030	0.8728530	H	4.7876100	-0.5700240	2.2450790
H	-7.9891820	2.0434780	1.5942340	C	3.0474470	-0.8045840	-0.0074680
C	-7.7002570	0.7014590	-0.0690910	O	3.7029890	-1.8089730	-0.2011810
H	-8.7328950	0.3644710	-0.0838160	Rh	-0.0247090	-1.3624960	-0.2583920
C	3.6216780	4.4667180	-3.1207940	N	1.9146300	-0.4180000	-0.8546650
H	3.4743270	5.2457670	-3.8761060	C	2.0370700	-1.6752040	-2.8889530
H	4.2172650	3.6676210	-3.5757470	O	2.3360010	-0.4404280	-2.2152730
H	4.2161770	4.8995310	-2.3077390	C	-1.6792550	-2.5315050	0.4823740
H	2.5438390	-2.1352550	-3.3431770	C	-0.8790020	-2.1295220	1.6128670
H	0.7555290	-2.1780800	-3.1015950	C	0.4220650	-2.7023590	1.4475370
H	1.4451500	-1.3324880	-4.5080450	C	0.3911440	-3.5675320	0.2666490
H	5.5511520	0.4697250	2.9033570	C	-0.8825640	-3.4621500	-0.3175150
C	3.7971130	2.0714280	4.2539660	C	-1.3403970	-1.3337540	2.7982560
H	4.3519080	3.0131510	4.1590420	H	-1.6963730	-2.0079640	3.5883160

H	-0.5312490	-0.7295500	3.2146540	C	-4.7366000	1.9900690	-0.2764280
H	-2.1600620	-0.6609050	2.5414660	C	1.5368500	2.0408490	-1.5307000
C	1.5392530	-2.6662290	2.4504720	H	0.9558580	2.9016390	-1.1911840
H	1.5459900	-1.7313650	3.0159590	H	1.0249460	1.6371150	-2.4082670
H	1.4305850	-3.4896430	3.1695390	C	-3.2525220	2.1995400	-0.4775480
H	2.5140670	-2.7771930	1.9702210	H	-3.0029510	3.2619490	-0.3889520
C	1.5392850	-4.4220870	-0.1857600	H	-2.9603540	1.8809520	-1.4838850
H	1.3796030	-4.8078190	-1.1950760	C	-0.9398050	1.5598610	0.3204390
H	2.4799260	-3.8650080	-0.1815150	C	2.9559720	2.4965150	-1.8999460
H	1.6582880	-5.2835840	0.4840760	H	3.4444550	2.9427810	-1.0233040
C	-3.1459240	-2.2989830	0.2626470	H	3.5627720	1.6342220	-2.1960290
H	-3.3476710	-1.9898410	-0.7667420	C	-5.4270780	1.0076290	-1.0003990
H	-3.7088040	-3.2231920	0.4491860	H	-4.8908770	0.4211450	-1.7431200
H	-3.5469030	-1.5346340	0.9305240	C	-6.7886600	0.7830400	-0.7888620
C	-1.3706430	-4.0753370	-1.5949770	H	-7.3058370	0.0210530	-1.3658750
H	-1.5815220	-3.2830230	-2.3228640	C	2.9453100	3.5212460	-3.0429350
H	-0.6306190	-4.7512410	-2.0290400	H	2.4644320	3.0731980	-3.9228080
H	-2.2927700	-4.6443530	-1.4301110	H	2.3187270	4.3778720	-2.7579380
F	-0.5850960	2.9108300	0.4100000	C	-5.4508140	2.7445630	0.6654580
F	-0.7288890	-0.9415830	-2.1078530	H	-4.9347950	3.5180860	1.2300710
C	1.4121020	0.9858580	-0.4101970	C	-6.8116250	2.5231070	0.8815180
C	-0.0159170	0.6598860	-0.0033700	H	-7.3469040	3.1225910	1.6130180
C	-2.4051430	1.4035580	0.5492500	C	-7.4859100	1.5395580	0.1548700
H	-2.6762660	1.7362200	1.5616020	H	-8.5461530	1.3685400	0.3185970
H	-2.6471600	0.3447420	0.4659730	C	4.3450040	4.0154450	-3.4214540

H	4.3055590	4.7422820	-4.2396450	C	2.3523190	0.3554050	-3.3146000
H	4.9837240	3.1853450	-3.7440950	O	1.9416140	1.5359580	-2.5927250
H	4.8385270	4.4993220	-2.5705540	C	0.8956540	-3.9478980	0.1247070
H	2.5993150	-2.5027710	-2.4499530	C	0.6705970	-3.2249670	1.3674270
H	0.9592520	-1.8447680	-2.8824350	C	1.6683480	-2.2127690	1.4814460
H	2.3864140	-1.4950100	-3.9090360	C	2.5185960	-2.2818720	0.3003760
H	4.7326940	1.3870430	3.7965490	C	2.0525980	-3.3786480	-0.5064630
C	3.1214690	3.5702520	3.6996030	C	-0.4226280	-3.5335270	2.3443310
H	3.9803890	4.2242070	3.5046920	H	-0.6023770	-2.6960660	3.0217620
H	2.2154310	4.1707260	3.5861840	H	-1.3586440	-3.7495500	1.8233820
H	3.1927700	3.2497610	4.7441640	H	-0.1596290	-4.4096690	2.9508520
TS43				C	1.8857370	-1.3270520	2.6713820
				H	0.9437580	-1.0729700	3.1620890
C	0.6432650	2.0738990	2.1194160	H	2.5170830	-1.8424750	3.4074780
C	1.3138610	1.8866950	0.9163320	H	2.3830170	-0.3944260	2.4034430
C	2.6953020	2.0571380	0.8386610	C	3.7859320	-1.5125690	0.0704080
C	3.4405780	2.4287270	1.9555760	H	3.9022570	-1.2197020	-0.9745730
C	2.7655740	2.6252050	3.1599180	H	3.8207100	-0.6031170	0.6705720
C	1.3704750	2.4569880	3.2579760	H	4.6545890	-2.1243890	0.3485650
H	-0.4317290	1.9259790	2.1846810	C	0.0480720	-5.0714750	-0.3900270
H	4.5150800	2.5632440	1.8755000	H	0.2763450	-5.2903000	-1.4351220
C	3.1425300	1.8254430	-0.5584230	H	0.2044450	-5.9861760	0.1957230
O	4.2471620	1.9802110	-1.0494660	H	-1.0123360	-4.8067740	-0.3314280
Rh	0.4722350	-1.8992310	-0.3350130	C	2.5997360	-3.7825320	-1.8433320
N	2.0093330	1.3443060	-1.2164740	H	3.6124200	-3.3993110	-1.9870090

H	2.6283820	-4.8717240	-1.9418640	H	-1.1091920	5.2842740	-1.1336560
H	1.9583470	-3.3731590	-2.6328560	C	-5.8755870	-0.8380610	-0.2996830
F	-1.5979920	-1.9640050	-0.3349940	H	-5.3948050	-1.7662980	-0.5997010
F	0.3064040	-1.7658590	-2.3210870	C	-7.2314330	-0.6415670	-0.5629830
C	-0.1041230	0.2829680	-0.4027280	H	-7.8008770	-1.4169140	-1.0680380
C	-2.7886700	0.2739770	-0.6431890	C	-7.8570840	0.5450640	-0.1740690
H	-3.1130520	-0.3266310	-1.4980770	H	-8.9134970	0.6975750	-0.3758030
H	-2.9356140	1.3296820	-0.9213250	C	0.4862430	6.4851700	-1.9646700
C	-5.1199400	0.1459500	0.3543860	H	-0.1801950	7.2482430	-2.3800550
C	-0.0725320	2.7153990	-1.0588610	H	1.3416310	6.3844320	-2.6417660
H	-0.9489820	2.8518820	-0.4135110	H	0.8661670	6.8597930	-1.0072730
H	-0.4353060	2.3871460	-2.0374540	H	3.4095940	0.1498110	-3.1179280
C	-3.6427770	-0.0609950	0.6041430	H	1.7108260	-0.4936450	-3.0622700
H	-3.4307810	-1.0998540	0.8644520	H	2.2285100	0.6300910	-4.3652450
H	-3.3124850	0.5655380	1.4409450	H	3.3231470	2.9170720	4.0463180
C	-1.3497210	0.1154450	-0.4699810	C	0.6634930	2.7134700	4.5684360
C	0.6679960	4.0490520	-1.2096310	H	0.4297230	3.7789140	4.6867730
H	1.0557830	4.3798910	-0.2376530	H	-0.2803710	2.1640950	4.6294060
H	1.5322240	3.9125580	-1.8692020	H	1.2835540	2.4226190	5.4217870
C	-5.7602030	1.3313700	0.7390060	C	0.7525270	1.5369500	-0.4585490
H	-5.1909690	2.1028830	1.2531770				
C	-7.1172030	1.5317200	0.4792740	44			
H	-7.5960750	2.4563210	0.7898060	C	1.3702010	2.5427450	1.8278330
C	-0.2373790	5.1464390	-1.7883890	C	1.7162500	2.1544400	0.5378310
H	-0.6334400	4.8145090	-2.7574740	C	3.0161920	2.3379990	0.0693360

C	3.9952520	2.9338520	0.8621290	H	3.6215950	-2.2345060	-1.9359080
C	3.6424000	3.3363720	2.1490980	H	4.1195600	-0.8628910	-0.9463780
C	2.3369070	3.1493890	2.6459890	H	4.8667330	-2.4494250	-0.6988470
H	0.3612550	2.3848280	2.2011260	C	0.2927670	-4.6287300	1.5815670
H	5.0000290	3.0762480	0.4755370	H	-0.0234500	-5.2128020	0.7156950
C	3.1113790	1.8366330	-1.3238600	H	0.6959640	-5.3190520	2.3333050
O	4.0563090	1.8812800	-2.0965830	H	-0.5990640	-4.1609510	2.0087310
Rh	0.8541430	-1.6992940	0.1377290	C	2.0860270	-4.5052300	-1.1105290
N	1.8770930	1.2378980	-1.5720910	H	3.0289870	-5.0635130	-1.1562200
C	1.7850280	-0.0694560	-3.5188440	H	1.2684950	-5.2236170	-1.0293670
O	1.4526670	1.1856260	-2.8983520	H	1.9619570	-3.9714440	-2.0568490
C	1.3162160	-3.5979820	1.2112500	F	-1.3453610	-1.2718080	0.6427810
C	1.6268710	-2.4124200	2.0217470	F	0.0054570	-1.9794020	-1.6932690
C	2.6545920	-1.6761290	1.3636420	C	0.1496360	0.2806290	-0.0771630
C	2.8788240	-2.3101570	0.0777230	C	-2.4965460	0.7075110	0.0547050
C	2.0984530	-3.5480460	0.0420720	H	-3.0077500	0.1410910	-0.7329040
C	1.0706380	-2.1322470	3.3862190	H	-2.4196230	1.7401560	-0.2832110
H	1.1431690	-1.0708870	3.6330440	C	-4.7698600	1.1120820	1.1234580
H	0.0200320	-2.4241220	3.4609860	C	-0.1348590	2.6363350	-1.1164940
H	1.6256850	-2.6951280	4.1483780	H	-0.7938440	2.9399470	-0.2967940
C	3.4599590	-0.5589910	1.9492110	H	-0.7556260	2.1595940	-1.8804940
H	2.8669900	0.0812450	2.6039850	C	-3.3473640	0.6417380	1.3465610
H	4.2810190	-0.9822280	2.5437870	H	-3.3553580	-0.3936770	1.7025390
H	3.8993100	0.0723190	1.1783770	H	-2.8746830	1.2449750	2.1313080
C	3.9233020	-1.9359690	-0.9297360	C	-1.1403850	0.0987060	0.1836310

C	0.5220920	3.8908390	-1.7088020	H	1.0994060	3.1047380	4.4236070
H	1.1507140	4.3825320	-0.9556460	H	2.8025930	3.4835630	4.7358560
H	1.1793110	3.6061740	-2.5375080	H	1.7412690	4.7006810	4.0291790
C	-5.2553700	2.2693980	1.7438080	C	0.8350940	1.5525620	-0.5547040
H	-4.6002450	2.8367670	2.4014310	O	-1.9411890	-3.6278620	-1.5743370
C	-6.5672970	2.7013960	1.5346980	C	-3.1987610	-3.1851410	-1.5269630
H	-6.9248730	3.6012820	2.0280150	O	-3.5241880	-2.0110570	-1.5723620
C	-0.5220770	4.8947160	-2.2199580	C	-4.1903010	-4.3244990	-1.4086900
H	-1.1549740	4.4062640	-2.9728390	H	-4.0383740	-5.0413720	-2.2207740
H	-1.1924350	5.1779240	-1.3964090	H	-4.0291210	-4.8611450	-0.4681520
C	-5.6305720	0.3926490	0.2782830	H	-5.2073990	-3.9346690	-1.4392860
H	-5.2674400	-0.5023530	-0.2223540	H	-1.2763090	-2.8756720	-1.6399150
C	-6.9399500	0.8237960	0.0668690				
H	-7.5928330	0.2559980	-0.5906330	TS45			
C	-7.4144870	1.9784910	0.6949850	C	-1.7948430	2.3076200	-1.7717060
H	-8.4354260	2.3111840	0.5295160	C	-2.1951040	1.7720580	-0.5526710
C	0.1073670	6.1550830	-2.8218250	C	-3.5477900	1.5959730	-0.2653670
H	-0.6575690	6.8522830	-3.1794480	C	-4.5352250	1.9675830	-1.1752600
H	0.7552360	5.9064090	-3.6696920	C	-4.1331130	2.5169120	-2.3916030
H	0.7205420	6.6835910	-2.0828220	C	-2.7708850	2.6951720	-2.7042470
H	2.8711020	-0.1992960	-3.5420000	H	-0.7401260	2.4308550	-2.0048870
H	1.2812250	-0.8953130	-3.0117620	H	-5.5840490	1.8298710	-0.9301980
H	1.4094080	0.0291190	-4.5404710	C	-3.6909310	1.0143270	1.0919170
H	4.3854570	3.8068800	2.7882330	O	-4.7050390	0.7902150	1.7309690
C	1.9763210	3.6290030	4.0329790	Rh	-0.3757880	-1.8305660	-0.1417420

N	-2.3853670	0.7235020	1.4959580	H	-2.1059910	-5.0733390	1.4154490
C	-2.1408690	-0.6205870	3.4055550	H	-0.4669560	-5.5486250	0.9387500
O	-2.1377710	0.7169070	2.8659770	H	-0.7069970	-4.1002300	1.9359520
C	-0.2871240	-3.7408980	-1.1661240	F	1.6608400	-1.2624720	-0.4482480
C	-0.7433340	-2.7130500	-2.0971890	F	0.1572270	-1.9487280	1.7817400
C	-1.9759960	-2.1923720	-1.6055700	C	-0.2686630	0.3466760	0.2274440
C	-2.2617560	-2.8316630	-0.3328360	C	2.3142580	1.1333190	0.1848250
C	-1.2342420	-3.8314230	-0.1066910	H	2.9317820	0.5450720	0.8729250
C	-0.0580010	-2.3539680	-3.3815320	H	2.1635000	2.1196300	0.6504580
H	-0.4249480	-1.4052960	-3.7790470	C	4.3386370	2.0677350	-1.0471480
H	1.0218400	-2.2621730	-3.2381050	C	-0.7171990	2.5759270	1.3599430
H	-0.2317290	-3.1266650	-4.1415030	H	-0.0138210	3.0352770	0.6550460
C	-2.8817350	-1.2454930	-2.3300680	H	-0.1336720	2.1931700	2.2024180
H	-2.3261990	-0.5191360	-2.9257480	C	3.0374800	1.3026480	-1.1734950
H	-3.5297210	-1.8138000	-3.0106370	H	3.2165680	0.3006870	-1.5739610
H	-3.5238930	-0.6926970	-1.6453910	H	2.3734770	1.8168040	-1.8779220
C	-3.5100940	-2.6871280	0.4855550	C	0.9813970	0.5460560	0.1182340
H	-3.3127030	-2.8958600	1.5389130	C	-1.6996770	3.6411940	1.8613080
H	-3.9371850	-1.6852590	0.4254890	H	-2.2934150	4.0319070	1.0250480
H	-4.2732120	-3.3982040	0.1407040	H	-2.4024420	3.1865320	2.5683400
C	0.9730980	-4.5389220	-1.3112790	C	4.4992270	3.3144260	-1.6649050
H	1.3611930	-4.8554480	-0.3414150	H	3.6793910	3.7321340	-2.2455170
H	0.7930690	-5.4324090	-1.9230770	C	5.6963480	4.0247710	-1.5513310
H	1.7543800	-3.9519740	-1.8001710	H	5.8011050	4.9890520	-2.0413490
C	-1.1248940	-4.6947340	1.1144350	C	-0.9773930	4.8071670	2.5523540

H	-0.3834890	4.4185400	3.3903290	H	4.4107530	-3.8342190	3.0838090
H	-0.2595250	5.2590540	1.8537090	H	5.3765950	-4.0827010	1.6299230
C	5.4081560	1.5445080	-0.3028910	H	5.8533220	-2.8189460	2.8065250
H	5.2990820	0.5849860	0.1959970	H	2.6023460	-2.1951560	0.4787940
C	6.6030310	2.2548300	-0.1861500				
H	7.4204000	1.8365000	0.3949320	46			
C	6.7532750	3.4957240	-0.8104770	C	1.7164460	3.7093040	-0.6006880
H	7.6860760	4.0451660	-0.7189890	C	1.0743070	2.4602190	-0.6769980
C	-1.9392420	5.8839940	3.0643120	C	1.3899180	1.6152450	-1.7651280
H	-1.3998770	6.6998070	3.5566620	C	2.3181190	2.0440340	-2.7232230
H	-2.6483520	5.4676330	3.7883890	C	2.9606830	3.2732880	-2.6070440
H	-2.5223210	6.3174950	2.2437240	C	2.6639170	4.1303050	-1.5380890
H	-3.1382740	-1.0593660	3.3037560	H	1.4764630	4.3740050	0.2256330
H	-1.3688700	-1.2289990	2.9271970	H	2.5182230	1.4033780	-3.5771800
H	-1.9142200	-0.4792560	4.4653690	H	3.6833100	3.5787690	-3.3601050
H	-4.8825630	2.8181690	-3.1191280	C	0.6489700	0.3255180	-2.0611350
C	-2.3690750	3.3283750	-4.0158990	O	-0.0882580	0.2503600	-3.0433150
H	-1.3532540	3.0441120	-4.3051820	Rh	1.4698330	-0.5980660	0.7670520
H	-3.0478410	3.0408100	-4.8245810	N	0.9670870	-0.7067580	-1.2222200
H	-2.3946670	4.4230500	-3.9466580	C	0.5566560	-2.9500040	-1.8870020
C	-1.3471970	1.3459550	0.6412290	O	0.0248290	-1.7843950	-1.4412230
O	3.1814670	-2.8895950	0.9004430	C	3.4382930	0.1277420	1.1270830
C	4.1556950	-2.3104910	1.6017300	C	3.6424080	-1.2254860	0.5973150
O	4.3362750	-1.1044040	1.6599640	C	3.0234970	-2.1256410	1.4748110
C	5.0140160	-3.3221830	2.3274770	C	2.4682880	-1.3564730	2.6003270

C	2.7864820	0.0120070	2.4251530	C	-2.4944230	0.1887380	0.9814250
C	4.3370620	-1.5626420	-0.6877150	H	-2.3674490	-0.3311810	0.0269990
H	4.5676620	-0.6610920	-1.2582280	H	-2.8228100	1.2021750	0.7440520
H	5.2813110	-2.0825160	-0.4841390	C	-4.9154780	-0.5317530	1.1700720
H	3.7066760	-2.2034890	-1.3095900	C	-1.0321960	3.1506020	0.5918070
C	2.9506860	-3.6161980	1.3219480	H	-0.5178750	4.0532650	0.9507240
H	2.0380490	-4.0207330	1.7691820	H	-1.6716630	2.8422790	1.4236580
H	2.9664600	-3.9029600	0.2684070	C	-3.5621770	-0.5125200	1.8478170
H	3.7991540	-4.1000210	1.8240380	H	-3.2359290	-1.5353220	2.0600430
C	1.7605080	-1.9714050	3.7697140	H	-3.6324880	0.0064890	2.8091020
H	1.2020520	-1.2283960	4.3415740	C	-1.1246570	0.2591170	1.6432780
H	1.0572770	-2.7452890	3.4500120	C	-1.8886760	3.5397210	-0.6281430
H	2.4868120	-2.4450360	4.4429460	H	-1.2300730	3.8702790	-1.4404170
C	4.1025110	1.3611290	0.6009110	H	-2.4096870	2.6514640	-1.0085930
H	3.6270130	2.2661350	0.9793630	C	-5.8405810	0.4993510	1.3830110
H	5.1546160	1.3706100	0.9182450	H	-5.5912480	1.3061850	2.0687570
H	4.0780380	1.4068380	-0.4890070	C	-7.0763010	0.5002080	0.7341410
C	2.5310270	1.1400760	3.3809990	H	-7.7812030	1.3067940	0.9162910
H	2.2656240	2.0565140	2.8487700	C	-2.9102260	4.6408040	-0.3163980
H	1.7083710	0.9086340	4.0609060	H	-3.5676640	4.3085570	0.4993970
H	3.4236180	1.3451640	3.9858220	H	-2.3832090	5.5276150	0.0627020
F	-0.7542570	-1.1047200	1.8920410	C	-5.2623130	-1.5656840	0.2894150
F	-1.2388480	0.8061910	2.9101850	H	-4.5593260	-2.3775890	0.1168380
C	0.0175250	2.0787820	0.3123710	C	-6.4963480	-1.5691660	-0.3619770
C	0.0264330	0.8505820	0.8716910	H	-6.7470900	-2.3812860	-1.0388120

C	-7.4080300	-0.5348890	-0.1418210	TS47			
H	-8.3700480	-0.5372700	-0.6462200	C	2.8238430	3.1740150	-0.4008390
C	-3.7608190	5.0309210	-1.5294210	C	1.8295660	2.1867620	-0.5413980
H	-4.4812090	5.8162570	-1.2773190	C	1.9351070	1.2706210	-1.6096910
H	-4.3235390	4.1713300	-1.9102170	C	3.0204350	1.3817000	-2.4915620
H	-3.1346960	5.4027060	-2.3483010	C	4.0096980	2.3418420	-2.3103310
C	3.3263650	5.4837510	-1.4239410	C	3.9242820	3.2620820	-1.2549400
H	2.9031190	6.1937770	-2.1452700	H	2.7445780	3.8887060	0.4141820
H	3.1949550	5.9125400	-0.4262890	H	3.0591590	0.7098700	-3.3432800
H	4.4007960	5.4230220	-1.6272660	H	4.8440550	2.3934670	-3.0060520
O	1.7433030	-3.1960070	-1.9372300	C	0.8603430	0.2803900	-2.0172810
C	-0.5586990	-3.8929860	-2.3644990	O	0.3732050	0.3683500	-3.1484420
C	-1.7554240	-3.8825840	-1.3913980	Rh	1.0612150	-0.9040000	0.8884230
H	-2.2080390	-2.8909510	-1.3271650	N	0.5753730	-0.6861390	-1.1104280
H	-2.5165470	-4.5873790	-1.7435060	C	-0.2676750	-2.5801260	-2.2320590
H	-1.4546880	-4.1897400	-0.3835780	O	-0.5558190	-1.4478030	-1.5485160
C	-1.0065440	-3.3669730	-3.7515470	C	3.1858600	-0.7843050	1.4120130
H	-0.1895910	-3.4385480	-4.4767570	C	2.9995840	-1.9298630	0.5596370
H	-1.8434840	-3.9693330	-4.1214800	C	2.0944590	-2.8330380	1.2084400
H	-1.3151170	-2.3202100	-3.6924380	C	1.7494990	-2.2559160	2.4942100
C	0.0111990	-5.3145170	-2.4907910	C	2.4187580	-1.0057400	2.6288260
H	0.3148290	-5.7103970	-1.5160070	C	3.6415610	-2.1598170	-0.7745710
H	-0.7495570	-5.9829750	-2.9071780	H	4.0728850	-1.2395410	-1.1726590
H	0.8862300	-5.3308030	-3.1440640	H	4.4481690	-2.8976190	-0.6758960
				H	2.9093090	-2.5325410	-1.4948070

C	1.6458060	-4.1734240	0.7075110	H	0.7171610	4.2539790	0.9828760
H	1.6367670	-4.2033250	-0.3835510	H	-0.7679960	3.4384230	1.4052010
H	2.3114760	-4.9687360	1.0700410	C	-3.4434980	0.1721710	1.8605510
H	0.6361700	-4.4027000	1.0602700	H	-3.1889850	-0.8898120	1.8807650
C	0.8000320	-2.8855960	3.4687520	H	-3.4652550	0.5247280	2.8966030
H	0.6771420	-2.2745710	4.3650670	C	-0.9534640	0.7795530	1.6666220
H	-0.1857760	-3.0098160	3.0092090	C	-0.6726050	4.1048590	-0.6611990
H	1.1654100	-3.8722600	3.7753850	H	0.0822010	4.1860120	-1.4521210
C	4.1845450	0.3153460	1.2126560	H	-1.4263260	3.3981900	-1.0325740
H	3.8562700	1.2462570	1.6788750	C	-5.6642710	1.3862340	1.6778200
H	5.1449190	0.0351760	1.6668380	H	-5.3753330	1.9905890	2.5350810
H	4.3600040	0.5202710	0.1559890	C	-6.8975660	1.6060370	1.0615350
C	2.4148720	-0.1044310	3.8291470	H	-7.5600510	2.3798120	1.4396650
H	2.4771790	0.9464050	3.5359120	C	-1.3219790	5.4748690	-0.4271020
H	1.5070000	-0.2291530	4.4227160	H	-2.0721950	5.3927690	0.3718780
H	3.2740630	-0.3206010	4.4773840	H	-0.5616220	6.1770250	-0.0579450
F	-0.9350810	-1.3330090	1.2978400	C	-5.1922980	-0.3837270	0.1144270
F	-0.9206520	0.5792160	2.9844770	H	-4.5326020	-1.1658140	-0.2540580
C	0.6622220	2.1837930	0.3874690	C	-6.4231930	-0.1666020	-0.5052850
C	0.2458070	1.0604760	1.0085150	H	-6.7148610	-0.7786330	-1.3542060
C	-2.3253250	0.9033860	1.0933840	C	-7.2802090	0.8301330	-0.0336320
H	-2.2758300	0.5757570	0.0527040	H	-8.2400760	0.9977530	-0.5136860
H	-2.5371370	1.9848460	1.0640360	C	-1.9792880	6.0472700	-1.6869840
C	-4.7946690	0.3906420	1.2137390	H	-2.4335390	7.0241040	-1.4912730
C	-0.0190810	3.5289640	0.6104520	H	-2.7660220	5.3821090	-2.0599370

H	-1.2471840	6.1745770	-2.4921160	C	4.9795590	0.4648370	-1.9291960
C	4.9830490	4.3228560	-1.0643130	C	5.1885250	1.4174370	-0.9191210
H	5.9768210	3.8783310	-0.9368220	H	4.2257830	2.5960790	0.5828130
H	5.0399270	4.9877460	-1.9340810	H	3.5314600	-0.6779210	-3.0368330
H	4.7782060	4.9409750	-0.1856660	H	5.8211550	0.1108420	-2.5199830
O	0.8503600	-3.0165560	-2.4133220	C	1.2488470	-0.0332720	-2.0126640
C	-1.5647760	-3.2555940	-2.7051180	O	1.0715290	0.0656720	-3.2296490
C	-1.2009490	-4.3895530	-3.6766230	Rh	0.3079400	-0.9862280	0.8823160
H	-0.5306780	-5.1139660	-3.2074640	N	0.3397310	-0.5725050	-1.1540450
H	-2.1104880	-4.9100160	-3.9949670	C	-1.1003710	-2.0087420	-2.3197730
H	-0.6977480	-4.0005010	-4.5664240	O	-0.8972190	-0.7643680	-1.8256900
C	-2.4705280	-2.2217490	-3.4081960	C	2.3192920	-1.7180380	1.6250370
H	-1.9432950	-1.7289280	-4.2302060	C	1.8144750	-2.7720120	0.7801250
H	-3.3550010	-2.7249470	-3.8147960	C	0.5717470	-3.1992840	1.3145540
H	-2.7990850	-1.4445110	-2.7150670	C	0.3197510	-2.4530350	2.5475280
C	-2.2841620	-3.8313320	-1.4626810	C	1.4137500	-1.5712520	2.7515610
H	-3.2252080	-4.3038370	-1.7655520	C	2.4491640	-3.3029030	-0.4679890
H	-1.6696370	-4.5923070	-0.9691080	H	3.3120720	-2.7047830	-0.7648330
H	-2.5023360	-3.0476750	-0.7324420	H	2.7891520	-4.3332960	-0.3068440
48				H	1.7240640	-3.3009820	-1.2869460
				C	-0.3375830	-4.2541700	0.7727720
C	4.0778430	1.8564840	-0.1994850	H	-0.0393210	-4.5608440	-0.2293590
C	2.7802040	1.3576720	-0.4273910	H	-0.3400130	-5.1301210	1.4340450
C	2.5860190	0.4161310	-1.4591830	H	-1.3571090	-3.8620090	0.7158670
C	3.7007230	-0.0003520	-2.2065330	C	-0.8728430	-2.6730760	3.4257840

H	-0.9230190	-1.9389270	4.2320610	C	-0.4782470	0.9614720	1.5728240
H	-1.7860980	-2.5942850	2.8291750	C	1.2414820	4.1374750	-0.6760860
H	-0.8399520	-3.6735600	3.8737900	H	2.0234250	3.9210900	-1.4142610
C	3.6960130	-1.1287020	1.5725090	H	0.3024470	3.7653030	-1.1058280
H	3.7164650	-0.1195450	1.9859870	C	-4.8178560	2.7737770	1.5728650
H	4.3782640	-1.7482210	2.1706450	H	-4.3092260	3.3218060	2.3633610
H	4.0868970	-1.0822080	0.5562240	C	-5.9680220	3.3094110	0.9908920
C	1.6886170	-0.7297770	3.9608110	H	-6.3471490	4.2704350	1.3281030
H	2.0990780	0.2451150	3.6890330	C	1.1449150	5.6529760	-0.4588250
H	0.7883050	-0.5617470	4.5515840	H	0.3687140	5.8650620	0.2893610
H	2.4253770	-1.2374490	4.5966710	H	2.0884100	6.0184340	-0.0300820
F	-1.6335930	-1.4750660	0.6321770	C	-4.9896460	0.8402960	0.1490940
F	-0.4996470	0.9886840	2.9578910	H	-4.6130560	-0.1262830	-0.1757700
C	1.6598780	1.8623100	0.4084410	C	-6.1400300	1.3716880	-0.4358410
C	0.7497390	1.0577680	0.9548860	H	-6.6535210	0.8170690	-1.2165140
C	-1.7926630	1.4122630	0.9806150	C	-6.6328640	2.6094180	-0.0174320
H	-1.8471000	1.0608270	-0.0517100	H	-7.5295220	3.0229240	-0.4704200
H	-1.7598640	2.5124250	0.9441980	C	0.8359650	6.4215390	-1.7476640
C	-4.3103360	1.5338010	1.1609670	H	0.7737530	7.4992280	-1.5646550
C	1.5382840	3.3668010	0.6242960	H	-0.1183660	6.1005020	-2.1795190
H	2.4681730	3.7523740	1.0634380	H	1.6118890	6.2551650	-2.5032390
H	0.7500720	3.5619970	1.3593480	C	6.5719440	1.9522990	-0.6341330
C	-3.0439980	0.9711540	1.7689680	H	7.2579430	1.1494240	-0.3399300
H	-3.0678580	-0.1199650	1.7697740	H	7.0021310	2.4306700	-1.5214650
H	-2.9521240	1.3104470	2.8056230	H	6.5587460	2.6921650	0.1709330

O	-0.3245090	-2.9335210	-2.1937630	C	-2.8157310	0.4759360	1.3648410
C	-2.4564600	-2.1204710	-3.0319310	O	-3.4245090	1.0034400	2.2980500
C	-2.2365860	-2.9365760	-4.3216200	Rh	-0.5714200	-1.3933560	0.2840130
H	-1.7678650	-3.8975280	-4.0983520	N	-2.0587240	-0.6546270	1.4631100
H	-3.1981000	-3.1180560	-4.8137200	C	-2.7403060	-1.7617480	3.4239550
H	-1.5913810	-2.3975420	-5.0228030	O	-1.7143910	-0.9859310	2.8077820
C	-3.0638420	-0.7486010	-3.3749970	C	-1.4112710	-2.2119530	-1.4764340
H	-2.3809070	-0.1558360	-3.9896530	C	-1.6696410	-3.2525990	-0.4761570
H	-3.9935520	-0.8954810	-3.9361310	C	-0.4320160	-3.6840030	0.0135460
H	-3.2955180	-0.1706320	-2.4773470	C	0.6328350	-2.9933650	-0.7356090
C	-3.3934020	-2.8943820	-2.0742810	C	0.0304200	-2.1553020	-1.6995680
H	-4.3816410	-3.0069000	-2.5336630	C	-3.0411510	-3.6891360	-0.0594140
H	-2.9949690	-3.8915710	-1.8645970	H	-3.5464820	-4.2056490	-0.8845940
H	-3.5031480	-2.3648930	-1.1235950	H	-3.0067530	-4.3731260	0.7913010
49				H	-3.6536230	-2.8289830	0.2257670
C	-2.2653640	2.1208260	-2.0618790	C	-0.1672940	-4.6844860	1.0995290
C	-1.9524390	1.5562490	-0.8121320	H	0.5709970	-4.3078330	1.8145700
C	-2.9971560	0.9971740	-0.0471570	H	-1.0745890	-4.9275590	1.6559690
C	-4.3084370	1.0474250	-0.5412370	H	0.2312280	-5.6171570	0.6802280
C	-4.5901660	1.5874020	-1.7916540	C	2.0939020	-3.2850600	-0.5582330
C	-3.5641710	2.1325090	-2.5777760	H	2.7201160	-2.5615830	-1.0839530
H	-1.4661810	2.5644120	-2.6515870	H	2.3803230	-3.2754360	0.4975310
H	-5.1118960	0.6690390	0.0842170	H	2.3357350	-4.2802390	-0.9535790
H	-5.6151420	1.6034080	-2.1552130	C	-2.4524610	-1.6244890	-2.3787490
				H	-2.6384450	-2.3055460	-3.2212600

H	-3.3973870	-1.4695610	-1.8555370	H	5.4521340	-1.5783330	0.3637940
H	-2.1397790	-0.6609110	-2.7834390	C	6.9942840	-0.6859470	-0.8459280
C	0.6987020	-1.3748740	-2.7922740	H	7.4872580	-1.6337700	-1.0443320
H	0.2356050	-0.3934850	-2.9193320	C	-0.1536440	5.3679380	0.9095500
H	1.7609450	-1.2196650	-2.5906710	H	0.9326980	5.3547750	1.0760910
H	0.6166790	-1.9114670	-3.7462590	H	-0.3044440	5.8311420	-0.0759570
F	1.3929300	1.5782950	1.8984490	C	5.7295260	1.7365870	-0.3091520
F	1.3512280	-0.6256620	1.7410140	H	5.2451000	2.6865700	-0.0944930
C	-0.5602780	1.6442170	-0.2684140	C	6.8775430	1.7100030	-1.1015980
C	0.0657330	0.5425050	0.1867800	H	7.2789840	2.6371460	-1.5013390
C	2.6624080	0.5914710	0.1699550	C	7.5138470	0.4970520	-1.3738870
H	2.6549840	1.4811120	-0.4683480	H	8.4101720	0.4753030	-1.9870610
H	2.6584030	-0.2730160	-0.4991240	C	-0.8232600	6.2284880	1.9860180
C	5.1941240	0.5556390	0.2247250	H	-0.4297390	7.2506800	1.9853370
C	0.0056670	3.0595530	-0.1909950	H	-0.6602870	5.8078640	2.9845130
H	-0.1182250	3.5464070	-1.1680830	H	-1.9059780	6.2868800	1.8276870
H	1.0794700	3.0389220	0.0101850	H	-2.3725910	-1.9851230	4.4295800
C	3.9274620	0.5838490	1.0525520	H	-3.6665180	-1.1839890	3.4876040
H	3.9126990	1.4714370	1.6927230	H	-2.9109910	-2.7007760	2.8809660
H	3.8947750	-0.2860480	1.7157870	C	-3.8647160	2.7414570	-3.9278690
C	1.3589380	0.5752700	0.9565630	H	-4.4150280	2.0438250	-4.5693840
C	-0.6807500	3.9279950	0.8819490	H	-4.4845410	3.6406630	-3.8287560
H	-1.7638560	3.9372800	0.7083440	H	-2.9482510	3.0275060	-4.4517540
H	-0.5280560	3.4584720	1.8604980				
C	5.8447340	-0.6539060	-0.0543210	TS50			

C	1.6608790	2.4190160	2.0227020	H	-1.4492770	-3.6576800	-1.0701500
C	1.5771430	1.7979800	0.7675670	H	-1.4794310	-4.6023630	0.4291320
C	2.8042760	1.4890300	0.1374120	H	-2.0947440	-2.9482510	0.4049610
C	4.0413040	1.7257400	0.7534650	C	-0.5371020	-1.7003270	2.5221350
C	4.0792850	2.3367950	1.9990580	H	-0.1917510	-0.7324340	2.8932720
C	2.8843880	2.6900980	2.6508980	H	-1.5398810	-1.5603310	2.1164480
H	0.7427030	2.6857540	2.5389540	H	-0.6209620	-2.3785890	3.3813420
H	4.9558720	1.4446630	0.2402510	C	3.8442580	-3.2582480	0.2483190
H	5.0345580	2.5379390	2.4765580	H	4.0010590	-3.6477760	-0.7600500
C	2.7339230	1.1242900	-1.4128110	H	4.4093010	-2.3250580	0.3299310
O	2.8238560	1.8608840	-2.3667630	H	4.2764640	-3.9745520	0.9589130
Rh	1.1598200	-1.3427880	-0.3468240	C	2.6369470	-1.4894740	2.6204390
N	2.6532270	-0.0884580	-0.9716560	H	3.5988030	-1.1491920	2.2292270
C	1.0408900	-0.6986350	-3.4567610	H	2.1086820	-0.6171100	3.0109600
O	1.6971970	-1.3433010	-2.3857060	H	2.8417380	-2.1642710	3.4625560
C	2.3848790	-3.0369210	0.5192380	F	-1.6258760	1.1530140	-2.0485830
C	1.2986640	-3.5870320	-0.2043110	F	-1.4615400	-1.0188060	-1.8059520
C	0.0566910	-3.0998930	0.3714430	C	0.2548290	1.5536380	0.1016640
C	0.4047020	-2.2700110	1.5018040	C	-0.0858260	0.3368310	-0.4013210
C	1.8343320	-2.1949270	1.5680090	C	-2.6673730	0.1410180	-0.1683900
C	1.4184720	-4.4491210	-1.4272340	H	-2.6578170	1.0192090	0.4819080
H	1.8519260	-3.8717450	-2.2523900	H	-2.5691640	-0.7289830	0.4854600
H	2.0616140	-5.3141990	-1.2335720	C	-5.1861950	-0.0430720	-0.0018480
H	0.4432990	-4.8190410	-1.7503410	C	-0.5772250	2.8370350	-0.0037250
C	-1.3126950	-3.6001080	0.0116360	H	-0.6101690	3.3337180	0.9752250

H	-1.6092410	2.6185710	-0.2740860	H	0.1897190	-1.3073920	-3.7970610
C	-4.0021470	0.0649450	-0.9380570	H	0.6616300	0.2953840	-3.2010680
H	-4.0966820	0.9546990	-1.5680520	H	1.7485090	-0.5836280	-4.2897240
H	-3.9741480	-0.7988060	-1.6093660	C	2.9226940	3.3686500	3.9982890
C	-1.4374110	0.1679530	-1.0789990	H	1.9675000	3.2781200	4.5225080
C	-0.0125020	3.8291640	-1.0401940	H	3.7060560	2.9479640	4.6365980
H	1.0334880	4.0620780	-0.8036980	H	3.1372700	4.4390890	3.8882000
H	-0.0030920	3.3392530	-2.0201910				
C	-5.6793990	-1.2952880	0.3906780	P2			
H	-5.2280950	-2.1967040	-0.0184470	C	-1.5488400	2.1403480	0.4731160
C	-6.7448030	-1.4000980	1.2862130	C	-1.7913730	0.9423750	-0.1883690
H	-7.1151540	-2.3806810	1.5727450	C	-2.5461180	0.9154250	-1.3594900
C	-0.8201790	5.1309220	-1.1164160	C	-3.0926660	2.0807960	-1.8909650
H	-1.8661380	4.8953580	-1.3571180	C	-2.8612570	3.2790740	-1.2203470
H	-0.8364700	5.6091620	-0.1266350	C	-2.0935450	3.3267320	-0.0402030
C	-5.7946900	1.1046950	0.5253980	H	-0.9408570	2.1648830	1.3734850
H	-5.4326930	2.0854490	0.2248970	H	-3.6784080	2.0415970	-2.8039590
C	-6.8602340	1.0056670	1.4211570	C	-2.6404480	-0.4785490	-1.8615200
H	-7.3206780	1.9079710	1.8142970	O	-3.2811380	-0.9316560	-2.7935730
C	-7.3383000	-0.2484230	1.8062300	N	-1.7714940	-1.1942870	-1.0402950
H	-8.1699510	-0.3272760	2.5005820	C	-1.0623220	-3.2290890	-1.8970930
C	-0.2690310	6.1173910	-2.1510320	O	-1.9136610	-2.5737170	-0.9447210
H	-0.8650520	7.0355680	-2.1873410	C	-1.3389560	-0.4715500	0.1801290
H	-0.2705940	5.6777980	-3.1545430	C	0.1212730	-0.5551200	0.3540450
H	0.7641480	6.3987300	-1.9178290	C	2.7628630	-0.7134730	0.7281440

H	3.1016560	-1.7421970	0.5501840	H	8.8874550	-0.2354790	0.5301920
H	3.0192920	-0.4894350	1.7715480	C	-5.7162230	-1.6357020	2.6717860
C	5.0422510	0.1333980	-0.0194310	H	-6.1251010	-2.0456040	3.6010320
C	-2.0441000	-1.0241650	1.4552230	H	-6.0852780	-2.2517750	1.8444210
H	-1.6910580	-0.4222970	2.3009440	H	-6.1286950	-0.6287520	2.5418800
H	-1.6687060	-2.0404170	1.6113820	H	-1.3646940	-2.9750830	-2.9165790
C	3.5454830	0.2477030	-0.2061930	H	-0.0139140	-2.9621900	-1.7308320
H	3.2742770	0.0229250	-1.2429440	H	-1.2111100	-4.2966150	-1.7198580
H	3.2149780	1.2728850	-0.0085200	C	-1.8752800	4.6436850	0.6667730
C	1.3134730	-0.6364840	0.5465920	H	-1.5667750	5.4259520	-0.0345700
C	-3.5749550	-1.0376990	1.4107610	H	-2.7969700	4.9902940	1.1495540
H	-3.9561570	-0.0216960	1.2494270	H	-1.1077620	4.5611970	1.4408060
H	-3.9101390	-1.6401480	0.5581140	H	-3.2757080	4.2033760	-1.6147540
C	5.7102820	0.9175440	0.9306120				
H	5.1480380	1.6426880	1.5145240	35Cl			
C	7.0849810	0.7866430	1.1298950	C	-2.5844610	2.3864450	-0.3413200
H	7.5850490	1.4075480	1.8678060	C	-2.2018690	1.2457410	0.3711220
C	-4.1852280	-1.6074500	2.6990440	C	-2.2824800	1.2733820	1.7681360
H	-3.8028050	-2.6239050	2.8619200	C	-2.7173630	2.4168330	2.4420890
H	-3.8448080	-1.0132700	3.5582670	C	-3.0984410	3.5438880	1.7184530
C	5.7896580	-0.7864770	-0.7672010	C	-3.0482410	3.5398670	0.3162440
H	5.2896590	-1.3977500	-1.5149450	H	-2.5254300	2.4100860	-1.4272830
C	7.1644530	-0.9211210	-0.5717900	H	-2.7423600	2.3967090	3.5281880
H	7.7265820	-1.6363330	-1.1655430	H	-3.4391850	4.4354920	2.2397000
C	7.8167280	-0.1347450	0.3790550	C	-1.8835050	0.0392370	2.5027320

O	-1.7421510	-0.0359970	3.7244020	H	-4.1075000	1.1492990	-2.4778040
Rh	-1.4983900	-0.5386230	-0.3978530	C	-1.6172350	0.2599270	-3.7273220
N	-1.7870510	-0.9933810	1.6032320	H	-2.0479190	1.2506270	-3.5590260
C	-2.0962410	-2.8701440	2.9930790	H	-0.5356750	0.3770380	-3.8295870
O	-1.2137050	-2.1855640	2.0987570	H	-1.9991670	-0.1011820	-4.6913790
C	-3.2131290	-0.7368320	-1.9119050	C	0.2846620	0.6729810	-0.6465440
C	-3.1884930	-1.8851000	-1.0591730	C	0.6140370	-0.3423970	0.0256090
C	-1.9648990	-2.6218150	-1.3145750	C	3.0781280	-0.4996580	0.1799940
C	-1.2199410	-1.8877320	-2.2736090	H	3.0767060	0.5876070	0.3105340
C	-1.9712090	-0.6967940	-2.6244980	H	3.0778940	-0.6969740	-0.8975000
C	-4.3275190	-2.3494750	-0.2007250	C	5.5965800	-0.4711690	0.2082370
H	-5.1040960	-2.8181650	-0.8196800	C	0.5618830	1.9784680	-1.2914590
H	-3.9954380	-3.0838210	0.5338150	H	-0.3080760	2.3163520	-1.8612770
H	-4.7858310	-1.5192230	0.3419680	H	1.3757670	1.8301580	-2.0161470
C	-1.6205820	-3.9507330	-0.7066820	C	4.3524060	-1.0879090	0.8135460
H	-1.4573060	-3.8530630	0.3696490	H	4.3320510	-0.9093040	1.8923690
H	-2.4279850	-4.6726590	-0.8762200	H	4.3618370	-2.1717410	0.6665590
H	-0.7086670	-4.3613870	-1.1438260	C	1.7285440	-1.0092930	0.7318070
C	0.0856120	-2.2796250	-2.8992940	C	0.9676820	3.0769730	-0.2853950
H	0.7447490	-1.4151520	-3.0208270	H	0.1637980	3.1970170	0.4482020
H	0.6174900	-3.0153770	-2.2951890	H	1.8550030	2.7488230	0.2702600
H	-0.0809400	-2.7065740	-3.8965710	C	6.1978570	-1.0325760	-0.9267480
C	-4.3959510	0.1627200	-2.1113470	H	5.7813690	-1.9408320	-1.3567670
H	-5.0761750	-0.2793680	-2.8514740	C	7.3272360	-0.4492110	-1.5030740
H	-4.9565010	0.3020780	-1.1843650	H	7.7822980	-0.9034570	-2.3789980

C	1.2545970	4.4173190	-0.9726140	C	1.4065280	1.3955490	-0.5993830
H	2.0447690	4.2828630	-1.7244750	C	0.5829830	1.5397580	-1.7345070
H	0.3594260	4.7391000	-1.5222720	C	0.6642070	2.6792630	-2.5361280
C	6.1586220	0.6918480	0.7531060	C	1.6099890	3.6622330	-2.2584780
H	5.7107780	1.1357700	1.6393430	C	2.4944730	3.5177840	-1.1739200
C	7.2880020	1.2786520	0.1804740	H	3.0241330	2.3101920	0.5124050
H	7.7122050	2.1763360	0.6218200	H	-0.0117350	2.7639010	-3.3821620
C	7.8757070	0.7099590	-0.9511280	H	1.6777020	4.5444920	-2.8903570
H	8.7572560	1.1630740	-1.3955580	C	-0.3241540	0.4082820	-2.0848170
C	1.6681500	5.5132590	0.0146370	O	-1.3840580	0.5337600	-2.7115640
H	1.8620570	6.4601740	-0.4995120	Rh	1.5932200	-0.6848290	-0.0555280
H	2.5795180	5.2353460	0.5558110	N	0.2503510	-0.7546220	-1.6611630
H	0.8835050	5.6905610	0.7583790	C	-0.7109520	-2.3250200	-3.1332460
H	-1.6056850	-3.8259210	3.1993790	O	-0.5834410	-1.8988620	-1.7725490
H	-2.2249640	-2.2997790	3.9151960	C	3.8393410	-0.9700650	-0.3392980
H	-3.0737580	-3.0496870	2.5275240	C	3.1354010	-2.0469200	-0.9391660
C	-3.5026710	4.7458250	-0.4744400	C	2.4041750	-2.7593690	0.1017050
H	-3.2250790	5.6799780	0.0243980	C	2.6849450	-2.1096570	1.3456130
H	-3.0676850	4.7574090	-1.4789780	C	3.5217730	-0.9737230	1.0735170
H	-4.5939170	4.7569680	-0.5920070	C	3.2106930	-2.4720710	-2.3754380
Cl	1.6551440	-2.8289200	0.4994290	H	4.0546770	-3.1584620	-2.5239350
Cl	1.6367250	-0.6527390	2.5161380	H	2.3012090	-2.9922660	-2.6802190
TS36^{Cl}				H	3.3497190	-1.6202410	-3.0450820
C	2.3707140	2.3930070	-0.3523240	C	1.6501840	-4.0394430	-0.1145390
				H	0.8609480	-3.9081580	-0.8591800

H	2.3268010	-4.8313250	-0.4599360	H	-4.1729470	-0.9373200	1.9036100
H	1.1762140	-4.3807000	0.8066490	C	-1.3808450	-0.8953400	1.4575630
C	2.2576420	-2.5478820	2.7158400	C	-0.5168670	3.2818530	1.3362590
H	1.9975560	-1.6943230	3.3477000	H	-0.1930310	3.5785790	0.3330230
H	1.3874830	-3.2028320	2.6785780	H	-1.5416320	2.9026700	1.2368730
H	3.0741690	-3.0891440	3.2113550	C	-6.3520540	-0.6035750	0.4678820
C	4.7972210	-0.0445900	-1.0289250	H	-6.5369570	-0.9426220	1.4849190
H	4.5819590	0.0258670	-2.0977000	C	-7.4190710	-0.1661970	-0.3160370
H	4.7542960	0.9674540	-0.6196920	H	-8.4257410	-0.1671570	0.0936600
H	5.8282010	-0.4051320	-0.9186950	C	-0.5111420	4.5036490	2.2641730
C	4.1340090	-0.0817440	2.1155150	H	-0.8207640	4.1979620	3.2727310
H	4.4376650	0.8810350	1.6978820	H	0.5172530	4.8792370	2.3604700
H	3.4437650	0.1075170	2.9416100	C	-4.8227240	-0.1619120	-1.3396040
H	5.0323430	-0.5487700	2.5405000	H	-3.8219550	-0.1378800	-1.7617810
C	0.4057420	0.9245170	0.9900930	C	-5.8912330	0.2810150	-2.1239350
C	-0.1337270	-0.2540300	0.9928670	H	-5.6987340	0.6315470	-3.1343000
C	-2.5504900	-0.5380410	0.5269150	C	-7.1917110	0.2793650	-1.6197220
H	-2.2309190	-0.8496230	-0.4708080	H	-8.0190580	0.6258230	-2.2329230
H	-2.6113310	0.5552360	0.5192340	C	-1.4225480	5.6310720	1.7689730
C	-5.0399730	-0.6140440	-0.0292310	H	-1.3964450	6.4916840	2.4453760
C	0.3852560	2.1492610	1.8628460	H	-2.4629050	5.2951950	1.6968650
H	1.4033730	2.5277840	1.9967820	H	-1.1182460	5.9776720	0.7749270
H	0.0269650	1.8283500	2.8469580	H	-1.2627300	-3.2681130	-3.0872700
C	-3.9201270	-1.1382930	0.8573460	H	-1.2664100	-1.5887590	-3.7184450
H	-3.8636490	-2.2296880	0.7602710	H	0.2740930	-2.4953690	-3.5850280

C	3.5498250	4.5658220	-0.9038180	C	1.2923380	-3.0367500	-0.3875740
H	4.2839830	4.6085560	-1.7171330	C	0.4151070	-2.8123320	0.7491140
H	3.1072010	5.5646310	-0.8204330	C	1.1992840	-2.2516520	1.7882850
H	4.0930170	4.3618850	0.0235750	C	3.8735000	-2.9818160	-0.8052980
Cl	-1.7737810	-0.2932900	3.1939440	H	4.1260500	-4.0494860	-0.8371620
Cl	-1.2127950	-2.7056520	1.5867250	H	3.7034940	-2.6490980	-1.8319140
37Cl				H	4.7433650	-2.4442840	-0.4218190
C	1.3819580	1.6896620	2.3260930	C	0.9538820	-3.7512230	-1.6625680
C	1.2917240	1.4660190	0.9281020	H	1.3155950	-3.1991320	-2.5339710
C	2.4975460	1.4145970	0.1770550	H	1.4228880	-4.7441450	-1.6687650
C	3.7288300	1.6163590	0.8373080	H	-0.1215360	-3.8840270	-1.7766760
C	3.7791140	1.8421880	2.2008120	C	-1.0211060	-3.2284620	0.8464770
C	2.5952950	1.8792240	2.9742150	H	-1.5560410	-2.6572610	1.6089010
H	0.4597650	1.7469650	2.8991230	H	-1.5428140	-3.1079230	-0.1036510
H	4.6392970	1.6226120	0.2451110	H	-1.0784330	-4.2878200	1.1305050
H	4.7381030	2.0106630	2.6855600	C	3.7473980	-1.8336120	2.2191120
C	2.4699920	1.3005470	-1.3439760	H	3.8929300	-2.5592190	3.0296360
O	2.7356600	2.2496820	-2.0801370	H	4.6790230	-1.7722750	1.6533540
Rh	1.3220970	-0.9090920	-0.0081760	H	3.5726240	-0.8566550	2.6789950
N	2.1774740	0.0177150	-1.6485840	C	0.7398000	-1.8970250	3.1727210
C	2.9501640	-0.2472670	-3.8456060	H	1.2834020	-1.0328950	3.5622040
O	1.8088820	-0.2538360	-2.9869660	H	-0.3257440	-1.6562300	3.1918760
C	2.5994080	-2.2520280	1.3521630	H	0.9056800	-2.7334610	3.8648130
C	2.6579190	-2.7542310	0.0414440	C	-0.0509590	1.4662600	0.2411500
				C	-0.3129180	0.3221150	-0.4209740

C	-2.8114050	-0.0985880	-0.3129210	C	-7.3054220	-0.7474840	1.9679940
H	-2.8854400	0.8068620	0.2967380	H	-8.0905760	-0.8414300	2.7127920
H	-2.5794440	-0.9155080	0.3777800	C	-0.2908250	6.4675490	-0.8006090
C	-5.2769400	-0.5041790	0.0268830	H	-0.8879380	7.3775660	-0.6780560
C	-0.8402210	2.7579600	0.3780040	H	-0.1504340	6.3010670	-1.8742220
H	-0.9607680	2.9796620	1.4492700	H	0.6975990	6.6553760	-0.3660090
H	-1.8459450	2.6449740	-0.0291630	H	2.5712400	-0.5415840	-4.8282620
C	-4.1664930	-0.3684340	-0.9942630	H	3.3935660	0.7507050	-3.8981990
H	-4.3896820	0.4512040	-1.6836570	H	3.7042850	-0.9728800	-3.5103260
H	-4.0968740	-1.2802280	-1.5940340	C	2.6640040	2.1532500	4.4581340
C	-1.5755820	0.0727080	-1.2169440	H	3.2885460	1.4145250	4.9739490
C	-0.1594970	3.9653160	-0.2979320	H	3.1048170	3.1369420	4.6570790
H	0.8439850	4.1077320	0.1231000	H	1.6714540	2.1337590	4.9161520
H	-0.0141930	3.7421640	-1.3606630	Cl	-1.4162050	-1.4169760	-2.2755110
C	-5.6538050	-1.7610640	0.5196960	Cl	-1.8924940	1.4532770	-2.4155540
H	-5.1610640	-2.6522510	0.1371490				
C	-6.6584100	-1.8845710	1.4811590	38^{Cl}			
H	-6.9400280	-2.8691600	1.8446520	C	-1.2174040	3.4602760	-0.6665140
C	-0.9650700	5.2608790	-0.1397120	C	-0.7331160	2.2935200	-0.0443580
H	-1.9658720	5.1201030	-0.5706000	C	-1.0439720	2.0808690	1.3160420
H	-1.1203490	5.4676000	0.9289780	C	-1.7884260	3.0498580	2.0037220
C	-5.9370940	0.6289590	0.5234620	C	-2.2697010	4.1867570	1.3634240
H	-5.6652710	1.6118160	0.1450620	C	-1.9950640	4.4067980	0.0058060
C	-6.9415070	0.5111730	1.4848850	H	-0.9751860	3.6386790	-1.7112300
H	-7.4444990	1.4016370	1.8519500	H	-1.9702910	2.9051970	3.0647800

H	-2.8500280	4.9170890	1.9226290	H	-3.5977450	1.9866210	-0.4932930
C	-0.4951540	0.9377340	2.1527510	H	-5.1856320	1.2360310	-0.2569430
O	0.2649430	1.1910120	3.0918500	H	-4.0583370	1.3926560	1.0986990
Rh	-1.5998910	-0.9962620	0.0222290	C	-2.8358670	0.3290600	-2.7752200
N	-1.0208240	-0.2909290	1.8716480	H	-2.5124760	1.3222890	-2.4569730
C	-0.9815900	-1.4119850	3.9387730	H	-2.0766760	-0.0700640	-3.4511060
O	-0.4069130	-1.3318420	2.6372980	H	-3.7676200	0.4455440	-3.3440640
C	-3.5734190	-0.1632340	-0.3071270	C	0.2059320	1.3755200	-0.7586440
C	-3.8143000	-1.3694750	0.4844040	C	0.0280270	0.0370190	-0.6822180
C	-3.3440890	-2.4652230	-0.2546040	C	2.4692210	-0.7938710	-0.3748840
C	-2.8516970	-1.9768630	-1.5513640	H	2.2908970	-0.6138010	0.6904550
C	-3.0584060	-0.5749390	-1.5995080	H	2.8907470	0.1265640	-0.7843180
C	-4.4496290	-1.3725360	1.8422350	C	4.8215370	-1.5780860	0.0740550
H	-5.5255910	-1.1707890	1.7645810	C	1.3409980	2.0757830	-1.4998120
H	-4.3276170	-2.3345230	2.3453390	H	0.8934660	2.7682110	-2.2267360
H	-4.0105830	-0.6016630	2.4811300	H	1.9026790	1.3604450	-2.1060680
C	-3.3464480	-3.9092280	0.1532290	C	3.4900960	-1.9337310	-0.5564670
H	-3.4871720	-4.0254970	1.2298720	H	3.0991300	-2.8492090	-0.1011030
H	-4.1558190	-4.4511920	-0.3525760	H	3.6263120	-2.1356760	-1.6232190
H	-2.4085910	-4.4031030	-0.1172210	C	1.0900730	-0.9725960	-1.0142860
C	-2.3784360	-2.8570420	-2.6712670	C	2.3004100	2.8828230	-0.6027780
H	-1.7715680	-2.2998880	-3.3876560	H	1.7280720	3.6317010	-0.0426960
H	-1.7705640	-3.6870780	-2.3023530	H	2.7462090	2.2216400	0.1511230
H	-3.2322290	-3.2865530	-3.2119010	C	5.8568320	-1.0320740	-0.6961490
C	-4.1254380	1.1880890	0.0292330	H	5.7093730	-0.8904480	-1.7644930

C	7.0732420	-0.6752370	-0.1115360	TS39^{Cl}			
H	7.8656520	-0.2570820	-0.7262230	C	-1.6897950	3.3941200	-0.6336030
C	3.4130260	3.5775130	-1.3987460	C	-1.0352730	2.3049310	-0.0255360
H	3.9853050	2.8251600	-1.9593510	C	-1.3131420	2.0194580	1.3267260
H	2.9614550	4.2371790	-2.1528650	C	-2.1978560	2.8536580	2.0260130
C	5.0343010	-1.7594060	1.4478180	C	-2.8478330	3.9120590	1.4013850
H	4.2420860	-2.1839680	2.0601780	C	-2.6075600	4.1960570	0.0488610
C	6.2481140	-1.4030520	2.0361670	H	-1.4759830	3.6244990	-1.6744410
H	6.3946350	-1.5520280	3.1022650	H	-2.3522730	2.6666980	3.0845100
C	7.2720350	-0.8592670	1.2576500	H	-3.5365010	4.5336780	1.9690170
H	8.2182370	-0.5837370	1.7145340	C	-0.5874130	0.9759500	2.1556870
C	4.3665760	4.3868920	-0.5139380	O	0.0644790	1.3584580	3.1345400
H	5.1489560	4.8716410	-1.1073560	Rh	-1.3631580	-1.1212000	-0.0158700
H	4.8578930	3.7456120	0.2261570	N	-0.8259080	-0.3234410	1.8276690
H	3.8294140	5.1694740	0.0337340	C	-0.6655150	-1.4260010	3.8976460
H	-0.7884750	-0.4966610	4.5055740	O	-0.0631000	-1.2245970	2.6231830
H	-2.0608350	-1.6072370	3.8853910	C	-3.4672650	-0.5490340	-0.2864410
H	-0.4844320	-2.2569420	4.4247400	C	-3.4631500	-1.7467490	0.5411640
C	-2.4982630	5.6472160	-0.6955510	C	-2.8748180	-2.7926690	-0.2057540
H	-2.0355520	6.5517920	-0.2830320	C	-2.5280620	-2.2728660	-1.5279550
H	-2.2760490	5.6207300	-1.7661220	C	-2.9382850	-0.9108330	-1.5818730
H	-3.5820070	5.7621600	-0.5801360	C	-4.0371270	-1.8219660	1.9236670
Cl	0.3760400	-2.5786520	-0.2533160	H	-5.1334310	-1.8544350	1.8789550
Cl	1.2437930	-1.2937970	-2.8236960	H	-3.6969770	-2.7129680	2.4553660
				H	-3.7509120	-0.9498180	2.5161160

C	-2.6430740	-4.2074250	0.2284690	C	3.6058580	-1.5303840	-0.8493560
H	-2.8881960	-4.3517310	1.2824440	H	3.2181700	-2.5205480	-0.5934870
H	-3.2627200	-4.8948000	-0.3606940	H	3.8085880	-1.5273870	-1.9244460
H	-1.5963420	-4.4950560	0.0835610	C	1.1819000	-0.5805430	-1.1932860
C	-1.9865810	-3.1049200	-2.6521630	C	1.9056510	3.3098680	-0.5443070
H	-1.5873660	-2.4818510	-3.4548700	H	1.2448020	3.9290730	0.0736000
H	-1.1816450	-3.7598180	-2.3092070	H	2.4584850	2.6697680	0.1557240
H	-2.7775800	-3.7356430	-3.0788430	C	5.9775420	-0.6376480	-0.7115910
C	-4.2150500	0.7073140	0.0398180	H	5.9115250	-0.3743490	-1.7650110
H	-3.8241570	1.5686970	-0.5026340	C	7.1491840	-0.3654390	-0.0024930
H	-5.2743050	0.5900350	-0.2290540	H	7.9871390	0.1091450	-0.5056990
H	-4.1652140	0.9397790	1.1043710	C	2.8862780	4.2073610	-1.3094090
C	-2.8926530	-0.0075030	-2.7780890	H	3.5400000	3.5843650	-1.9360450
H	-2.7136050	1.0290430	-2.4848170	H	2.3237900	4.8478650	-2.0030870
H	-2.1074550	-0.3021030	-3.4773600	C	4.9937530	-1.5923970	1.2698020
H	-3.8504690	-0.0432250	-3.3133510	H	4.1564870	-2.0748350	1.7686090
C	0.0261770	1.5595430	-0.7601430	C	6.1618040	-1.3200470	1.9819210
C	0.0761040	0.2075080	-0.7636990	H	6.2278280	-1.5904580	3.0319990
C	2.5257800	-0.4862950	-0.5197180	C	7.2439140	-0.7054720	1.3475270
H	2.3340020	-0.4458270	0.5556880	H	8.1545740	-0.4957160	1.9013040
H	2.8945260	0.5122600	-0.8024110	C	3.7443280	5.0805230	-0.3881740
C	4.8859120	-1.2538050	-0.0868240	H	4.4291150	5.7135240	-0.9621710
C	1.0527030	2.4297930	-1.4796770	H	4.3469740	4.4670160	0.2906030
H	0.5247290	3.0880750	-2.1829590	H	3.1201500	5.7370000	0.2282320
H	1.7052370	1.8109390	-2.1041120	H	-0.6870190	-0.4951660	4.4720800

H	-1.6785080	-1.8379440	3.7993780	C	-1.3907860	-1.9179150	-1.7133430
H	-0.0281830	-2.1564240	4.4047850	C	-2.1231390	-0.7280730	-2.0765120
C	-3.2945990	5.3557920	-0.6340610	C	-3.3999190	-0.7825660	-1.4129530
H	-2.9440060	6.3155640	-0.2356330	C	-3.4161020	-1.9318800	-0.5712440
H	-3.1055210	5.3566270	-1.7113410	C	-0.1213350	-2.3531320	-2.3795630
H	-4.3793400	5.3246310	-0.4828760	H	-0.3559690	-2.7479070	-3.3768460
Cl	1.1943290	-1.1253660	-2.8707240	H	0.5685840	-1.5166300	-2.5122190
Cl	0.5664340	-2.6912600	-0.1075310	H	0.3918570	-3.1314280	-1.8163910
40Cl				C	-1.7657450	0.2013500	-3.1967250
				H	-0.6884680	0.3649080	-3.2611440
C	1.0549680	1.8841860	-1.5129440	H	-2.0970540	-0.2216590	-4.1550290
C	-0.0196720	1.7352710	-0.6281750	H	-2.2411210	1.1760300	-3.0804670
C	-1.1529710	2.5572640	-0.7707320	C	-4.5130290	0.1915900	-1.6339210
C	-1.1667630	3.5347960	-1.7682310	H	-5.3370340	0.0313200	-0.9377320
C	-0.0898200	3.6760040	-2.6416460	H	-4.1731120	1.2227850	-1.5110480
C	1.0371370	2.8501630	-2.5296850	H	-4.9020390	0.0803890	-2.6536900
H	1.9307990	1.2513690	-1.3930180	C	-1.9066210	-4.0105590	-0.1966840
H	-2.0338780	4.1845020	-1.8351170	H	-1.8834360	-3.9750880	0.8962910
C	-2.3106350	2.4752980	0.1853050	H	-2.7086850	-4.6955200	-0.4984480
O	-2.9401440	3.4958530	0.4724310	H	-0.9599930	-4.4216940	-0.5458280
Rh	-1.7080690	-0.6174670	0.1588060	C	-4.5503850	-2.4589660	0.2545760
N	-2.6033680	1.2277280	0.6955930	H	-4.2264790	-2.6457300	1.2828360
C	-4.5731420	0.9706280	1.9422150	H	-5.3942840	-1.7675670	0.2781560
O	-3.2053430	1.3503190	1.9500940	H	-4.9083760	-3.4077100	-0.1645290
C	-2.1680630	-2.6498460	-0.7679180	C	0.0493660	0.7920470	0.5327190

C	0.4223470	-0.5365280	0.4286560	H	8.0889680	-2.1263390	1.0980380
C	2.8887830	-0.9829970	0.6495040	C	7.8888190	-0.3865990	-0.1607520
H	3.3215230	-1.3285530	1.5966130	H	8.9304600	-0.0942970	-0.0644850
H	2.9524960	0.1080430	0.6444760	C	2.7743310	3.4770620	3.9277330
C	5.1895040	-1.1492350	-0.4161470	H	2.7219180	4.0198850	4.8771120
C	0.0875600	1.4379870	1.9259090	H	3.0961560	4.1866780	3.1567090
H	-0.1645730	0.6825160	2.6728530	H	3.5566910	2.7152720	4.0233470
H	-0.6755220	2.2161010	1.9922350	H	-5.1505120	1.5998020	1.2551740
C	3.7321770	-1.5441450	-0.5219300	H	-4.6895110	-0.0883480	1.6895260
H	3.6412440	-2.6349540	-0.5344890	H	-4.9195010	1.1301620	2.9663250
H	3.3130390	-1.1782460	-1.4672270	H	-0.1196350	4.4384990	-3.4160520
C	1.4289820	-1.3804570	0.6034780	C	2.2246180	3.0268060	-3.4465210
C	1.4560440	2.0725050	2.2459400	H	2.9355120	3.7534400	-3.0335790
H	2.2277100	1.2960360	2.3070430	H	2.7671420	2.0870940	-3.5896220
H	1.7541780	2.7541140	1.4377520	H	1.9194360	3.3959850	-4.4301650
C	5.6782600	-0.0083020	-1.0663190	Cl	-1.8515180	-1.4774090	2.3944170
H	5.0059910	0.5848150	-1.6827550	Cl	1.1942030	-3.1246720	0.8094090
C	7.0155720	0.3718990	-0.9419260				
H	7.3756210	1.2576070	-1.4580290	TS41^{Cl}			
C	1.4243510	2.8463140	3.5722490	C	-1.4153560	1.5872730	1.6691450
H	0.6557300	3.6277610	3.5142370	C	-0.2877880	1.6139570	0.8393630
H	1.1106170	2.1682380	4.3766500	C	0.8280420	2.3764320	1.2097860
C	6.0781950	-1.9029900	0.3637540	C	0.7862280	3.1479730	2.3725930
H	5.7183560	-2.7958620	0.8699730	C	-0.3486840	3.1367320	3.1784780
C	7.4154660	-1.5266310	0.4921500	C	-1.4642750	2.3533410	2.8421720

H	-2.2732930	0.9828320	1.3893740	C	2.0597040	-4.0983210	-0.1595200
H	1.6542390	3.7508330	2.6211020	H	2.0453070	-3.9793890	-1.2463920
C	2.0146000	2.3955360	0.3071010	H	2.8558230	-4.8083750	0.0981480
O	2.8342730	3.3182880	0.3297570	H	1.1073020	-4.5309220	0.1463540
Rh	1.7073840	-0.7600310	-0.1596180	C	4.6193660	-2.3715580	-0.6265640
N	2.0303820	1.3463260	-0.5853330	H	4.2200020	-2.5354210	-1.6316050
C	3.9936880	1.3302860	-1.9069830	H	5.3913650	-1.6017990	-0.6856660
O	2.6236310	1.7135330	-1.7942170	H	5.0984050	-3.3011680	-0.2942940
C	2.3121120	-2.7841640	0.5170890	C	-0.2755690	0.8705990	-0.4558540
C	1.5640150	-2.1784890	1.5725160	C	-0.3885280	-0.5279450	-0.4628630
C	2.2578450	-0.9863640	1.9895300	C	-2.8560740	-0.9776290	-0.8535080
C	3.4952330	-0.9094700	1.2396030	H	-3.2276790	-1.3136370	-1.8293950
C	3.5231020	-1.9929750	0.3222150	H	-2.9429830	0.1136340	-0.8377110
C	0.3394980	-2.7251580	2.2420520	C	-5.2186850	-1.1887530	0.0613140
H	0.6358700	-3.3039980	3.1267920	C	-0.4984160	1.5852240	-1.7803710
H	-0.3230130	-1.9247700	2.5796490	H	-1.5097400	1.2765570	-2.0913130
H	-0.2279040	-3.3794530	1.5808550	H	0.1798170	1.1316220	-2.5116270
C	1.9090340	-0.1500880	3.1847710	C	-3.7663240	-1.5695250	0.2518180
H	0.8339280	0.0304930	3.2582060	H	-3.6612640	-2.6590480	0.2465580
H	2.2263210	-0.6574750	4.1060310	H	-3.4121540	-1.2214180	1.2297410
H	2.4055600	0.8205950	3.1539770	C	-1.3962260	-1.3553560	-0.7318990
C	4.5586350	0.1252240	1.4539110	C	-0.4032060	3.1131480	-1.8227510
H	5.3316390	0.0717090	0.6858690	H	-1.0409170	3.5543740	-1.0454050
H	4.1524530	1.1402840	1.4451260	H	0.6222040	3.4341250	-1.6176310
H	5.0411750	-0.0331420	2.4264820	C	-5.7627260	-0.0682620	0.7032970

H	-5.1392620	0.5178350	1.3752980	Cl	-1.1423140	-3.0948920	-0.9892120
C	-7.0936350	0.3007950	0.5007530				
H	-7.4969950	1.1705400	1.0119960	42^{Cl}			
C	-0.8254690	3.6609550	-3.1943280	C	-2.1563600	1.4983760	1.3113980
H	-0.1911980	3.2124720	-3.9699910	C	-0.8466800	1.5810290	0.8313090
H	-1.8538030	3.3431130	-3.4169190	C	0.1128800	2.2426470	1.5965410
C	-6.0460130	-1.9333930	-0.7915920	C	-0.1876250	2.8232650	2.8343620
H	-5.6432570	-2.8100770	-1.2937190	C	-1.4898140	2.7330820	3.2995270
C	-7.3766300	-1.5684170	-0.9980530	C	-2.4872470	2.0808720	2.5415900
H	-8.0021860	-2.1611200	-1.6596880	H	-2.9353990	1.0092280	0.7383300
C	-7.9051970	-0.4487470	-0.3521690	H	0.5864330	3.3391330	3.3939750
H	-8.9418790	-0.1654390	-0.5095520	C	1.3834460	2.3001040	0.8876260
C	-0.7328430	5.1875430	-3.2770400	O	2.4018950	2.8901900	1.1878290
H	-1.0346060	5.5522730	-4.2643620	Rh	2.0078220	-0.5305310	-0.1974660
H	0.2912210	5.5303130	-3.0925180	N	1.2396550	1.5256970	-0.3510520
H	-1.3806150	5.6656390	-2.5330610	C	3.0024720	2.3787060	-1.7518600
H	4.5990050	1.8587390	-1.1640920	O	1.5994400	2.3734230	-1.4474410
H	4.1007550	0.2456260	-1.8172800	C	3.0351620	-2.4068110	0.2754780
H	4.2884920	1.6342930	-2.9141540	C	2.3333560	-1.9792630	1.4531720
H	-0.3741850	3.7384880	4.0835680	C	2.8718840	-0.7078790	1.8406660
C	-2.7048330	2.3629380	3.7040330	C	4.0106390	-0.4131500	0.9701040
H	-3.3750120	3.1837590	3.4196000	C	4.1098090	-1.4440070	0.0222280
H	-3.2700520	1.4312000	3.6066050	C	1.3066290	-2.7511080	2.2276510
H	-2.4561520	2.5003220	4.7606100	H	1.7899900	-3.2741730	3.0636550
Cl	1.7906250	-1.3087840	-2.5059670	H	0.5410100	-2.0931820	2.6464670

H	0.8039120	-3.4897990	1.6050170	H	-0.2320670	1.3033630	-2.5784050
C	2.5454150	0.0285980	3.1078530	C	-3.2868440	-2.0553760	0.2826330
H	1.4923410	-0.0828890	3.3776170	H	-3.0180610	-3.1166920	0.2626760
H	3.1439690	-0.3673440	3.9397200	H	-3.0003650	-1.6774510	1.2706960
H	2.7660090	1.0947980	3.0245190	C	-0.9617420	-1.4166660	-0.6132580
C	4.9307590	0.7597530	1.1423800	C	-1.2757090	3.0509480	-1.8004270
H	5.5773300	0.8949140	0.2725660	H	-2.0251380	3.2729530	-1.0290320
H	4.3743230	1.6863520	1.3005390	H	-0.3973070	3.6626330	-1.5719970
H	5.5781730	0.6049470	2.0154320	C	-5.5626810	-1.2148340	1.0309280
C	2.9259970	-3.7223930	-0.4370030	H	-5.0901730	-0.8235720	1.9289160
H	2.8370090	-3.5741240	-1.5164570	C	-6.9377570	-1.0510520	0.8463970
H	3.8234840	-4.3259150	-0.2476040	H	-7.5242640	-0.5241500	1.5942860
H	2.0583840	-4.2909010	-0.1032270	C	-1.8307420	3.4619740	-3.1713140
C	5.1200530	-1.5947000	-1.0738460	H	-1.0774080	3.2503350	-3.9414580
H	4.6229750	-1.6986550	-2.0434600	H	-2.7005210	2.8367890	-3.4169240
H	5.7913510	-0.7348340	-1.1258570	C	-5.4190370	-2.4163570	-1.0479320
H	5.7322010	-2.4895670	-0.9071680	H	-4.8367960	-2.9614320	-1.7869260
C	-0.2457790	1.0392320	-0.4606760	C	-6.7909110	-2.2532840	-1.2384260
C	-0.0265630	-0.4809450	-0.4145610	H	-7.2646840	-2.6667920	-2.1244970
C	-2.4587390	-1.3166110	-0.7987720	C	-7.5563140	-1.5667640	-0.2924550
H	-2.7192920	-1.7227540	-1.7843540	H	-8.6250680	-1.4410980	-0.4401440
H	-2.7619240	-0.2692220	-0.8098930	C	-2.2293750	4.9396890	-3.2369150
C	-4.7802390	-1.8940660	0.0875240	H	-2.6163870	5.2061160	-4.2259130
C	-0.9063940	1.5599390	-1.7580110	H	-1.3718620	5.5897700	-3.0288060
H	-1.8123660	0.9708720	-1.9153660	H	-3.0073370	5.1746140	-2.5011640

H	3.5752610	2.8523030	-0.9525610
H	3.3530760	1.3681230	-1.9666570
H	3.0574790	2.9823850	-2.6611470
H	-1.7581230	3.1801570	4.2530360
C	-3.9036900	2.0280870	3.0611560
H	-4.5814080	1.5682750	2.3380370
H	-3.9594790	1.4515440	3.9922150
H	-4.2783030	3.0329790	3.2854230
Cl	2.0448250	-0.7822720	-2.6040300
Cl	-0.4589900	-3.1323840	-0.7803410

2'F

C	2.3382970	0.4292810	0.4369660
C	1.1805450	0.0923450	0.5167360
C	3.7468630	0.8068190	0.3455520
H	4.0780670	1.1865680	1.3214370
H	3.8511470	1.6441960	-0.3576330
C	4.6625610	-0.3553910	-0.0940130
H	4.5472980	-1.1863940	0.6122340
H	4.3234630	-0.7286070	-1.0681170
C	6.1358750	0.0581360	-0.1780750
H	6.4628690	0.4360600	0.8001170
H	6.2377250	0.8985440	-0.8781870
C	7.0524220	-1.0875400	-0.6169890
H	8.0968760	-0.7644190	-0.6692320

H	6.9986020	-1.9285020	0.0832270
H	6.7701240	-1.4634460	-1.6066780
C	-0.2214250	-0.3156340	0.5857460
F	-0.6862250	-0.1634430	1.8669610
F	-0.3225750	-1.6558450	0.2840810
C	-1.1501920	0.4436590	-0.3904290
H	-0.7528480	0.2380670	-1.3969660
C	-2.5856900	-0.0473000	-0.3063120
C	-3.4402450	0.4448970	0.6875320
C	-3.0614500	-1.0089190	-1.2030600
C	-4.7538270	-0.0137750	0.7742410
H	-3.0659100	1.1896600	1.3812910
C	-4.3742680	-1.4724570	-1.1132070
H	-2.4013160	-1.3978140	-1.9740700
C	-5.2237200	-0.9740760	-0.1244870
H	-5.4110680	0.3759430	1.5463200
H	-4.7337280	-2.2179870	-1.8165620
H	-6.2474720	-1.3304240	-0.0555800
O	-1.0087850	1.8134750	-0.0707330
C	-1.4564040	2.6866430	-1.0944650
H	-2.5265270	2.5591350	-1.3037450
H	-1.2802670	3.7037990	-0.7386790
H	-0.8936080	2.5312850	-2.0271200

2'Cl

C	2.3934150	-0.1332480	0.7503760	C	-5.1947000	0.0904860	-0.8929630
C	1.2169820	-0.3728950	0.6031190	H	-5.4587870	0.6272540	1.1783230
C	3.8172780	0.1431190	0.9229040	H	-4.6143660	-0.3892010	-2.9138240
H	4.2346860	-0.5761090	1.6404980	H	-6.2575230	-0.0272700	-1.0827750
H	3.9382630	1.1344460	1.3804910	O	-0.7066980	1.6199740	0.7857800
C	4.6196440	0.0804380	-0.3944760	C	-0.8530390	2.9235570	0.2434350
H	4.4879450	-0.9103720	-0.8456780	H	-1.8800690	3.1145410	-0.0938560
H	4.1983120	0.8025940	-1.1045590	H	-0.6026220	3.6222940	1.0443240
C	6.1109360	0.3646310	-0.1845100	H	-0.1663390	3.0842500	-0.6008670
H	6.5192420	-0.3574140	0.5354990	Cl	-0.9010840	-1.2140650	2.0055900
H	6.2301430	1.3544280	0.2767110	Cl	-0.3571600	-2.0317280	-0.7905640
C	6.9191290	0.3043130	-1.4838380				
H	7.9788340	0.5101610	-1.3033100	TS10^F			
H	6.8466770	-0.6846710	-1.9497990	C	3.3258420	-1.6389000	0.0367840
H	6.5564030	1.0393630	-2.2109770	C	2.3143290	-0.7450040	0.4380380
C	-0.1876230	-0.6574460	0.4186000	C	2.4593790	-0.0919480	1.6773200
C	-0.9638190	0.5835040	-0.1402540	C	3.5492380	-0.3686410	2.5056780
H	-0.4611490	0.7956640	-1.0969670	C	4.5305060	-1.2650580	2.0937620
C	-2.4496810	0.3921340	-0.3999860	C	4.4401650	-1.8984980	0.8405240
C	-3.3816140	0.6098410	0.6228580	H	3.2403010	-2.1619280	-0.9129530
C	-2.9087090	0.0424610	-1.6751950	H	3.6079760	0.1429780	3.4619680
C	-4.7456720	0.4573370	0.3770480	H	5.3810080	-1.4736470	2.7383630
H	-3.0288080	0.9069090	1.6036380	C	1.4465410	0.9354340	2.0593560
C	-4.2728830	-0.1142150	-1.9203550	O	1.2040710	1.2716820	3.2191050
H	-2.1949820	-0.1122710	-2.4791530	Rh	1.0732950	0.4167620	-0.8893770

N	0.8911350	1.4461270	0.9195760	H	3.8115740	2.9324830	-1.1963970
C	-0.1388150	3.5143570	1.4083020	C	-0.3125010	3.1762800	-2.1605930
O	0.8548180	4.1397960	1.1056960	H	0.0232390	3.8186190	-1.3451440
O	-0.2969890	2.1759990	1.2282640	H	-0.3544850	3.7878260	-3.0720270
C	-1.3859350	4.1093870	2.0792680	H	-1.3262170	2.8381390	-1.9343440
C	-1.3692120	5.6346150	1.8893440	C	-0.9913180	0.3732320	-3.5994620
H	-1.4529640	5.9062050	0.8317340	H	-1.2742090	-0.6450500	-3.3207900
H	-2.2136140	6.0835600	2.4230340	H	-1.7956970	1.0364720	-3.2805360
H	-0.4426430	6.0687950	2.2712890	H	-0.9275010	0.4197930	-4.6945720
C	-1.2831160	3.7590830	3.5846720	C	4.0669720	0.4596230	-2.5489560
H	-1.2049710	2.6800050	3.7315100	H	4.5241330	0.7834850	-3.4929350
H	-0.3975690	4.2200360	4.0325310	H	4.6138850	0.9355530	-1.7324620
H	-2.1695630	4.1339820	4.1086060	H	4.2183050	-0.6181180	-2.4638130
C	-2.6801680	3.5112260	1.4904500	C	1.6715970	-1.3326800	-3.7174260
H	-2.7725060	3.7381490	0.4224200	H	2.4997370	-1.9121970	-3.3009990
H	-2.7161590	2.4275060	1.6105990	H	0.7587060	-1.9247180	-3.6133220
H	-3.5460580	3.9489880	1.9996020	H	1.8671520	-1.2116690	-4.7914190
C	2.6117060	0.8222860	-2.5295590	F	-2.2444350	-0.1972320	1.2768770
C	2.0601390	2.0486980	-2.0807550	F	-2.3581160	0.3994620	-0.8411650
C	0.6232440	2.0190160	-2.3532870	C	0.5142930	-1.5444420	0.1561120
C	0.3227320	0.7796860	-2.9982950	C	-0.4343860	-0.7128330	-0.0993380
C	1.5308790	0.0036490	-3.0459310	C	-2.7140670	-1.8852380	-0.2814260
C	2.7998940	3.2153770	-1.4966790	H	-2.4040190	-2.6040600	0.4932940
H	2.8859500	4.0209200	-2.2378300	C	0.6871100	-3.0136530	0.4083480
H	2.2851410	3.6099390	-0.6165480	H	1.5126980	-3.4032780	-0.1950270

H	-0.2234180	-3.5045580	0.0414840
C	-1.9094120	-0.5896660	-0.0007700
C	0.9151000	-3.3791780	1.8870950
H	1.8239050	-2.8874620	2.2484130
H	0.0872430	-2.9794130	2.4865880
C	1.0252420	-4.8942900	2.1003350
H	0.1187350	-5.3856940	1.7195440
H	1.8580890	-5.2844080	1.4988620
C	1.2336110	-5.2750080	3.5695180
H	1.3116710	-6.3600470	3.6936730
H	0.4005830	-4.9269470	4.1903570
H	2.1502760	-4.8258230	3.9672630
C	5.5288390	-2.8403930	0.3792770
H	5.7536310	-3.5944580	1.1415770
H	5.2458140	-3.3643760	-0.5383730
H	6.4622630	-2.3007000	0.1787980
C	-4.2121740	-1.6560330	-0.1690420
C	-4.9401200	-1.1573070	-1.2567760
C	-4.8756740	-1.9199550	1.0338510
C	-6.3121020	-0.9354740	-1.1424240
H	-4.4253130	-0.9535010	-2.1896790
C	-6.2470890	-1.6905880	1.1512380
H	-4.3165400	-2.3028570	1.8836330
C	-6.9685810	-1.1992730	0.0620570
H	-6.8691220	-0.5523790	-1.9928340

H	-6.7509030	-1.8987550	2.0907020
H	-8.0370080	-1.0243570	0.1502980
O	-2.3055340	-2.3441290	-1.5597350
C	-2.7312760	-3.6665630	-1.8583920
H	-3.8245300	-3.7456010	-1.8936860
H	-2.3202910	-3.9144900	-2.8391250
H	-2.3493550	-4.3849620	-1.1177650
TS10^{Cl}			
C	-2.6787900	-2.5673930	-0.0063890
C	-2.0213250	-1.3860330	-0.4004590
C	-2.4197750	-0.7774450	-1.6058640
C	-3.3935660	-1.3686950	-2.4142940
C	-4.0148390	-2.5472900	-2.0143750
C	-3.6787840	-3.1517450	-0.7891470
H	-2.3940690	-3.0577930	0.9211810
H	-3.6529630	-0.8718720	-3.3446160
H	-4.7754610	-3.0018220	-2.6445950
C	-1.8360810	0.5462100	-1.9707850
O	-1.8168770	1.0018490	-3.1155320
Rh	-1.1678850	0.0697430	0.9392060
N	-1.4017570	1.1596550	-0.8321170
C	-1.2999480	3.4682490	-1.2816800
O	-2.4408650	3.6373010	-0.9068680
O	-0.6074890	2.3032400	-1.1460020

C	-0.4635420	4.5268500	-2.0150640	H	0.1561400	3.2069380	2.0454700
C	-0.9644610	5.9213130	-1.6018540	C	0.7924390	0.7597360	3.6891490
H	-0.7643350	6.1182480	-0.5427830	H	1.4861350	0.0088150	3.3029870
H	-0.4512530	6.6891160	-2.1903140	H	1.2315370	1.7408360	3.5058250
H	-2.0402520	6.0152220	-1.7632100	H	0.7118550	0.6249160	4.7758520
C	-0.7259440	4.2939620	-3.5251830	C	-3.9291970	-1.0388300	2.6500170
H	-0.4739280	3.2706530	-3.8123290	H	-4.4993910	-0.8377140	3.5662010
H	-1.7805680	4.4577750	-3.7658190	H	-4.5888280	-0.8553790	1.7995140
H	-0.1234770	4.9957270	-4.1128360	H	-3.6743490	-2.1001190	2.6505470
C	1.0421790	4.3924980	-1.7229010	C	-1.0044240	-1.8317640	3.7366900
H	1.2560970	4.5109580	-0.6555790	H	-1.5693860	-2.6721890	3.3247810
H	1.4299080	3.4223560	-2.0372980	H	0.0592830	-2.0389850	3.5950430
H	1.5852980	5.1761410	-2.2627860	H	-1.1977370	-1.8081910	4.8176920
C	-2.7087210	-0.1671880	2.6115580	C	-0.0628270	-1.5762870	-0.1734610
C	-2.6679970	1.1842380	2.1862020	C	0.6104050	-0.4975350	0.0583780
C	-1.3238010	1.6938720	2.4528350	C	3.0761320	-1.0652710	0.3628560
C	-0.5701420	0.6488620	3.0701340	H	2.8930610	-1.9553890	-0.2563730
C	-1.3910030	-0.5293440	3.0955820	C	0.2101840	-3.0207490	-0.4870760
C	-3.8099350	1.9928610	1.6468050	H	-0.4564320	-3.6665720	0.0911610
H	-4.1809900	2.6862490	2.4131520	H	1.2277840	-3.2434970	-0.1422050
H	-3.5056800	2.5744720	0.7728350	C	2.0065450	-0.0265770	-0.1305800
H	-4.6422930	1.3496370	1.3514370	C	0.0907920	-3.3678520	-1.9839180
C	-0.9045100	3.1255090	2.2915980	H	-0.9270290	-3.1555820	-2.3260420
H	-1.4762350	3.6127880	1.5004420	H	0.7554290	-2.7092140	-2.5562740
H	-1.0812910	3.6796590	3.2232980	C	0.4371150	-4.8345870	-2.2716590

H	1.4561810	-5.0483210	-1.9197270	H	3.0674050	-3.4128270	1.6166860
H	-0.2294460	-5.4854910	-1.6887580	Cl	2.2870490	1.5774140	0.6714470
C	0.3252450	-5.1887310	-3.7580570	Cl	2.2846120	0.2029460	-1.9334740
H	0.5713860	-6.2402980	-3.9381650				
H	1.0052270	-4.5780090	-4.3622490	TS52			
H	-0.6908400	-5.0141620	-4.1286150	C	1.2464650	2.5682800	2.1798100
C	-4.3893210	-4.4057540	-0.3335970	C	1.3774520	1.9888800	0.9116240
H	-4.4118030	-5.1615620	-1.1261690	C	2.6682350	1.8729670	0.3681280
H	-3.9036640	-4.8497950	0.5404600	C	3.7943580	2.3053850	1.0780820
H	-5.4311790	-4.1958280	-0.0625800	C	3.6397890	2.8771630	2.3372590
C	4.5358920	-0.6694270	0.1931280	C	2.3622270	3.0065970	2.9066270
C	5.1983720	0.0775850	1.1766970	H	0.2567860	2.6705630	2.6137370
C	5.2524740	-1.0938690	-0.9325520	H	4.7797160	2.1916750	0.6398220
C	6.5442140	0.4098680	1.0238460	H	4.5095630	3.2177820	2.8884380
H	4.6552820	0.3885690	2.0619230	C	2.7978260	1.2109680	-1.0119660
C	6.5970830	-0.7564430	-1.0891550	O	2.9988950	1.7447190	-2.1012680
H	4.7536770	-1.6855440	-1.6948750	Rh	1.2942370	-1.2231240	-0.2929170
C	7.2459330	-0.0011510	-0.1113530	N	2.7579850	-0.0832600	-0.5614500
H	7.0455580	0.9903360	1.7931240	C	1.0215270	-0.3145860	-3.3051480
H	7.1371320	-1.0885980	-1.9710350	O	1.7775070	-1.1036560	-2.3236000
H	8.2938370	0.2595110	-0.2292680	C	2.3053260	-2.5351680	1.2704560
O	2.7442300	-1.3504480	1.7135660	C	2.3533060	-3.2268990	0.0207490
C	3.3500280	-2.5347370	2.2154900	C	0.9830750	-3.4950350	-0.3881590
H	4.4435170	-2.4573640	2.2341700	C	0.0992130	-2.9943680	0.6137810
H	2.9814590	-2.6660040	3.2350370	C	0.9089340	-2.3255650	1.6204280

C	3.5748270	-3.6066460	-0.7702190	H	-2.6993400	0.9233450	0.4171140
H	3.4751320	-3.2696070	-1.8076060	H	-2.4416640	-0.8024070	0.6670540
H	4.4694490	-3.1397590	-0.3495200	C	-5.1130090	-0.2930310	0.0162090
H	3.7205800	-4.6952420	-0.7675510	C	-0.7252950	2.8008070	-0.1875560
C	0.6015560	-4.1568170	-1.6810920	H	-0.7539750	3.4703260	0.6797840
H	1.0060450	-3.5740320	-2.5176280	H	-1.7448800	2.5070730	-0.4347670
H	1.0104590	-5.1739610	-1.7328850	C	-3.8990460	-0.3359260	-0.8910420
H	-0.4844490	-4.2066940	-1.7890210	H	-3.9827110	0.4115450	-1.6854830
C	-1.3798470	-3.2657600	0.6817310	H	-3.8028240	-1.3186780	-1.3629400
H	-1.8469930	-2.6871360	1.4830850	C	-1.3733290	0.0078960	-0.9956990
H	-1.8669720	-3.0107560	-0.2606070	C	-0.1526110	3.5701920	-1.4101690
H	-1.5537780	-4.3290740	0.8948500	H	0.9137820	3.7757890	-1.2608020
C	3.4917830	-2.0443280	2.0522740	H	-0.2465640	2.9096760	-2.2779940
H	4.2785590	-1.6895710	1.3806080	C	-5.5295250	-1.4367140	0.7115130
H	3.2115660	-1.2147990	2.7070980	H	-5.0023410	-2.3735230	0.5595870
H	3.9008290	-2.8520800	2.6739370	C	-6.6177500	-1.3841260	1.5846860
C	0.4038600	-1.7175550	2.9021110	H	-6.9314610	-2.2786110	2.1109980
H	1.0492200	-0.8954290	3.2250310	C	-0.9073670	4.8896910	-1.6736830
H	-0.6042000	-1.3151630	2.7695030	H	-1.9762030	4.6744160	-1.8085140
H	0.3727740	-2.4684560	3.7040820	H	-0.8142480	5.5431910	-0.7955620
F	-1.6490500	0.9137290	-2.0629470	C	-5.8115130	0.9060210	0.2144990
F	-1.2973990	-1.2683840	-1.6540690	H	-5.5031170	1.7962400	-0.3244590
C	0.1587310	1.5819480	0.1337570	C	-6.9001070	0.9620420	1.0867450
C	-0.0670490	0.3247030	-0.3149810	H	-7.4332470	1.8958730	1.2250670
C	-2.6045150	-0.0375250	-0.0921170	C	-7.3057890	-0.1834320	1.7756690

H	-8.1527770	-0.1421480	2.4506430	Rh	1.5523870	-1.1356790	-0.4118660
C	-0.3670410	5.6200120	-2.9224670	N	2.8003630	0.1889160	-0.6629260
H	-0.9090190	6.5558700	-3.0995860	C	1.1932510	-0.9717440	-3.3605500
H	-0.4730660	4.9866600	-3.8107240	O	1.3672410	-1.8222200	-2.2510770
H	0.6963700	5.8551190	-2.7985130	C	2.8413510	-1.9330010	1.4038890
H	0.0619450	-0.7928920	-3.5206080	C	2.8933570	-2.9481250	0.4074160
H	0.8471130	0.7085080	-2.9670760	C	1.5531780	-3.4397250	0.1986120
H	1.6381340	-0.2705840	-4.2103860	C	0.6698440	-2.7142130	1.0403860
C	2.1899980	3.6386400	4.2756500	C	1.4605340	-1.7274760	1.7616870
H	1.2813010	3.2746210	4.7652070	C	4.1215000	-3.4657200	-0.2807390
H	3.0458840	3.4169730	4.9212600	H	3.9300150	-3.6403820	-1.3429680
H	2.1107220	4.7299000	4.1838810	H	4.9506510	-2.7595060	-0.1996000
53				H	4.4456320	-4.4178360	0.1595790
C	0.6327660	2.8239090	1.8641370	C	1.1781690	-4.4906570	-0.7949170
C	0.9826170	2.1610980	0.6747040	H	1.1555060	-4.0375440	-1.7972300
C	2.3077650	2.2824220	0.2272700	H	1.9069060	-5.3070280	-0.8020790
C	3.2371310	3.0526900	0.9399690	H	0.1908060	-4.9086130	-0.5863210
C	2.8644940	3.6929860	2.1153910	C	-0.7575920	-3.0794310	1.3252900
C	1.5532570	3.5731340	2.6038390	H	-1.2631620	-2.2968060	1.8937140
H	-0.3894600	2.7522220	2.2267030	H	-1.3240760	-3.2561830	0.4101390
H	4.2497380	3.1434570	0.5577510	H	-0.7951750	-3.9939480	1.9315660
H	3.5914290	4.2890970	2.6616040	C	4.0250660	-1.1776160	1.9257960
C	2.7501760	1.5100310	-0.9812290	H	4.4723670	-0.5687860	1.1314920
O	3.1633580	1.9912900	-2.0330300	H	3.7467600	-0.5095230	2.7433290
				H	4.7883170	-1.8692060	2.2983290

C	0.9564930	-0.8600440	2.8785350	H	-6.7597300	-2.8754630	2.1956480
H	1.5668710	0.0366470	2.9985480	C	-1.7042070	4.6191400	-1.8520490
H	-0.0681670	-0.5314200	2.6926270	H	-2.5063250	4.0845290	-2.3791490
H	0.9661340	-1.4107080	3.8287380	H	-2.1678340	5.0588510	-0.9575860
F	-1.6791100	0.2340090	-2.3216990	C	-5.8728950	0.2732610	0.1257160
F	-1.1982840	-1.7294750	-1.4696190	H	-5.6330420	1.1556700	-0.4634320
C	-0.0916170	1.4821470	-0.1277750	C	-6.9642940	0.2980540	0.9948320
C	-0.0803530	0.1818240	-0.5186900	H	-7.5663870	1.1985510	1.0799270
C	-2.6103960	-0.3690050	-0.2180520	C	-7.2870000	-0.8332110	1.7470220
H	-2.7799150	0.6420990	0.1519570	H	-8.1389780	-0.8174230	2.4206800
H	-2.3956160	-0.9859100	0.6570950	C	-1.1621450	5.7377300	-2.7478360
C	-5.0832910	-0.8775160	-0.0087980	H	-1.9541480	6.4346930	-3.0416020
C	-1.1776620	2.4999150	-0.5191270	H	-0.7187350	5.3305220	-3.6632170
H	-1.6071660	2.9585200	0.3818070	H	-0.3841960	6.3138480	-2.2341110
H	-1.9924630	2.0277740	-1.0614080	H	0.2249050	-0.4614110	-3.3695000
C	-3.8798220	-0.8877280	-0.9260400	H	1.9901490	-0.2136190	-3.4069730
H	-4.0724960	-0.2643140	-1.8047020	H	1.2493340	-1.6004500	-4.2614540
H	-3.6940830	-1.9020770	-1.2919650	C	1.1471310	4.2556440	3.8889460
C	-1.3671910	-0.4006980	-1.1182380	H	0.1079910	4.0364750	4.1489990
C	-0.6214470	3.6197800	-1.4241820	H	1.7776720	3.9372020	4.7270200
H	0.1843460	4.1566290	-0.9104920	H	1.2489280	5.3442610	3.8086640
H	-0.1697550	3.1632270	-2.3138960				
C	-5.4206930	-2.0063330	0.7505360	TS54			
H	-4.8268050	-2.9122510	0.6503140	C	2.5619560	2.4222540	1.6651160
C	-6.5116350	-1.9872030	1.6210210	C	2.0819530	1.5960480	0.6128750

C	3.0377080	0.7720830	-0.0516210	H	-0.6209490	-5.7433400	-0.1911590
C	4.3876710	0.7990170	0.3607470	C	-2.1543620	-3.1562010	1.1667950
C	4.8073690	1.5879370	1.4124660	H	-2.6333870	-2.3127970	1.6699920
C	3.8839170	2.4213200	2.0842030	H	-2.6083100	-3.2578110	0.1763360
H	1.8577820	3.0677790	2.1817820	H	-2.4023220	-4.0640060	1.7323550
H	5.0915700	0.1869360	-0.1937050	C	2.7227550	-1.7677120	2.0997300
H	5.8507830	1.5820340	1.7177170	H	2.9894070	-2.4195590	2.9437910
C	2.7582430	0.0076650	-1.2799700	H	3.5821720	-1.7217740	1.4300460
O	3.6415600	-0.3624970	-2.0577640	H	2.5544210	-0.7623710	2.4905490
Rh	0.3637010	-1.5059150	-0.2216720	C	-0.2741240	-1.2744210	3.0302810
N	1.3998660	-0.2814370	-1.5513010	H	0.2203520	-0.2996830	2.9785840
C	1.4084910	-1.7758890	-3.4077310	H	-1.3532630	-1.1015460	3.0252310
O	1.1464150	-0.4506190	-2.9351610	H	-0.0174080	-1.7287830	3.9961250
C	1.5053170	-2.3117040	1.4156250	F	-1.2438540	1.3976320	-2.2398230
C	1.5219900	-3.3903520	0.4146620	F	-1.2695750	-0.7770430	-1.7528600
C	0.1991040	-3.7902560	0.1994660	C	0.7026690	1.6571110	0.1701310
C	-0.6657950	-2.9805700	1.0731860	C	0.1927530	0.5529260	-0.4986760
C	0.1490790	-2.1573720	1.8943460	C	-2.3934310	0.6801060	-0.2872520
C	2.7697270	-3.9097240	-0.2371950	H	-2.3150230	1.5891290	0.3104940
H	3.3787370	-4.4739130	0.4805150	H	-2.3760310	-0.1559130	0.4155850
H	2.5410640	-4.5752410	-1.0728430	C	-4.9156810	0.7228550	-0.1576850
H	3.3867320	-3.0918800	-0.6221170	C	0.0120590	3.0173130	0.2015830
C	-0.3044180	-4.8468960	-0.7404010	H	0.0170810	3.4248680	1.2219750
H	-1.1700780	-4.4995770	-1.3137470	H	-1.0418730	2.9330790	-0.0675590
H	0.4648820	-5.1513400	-1.4537290	C	-3.7169640	0.6901330	-1.0816050

H	-3.7262140	1.5603490	-1.7452490	H	0.8388070	-2.5167760	-2.8309670
H	-3.7625680	-0.1978070	-1.7198600	C	4.3421870	3.2933070	3.2288930
C	-1.1585040	0.5457790	-1.1773920	H	4.7982910	2.6961960	4.0274660
C	0.6452430	4.0533960	-0.7519120	H	5.1008360	4.0127910	2.8980680
H	1.7118960	4.1605980	-0.5199810	H	3.5123360	3.8576950	3.6631310
H	0.5868340	3.6638050	-1.7764470				
C	-5.5432100	-0.4635780	0.2463830	55			
H	-5.1870830	-1.4142630	-0.1445930	C	1.9769300	3.6431820	0.8387720
C	-6.6232240	-0.4396680	1.1303830	C	1.7315650	2.3959810	0.1762890
H	-7.0996870	-1.3702770	1.4263790	C	2.8916020	1.7214580	-0.3290190
C	-0.0353750	5.4263160	-0.6829330	C	4.1869120	2.2650310	-0.1411050
H	-1.1055510	5.3144280	-0.9080470	C	4.3696880	3.4575460	0.5141700
H	0.0189040	5.8075140	0.3466940	C	3.2410730	4.1696610	1.0088550
C	-5.4031540	1.9376710	0.3440580	H	1.1383380	4.2188410	1.2127160
H	-4.9358740	2.8695560	0.0335660	H	5.0259690	1.7090530	-0.5464480
C	-6.4821850	1.9668180	1.2283880	H	5.3671990	3.8672850	0.6477980
H	-6.8475970	2.9190930	1.6026150	C	2.7909890	0.5072910	-1.0791050
C	-7.0952780	0.7769730	1.6260220	O	3.7167620	-0.1595250	-1.5434580
H	-7.9376220	0.7984210	2.3114150	Rh	0.8414470	-1.5055770	-0.0604430
C	0.5803760	6.4523340	-1.6399100	N	1.4279030	0.0272450	-1.3538160
H	0.0769370	7.4223970	-1.5676350	C	1.6922380	-1.3133830	-3.3445030
H	0.5073030	6.1153760	-2.6800700	O	1.2654590	-0.0616840	-2.8003020
H	1.6421980	6.6106380	-1.4197250	C	2.2887450	-1.8992720	1.4741900
H	1.0569360	-1.7733960	-4.4425300	C	2.4434390	-3.0350950	0.5543340
H	2.4768680	-1.9948860	-3.3649100	C	1.2185210	-3.7161170	0.5233420

C	0.2944890	-3.0348160	1.4443560	C	0.2810690	0.6159460	-0.6771590
C	0.9960260	-1.9984920	2.1176050	C	-2.3377280	0.1404170	-0.4786060
C	3.7048140	-3.3493800	-0.1953430	H	-2.6657190	1.1694250	-0.3414180
H	4.4784030	-3.7311280	0.4842020	H	-2.1367090	-0.2846440	0.5078410
H	3.5358350	-4.1091780	-0.9626650	C	-4.7634900	-0.5470610	-0.3848940
H	4.0961680	-2.4549120	-0.6873010	C	-0.7443500	2.5566200	0.6775890
C	0.8699190	-4.9409030	-0.2715870	H	-0.3902760	3.0687460	1.5780150
H	1.5931410	-5.1214270	-1.0703790	H	-1.4720070	1.8382430	1.0595170
H	0.8518430	-5.8336600	0.3680820	C	-3.4765420	-0.6365630	-1.1777500
H	-0.1197310	-4.8583280	-0.7323820	H	-3.6213090	-0.2217680	-2.1804480
C	-1.0944780	-3.5208180	1.7501270	H	-3.1887850	-1.6838750	-1.3015110
H	-1.7036310	-2.7402790	2.2134790	C	-1.0445360	0.1485910	-1.2908360
H	-1.6115310	-3.8589050	0.8468510	C	-1.4566870	3.5920560	-0.2206420
H	-1.0664370	-4.3724500	2.4431100	H	-0.7276930	4.3532400	-0.5274790
C	3.4170160	-1.0141930	1.9182890	H	-1.7847080	3.1098150	-1.1510180
H	3.9938880	-1.5123140	2.7098930	C	-5.0923890	-1.5283950	0.5598330
H	4.1005430	-0.7940150	1.0960030	H	-4.4303520	-2.3809960	0.6952060
H	3.0542910	-0.0644910	2.3177670	C	-6.2600030	-1.4315960	1.3185790
C	0.5162180	-1.1576920	3.2635300	H	-6.4996580	-2.2056180	2.0424830
H	0.8483900	-0.1196700	3.1682550	C	-2.6520410	4.2665830	0.4640150
H	-0.5752170	-1.1516150	3.3285160	H	-3.3852490	3.5007540	0.7551700
H	0.8995840	-1.5381330	4.2204470	H	-2.3173030	4.7324760	1.4012590
F	-1.3038020	0.7665570	-2.4838390	C	-5.6381780	0.5355530	-0.5531360
F	-0.8274650	-1.2357310	-1.6370850	H	-5.4039510	1.3016180	-1.2889590
C	0.4273950	1.8463030	0.0251180	C	-6.8066950	0.6368100	0.2029390

H	-7.4742830	1.4809040	0.0540500	C	0.1057260	-2.0650640	1.3119990
C	-7.1208710	-0.3468980	1.1429070	O	0.7253270	-3.0677510	1.6473690
H	-8.0315920	-0.2709760	1.7299130	Rh	-0.2107700	0.5786590	0.0144740
C	-3.3359980	5.3195670	-0.4141940	N	0.6319440	-0.7577830	1.3174130
H	-4.1878570	5.7789380	0.0982170	C	2.3011830	-0.8402280	-0.2853390
H	-3.7066010	4.8776750	-1.3463310	O	1.4433580	-0.4482510	-1.0943420
H	-2.6392490	6.1205350	-0.6859930	O	2.0771980	-0.8891540	1.0191270
H	1.2512960	-1.3350740	-4.3450260	C	3.6748780	-1.3557890	-0.7020060
H	2.7805620	-1.3695460	-3.3956050	C	4.0575870	-0.7744070	-2.0728220
H	1.3021130	-2.1471610	-2.7495770	H	4.1722350	0.3137870	-2.0270350
C	3.4453440	5.4944480	1.7026200	H	5.0125900	-1.2002920	-2.3962010
H	4.0983040	5.3863670	2.5771390	H	3.3017690	-1.0046570	-2.8268740
H	3.9282990	6.2182930	1.0349670	C	3.5285730	-2.8983240	-0.7928720
H	2.4988510	5.9261930	2.0391910	H	3.1702460	-3.3152920	0.1519150
				H	2.8230570	-3.1786340	-1.5809380
56				H	4.5024300	-3.3383590	-1.0315060
C	-2.7255920	-1.0456190	-0.8729750	C	4.7371430	-0.9957290	0.3562510
C	-1.5566860	-0.9650440	-0.1008090	H	4.8386290	0.0888770	0.4693800
C	-1.2606590	-2.0562240	0.7370330	H	4.4901210	-1.4203140	1.3311140
C	-2.1101410	-3.1646180	0.8374150	H	5.7071320	-1.3928390	0.0403760
C	-3.2833920	-3.1958730	0.0950130	C	-1.6448770	2.2763920	-0.1933050
C	-3.5969650	-2.1420090	-0.7822320	C	-0.5311450	2.5338380	-1.0336780
H	-2.9761010	-0.2552040	-1.5754760	C	0.6539700	2.6989980	-0.1848480
H	-1.8183230	-3.9953820	1.4740170	C	0.2729070	2.4772130	1.1514710
H	-3.9526750	-4.0500030	0.1682660	C	-1.1453220	2.1185750	1.1587560

C	-0.5498720	2.7640560	-2.5171190	TS57			
H	0.3279670	2.3224760	-2.9971030	C	-1.4301890	1.5873170	-1.2574720
H	-1.4357080	2.3233370	-2.9800800	C	-0.6937990	1.3849040	-0.0928520
H	-0.5488550	3.8373100	-2.7498160	C	-0.9676440	2.1648020	1.0371210
C	2.0159380	3.0579140	-0.7036950	C	-1.9520370	3.1548130	1.0147250
H	2.2951190	2.4322500	-1.5573030	C	-2.6663810	3.3682690	-0.1603760
H	2.0431830	4.1016920	-1.0414350	C	-2.4198230	2.5883600	-1.3036020
H	2.7838290	2.9387350	0.0641920	H	-1.2783580	0.9633810	-2.1335430
C	1.1337720	2.5277350	2.3791520	H	-2.1526250	3.7270220	1.9163920
H	1.0334510	1.6082620	2.9632190	H	-3.4366860	4.1345250	-0.1959190
H	2.1896900	2.6488680	2.1277640	C	-0.1938370	1.7502320	2.2176560
H	0.8435390	3.3691770	3.0202670	O	-0.3369580	2.1085180	3.3772760
C	-3.0910710	2.2744570	-0.5877580	Rh	0.7505760	-0.0162810	0.2510960
H	-3.5280720	3.2605050	-0.3820860	N	0.8063210	0.7919380	1.8892360
H	-3.2240910	2.0734390	-1.6532970	C	-1.6823860	-1.6013240	0.6875320
H	-3.6662380	1.5328040	-0.0303580	O	-0.6401840	-1.4618330	-0.1195390
C	-1.9777040	1.9286130	2.3936740	O	-1.8707230	-0.9482200	1.7024020
H	-2.8819680	1.3549960	2.1788510	C	-2.6603260	-2.7141640	0.2227570
H	-1.4199640	1.3922020	3.1652390	C	-1.9343720	-4.0753810	0.2764300
H	-2.2834750	2.8971080	2.8121780	H	-1.5806900	-4.2939130	1.2899240
C	-4.8606110	-2.1935720	-1.6101160	H	-2.6200030	-4.8778290	-0.0187770
H	-4.8826390	-1.3952510	-2.3576960	H	-1.0745360	-4.0973770	-0.3988730
H	-4.9553980	-3.1502580	-2.1356950	C	-3.1194510	-2.4227610	-1.2205320
H	-5.7533590	-2.0850210	-0.9814790	H	-3.6131500	-1.4471960	-1.2868120
				H	-2.2747180	-2.4242120	-1.9140930

H	-3.8362540	-3.1846550	-1.5476250	H	0.9301250	1.5880050	-2.9455960
C	-3.8742290	-2.7367160	1.1651090	C	2.7027410	2.4047040	-0.7586860
H	-3.5684030	-2.9214170	2.1975160	H	1.8474930	2.9054270	-1.2179720
H	-4.4046430	-1.7810690	1.1471020	H	2.8465330	2.8330170	0.2355170
H	-4.5689030	-3.5268130	0.8579380	H	3.5918370	2.6370430	-1.3598090
C	1.8930780	0.0938500	-1.7263640	C	-3.1991950	2.8305180	-2.5752600
C	2.0725560	-1.2596440	-1.3442510	H	-3.2416570	1.9315260	-3.1974040
C	2.8064920	-1.2999760	-0.0997970	H	-4.2251920	3.1449890	-2.3614320
C	3.1173560	0.0310980	0.2767660	H	-2.7366850	3.6235670	-3.1770870
C	2.4976960	0.9196050	-0.6862910	58			
C	1.5682750	-2.4647940	-2.0752350	C	-0.7449260	2.3495720	-1.1125120
H	0.6100490	-2.7860750	-1.6482940	C	-0.5072540	1.5436820	0.0028020
H	1.4114060	-2.2530270	-3.1356360	C	-1.2004780	1.8177150	1.1919930
H	2.2746410	-3.2961900	-1.9944570	C	-2.1010370	2.8850100	1.2845020
C	3.1953800	-2.5584090	0.6199780	C	-2.3220140	3.6811590	0.1673020
H	2.3695170	-3.2751870	0.6396090	C	-1.6560150	3.4177310	-1.0448800
H	4.0421280	-3.0482880	0.1218210	H	-0.2458500	2.1507540	-2.0574490
H	3.4859910	-2.3568930	1.6526960	H	-2.6101980	3.0704860	2.2264230
C	3.8537380	0.4795200	1.4958610	H	-3.0191480	4.5137570	0.2214920
H	3.1340900	0.8718960	2.2305640	C	-0.9045960	0.8778440	2.2831470
H	4.3997570	-0.3437210	1.9611370	O	-1.3102920	0.9169070	3.4296350
H	4.5696720	1.2722950	1.2579840	Rh	0.6863380	-0.0958040	0.1487870
C	1.3665270	0.5919410	-3.0394810	N	0.0455600	-0.1502630	1.8789720
H	2.1797630	0.6548600	-3.7747850	C	-1.7686380	-1.6231080	0.1597520
H	0.6012430	-0.0729150	-3.4475740	O	-0.8635230	-1.1813470	-0.6634740

O	-1.8074120	-1.3978280	1.3781120	H	3.2680670	-3.5527630	-0.6964110
C	-2.8665600	-2.4983860	-0.5016120	H	2.3849250	-3.4605720	0.8351150
C	-2.1860610	-3.6941630	-1.1995260	C	3.1207040	-1.0750610	2.2371160
H	-1.6444260	-4.3170600	-0.4790710	H	2.2598370	-0.8264140	2.8725850
H	-2.9437790	-4.3224740	-1.6804780	H	3.3185300	-2.1433520	2.3490110
H	-1.4820800	-3.3567130	-1.9641710	H	3.9932020	-0.5302630	2.6118530
C	-3.6009200	-1.6295810	-1.5448610	C	2.5609000	1.7161250	-2.0852890
H	-4.0845240	-0.7688500	-1.0711110	H	3.6050440	1.9266980	-2.3512710
H	-2.9104180	-1.2589070	-2.3062240	H	2.0210260	1.5131130	-3.0136460
H	-4.3789820	-2.2234130	-2.0373680	H	2.1438840	2.6256500	-1.6469440
C	-3.8560480	-3.0002730	0.5610240	C	3.1746460	1.8757370	1.0403380
H	-3.3524350	-3.6077020	1.3175960	H	2.6596220	2.7641810	0.6672110
H	-4.3409590	-2.1673170	1.0758970	H	2.9613010	1.7914720	2.1085120
H	-4.6299000	-3.6122220	0.0843330	H	4.2541850	2.0433420	0.9260710
C	2.4928020	0.5588350	-1.1330720	C	-1.9444950	4.2589790	-2.2662460
C	2.2846960	-0.8001360	-1.4474650	H	-1.1757510	4.1313900	-3.0337990
C	2.4935980	-1.5954000	-0.2420640	H	-2.9071300	3.9836380	-2.7149390
C	2.8338880	-0.7182680	0.8106850	H	-2.0011200	5.3231250	-2.0140330
C	2.7468180	0.6401010	0.2995770				
C	1.9462170	-1.3845740	-2.7874210	TS59			
H	1.0904820	-2.0634650	-2.7175220	C	2.4979930	-1.1637810	1.0871230
H	1.6972810	-0.6096060	-3.5155460	C	1.4995540	-0.8938670	0.1417090
H	2.7918620	-1.9591580	-3.1857890	C	1.4989780	-1.6981470	-1.0169280
C	2.4076480	-3.0934290	-0.1928570	C	2.5388810	-2.5747720	-1.3707090
H	1.5059100	-3.4568920	-0.6953130	C	3.5062250	-2.8066320	-0.4074640

C	3.4825210	-2.1290460	0.8378910	C	-0.7409870	2.4519980	0.7967770
H	2.5306130	-0.6131090	2.0234760	C	-0.6367630	2.7120670	-0.5977120
H	2.5264170	-3.1121070	-2.3132820	C	0.7587690	2.5799090	-0.9590940
H	4.2861770	-3.5396080	-0.5966600	C	1.5133610	2.2957040	0.2268000
C	0.1371960	-1.7414770	-1.8360800	C	-2.0072920	2.5026660	1.5972840
O	-0.4391490	-2.7175050	-2.2519940	H	-1.9223930	1.9233810	2.5196030
Rh	0.1555460	0.5819240	-0.1637130	H	-2.2328420	3.5404560	1.8759690
N	0.2329740	-0.4375270	-1.9025020	H	-2.8428550	2.1044760	1.0199760
C	-2.4534150	-0.7139200	0.1562950	C	-1.7684780	3.0852230	-1.5098870
O	-1.2095320	-0.8312910	0.5377650	H	-2.6277200	2.4342660	-1.3349240
O	-2.9021260	0.2152070	-0.5237140	H	-2.0721650	4.1276020	-1.3465670
C	-3.3897600	-1.8650310	0.6070030	H	-1.4815940	2.9860810	-2.5594770
C	-4.5944900	-1.2340180	1.3341910	C	1.3170420	2.8073060	-2.3332010
H	-5.0804010	-0.4912820	0.6971530	H	0.6677060	2.3790060	-3.1005140
H	-5.3267330	-2.0064640	1.5955380	H	1.4109340	3.8818750	-2.5341810
H	-4.2840900	-0.7407090	2.2630220	H	2.3057380	2.3577090	-2.4473130
C	-2.6879190	-2.8764990	1.5264560	C	0.9267900	2.0199790	2.7760670
H	-1.8364280	-3.3441780	1.0260020	H	1.0189340	3.0013790	3.2602130
H	-2.3176980	-2.3993800	2.4389660	H	0.1638380	1.4551080	3.3172970
H	-3.3926000	-3.6654100	1.8155760	H	1.8800450	1.5022940	2.9088850
C	-3.8751450	-2.5730110	-0.6780790	C	3.0093490	2.2542260	0.3351560
H	-4.3869240	-1.8656890	-1.3357730	H	3.3425930	1.5349580	1.0864120
H	-3.0345020	-3.0062420	-1.2296360	H	3.4747740	1.9793930	-0.6141200
H	-4.5710580	-3.3804640	-0.4219900	H	3.3969970	3.2399470	0.6229090
C	0.5781740	2.1705740	1.3227770	C	4.5229560	-2.4562890	1.8792480

H 4.2997210 -3.4170800 2.3596070

H 5.5197500 -2.5442710 1.4343710

H 4.5606090 -1.6961170 2.6638750

60

C 2.7808940 -3.4415510 -0.4826290

C 2.3337690 -2.2060570 0.0343060

C 3.2160490 -1.1131930 -0.0515600

C 4.4921300 -1.2950450 -0.6181190

C 4.8935130 -2.5184470 -1.1337860

C 4.0296290 -3.6219660 -1.0758570

H 2.1089940 -4.2939220 -0.4294240

H 5.1641890 -0.4437730 -0.6271800

H 5.8829900 -2.6229140 -1.5725110

C -0.9514330 1.4769310 1.6934180

O 0.0426950 0.9338260 2.3541240

O -1.0806540 1.3833150 0.4598800

C -1.9602530 2.2180300 2.5747260

C -2.5645030 1.1982940 3.5702440

H -1.7927900 0.7762750 4.2176460

H -3.3072500 1.7039140 4.1958670

H -3.0553160 0.3703650 3.0520920

C -3.0664900 2.8445490 1.7124860

H -2.6544000 3.5525070 0.9877720

H -3.6300840 2.0878590 1.1602470

H -3.7665500 3.3853010 2.3574810

C -1.2180490 3.3181590 3.3674870

H -0.4085290 2.8964530 3.9671350

H -0.7947960 4.0766690 2.7020560

H -1.9236880 3.8177690 4.0391780

C 1.0650790 0.6312140 -3.0632600

C -0.0343690 1.5078870 -2.9006750

C -1.2251910 0.6842720 -2.7459750

C -0.8538770 -0.6902000 -2.8427520

C 0.5873480 -0.7342240 -2.9428950

C -0.0206700 3.0073050 -2.9760300

H 0.9643220 3.4033550 -2.7219410

H -0.2762880 3.3551060 -3.9858820

H -0.7479130 3.4459350 -2.2866180

C -2.6095760 1.2442380 -2.6098920

H -2.6522280 1.9848960 -1.8058390

H -2.9027390 1.7475430 -3.5397190

H -3.3518480 0.4736810 -2.3955200

C -1.7461750 -1.8817770 -3.0489480

H -1.6065750 -2.2620270 -4.0690630

H -1.5173160 -2.6993280 -2.3605660

H -2.8029650 -1.6281460 -2.9438210

C 2.4758740 0.9777860 -3.4222140

H 2.6781410 2.0414850 -3.3284770

H 3.1953950 0.4514220 -2.7913080

H	2.6538980	0.6675890	-4.4609270	C	-6.8465330	-1.0354870	-1.6943020
C	1.3873750	-1.9593800	-3.2652210	H	-7.2149350	-1.3984130	-2.6500450
H	2.4315990	-1.8507150	-2.9702040	C	1.6217580	-3.6117140	4.2778330
H	0.9885370	-2.8399270	-2.7588340	H	0.6013390	-3.9535120	4.4988370
H	1.3598160	-2.1484310	-4.3479540	H	2.1843620	-4.5066070	3.9775740
F	-1.6420580	-3.2484370	0.5524880	C	-5.9054800	-0.1380490	0.7679490
F	-1.5271840	-1.7126330	2.1544910	H	-5.5512480	0.2073840	1.7363820
C	0.9719130	-2.2284560	0.6743620	C	-7.0101110	0.4781440	0.1763890
C	-0.0776890	-1.4827140	0.2397950	H	-7.5051690	1.3013520	0.6842920
C	-2.7252760	-1.2221270	0.2030930	C	-7.4829570	0.0332180	-1.0592830
H	-2.7064710	-1.3302230	-0.8782780	H	-8.3445000	0.5086470	-1.5192140
H	-2.7049100	-0.1542830	0.4112170	C	2.2468080	-3.0158170	5.5434710
C	-5.2511260	-1.2067890	0.1397400	H	2.2653710	-3.7424400	6.3628660
C	0.9212770	-3.2195890	1.8454220	H	1.6834600	-2.1405880	5.8867180
H	1.4601500	-4.1359130	1.5796970	H	3.2778610	-2.6921940	5.3609650
H	-0.0965180	-3.5123980	2.0868740	C	4.4516720	-4.9674500	-1.6177100
C	-4.0254990	-1.8459970	0.7558440	H	5.2587840	-5.4009770	-1.0148220
H	-4.0195780	-2.9201050	0.5501860	H	3.6210400	-5.6787740	-1.6189410
H	-4.0486300	-1.7330250	1.8441830	H	4.8282910	-4.8856670	-2.6434750
C	-1.4662580	-1.8725010	0.7639670	H	0.6990020	0.5701520	1.6912280
C	1.5804080	-2.6221790	3.1062200	C	2.9747220	0.2840650	0.4469610
H	2.6017540	-2.2922570	2.8741320	O	3.8879810	0.9232780	0.9695640
H	1.0204410	-1.7269480	3.4040480	Rh	0.1128400	0.1758650	-1.0314000
C	-5.7430320	-1.6480290	-1.0980010	N	1.7190490	0.7952290	0.2049810
H	-5.2628840	-2.4904480	-1.5916270	C	2.5214270	3.0420000	-0.0962650

O	1.6872000	2.1954010	0.5749860	H	5.8098610	-2.7528400	-1.5754490
O	3.0642870	2.7799380	-1.1440540	C	-0.8779050	1.3412020	1.7362930
C	2.6273460	4.3898140	0.6373360	O	0.0588800	0.7152050	2.3190230
C	1.3000730	5.1589750	0.4477170	O	-1.0252530	1.3791700	0.4697270
H	0.4535480	4.6005730	0.8557100	C	-1.8859000	2.0900760	2.6325090
H	1.3542720	6.1236930	0.9638970	C	-2.5201040	1.0597820	3.5941500
H	1.1020610	5.3553660	-0.6115910	H	-1.7520400	0.5727060	4.1988080
C	3.7827830	5.1868140	0.0081910	H	-3.2262400	1.5653360	4.2619750
H	4.7343580	4.6636180	0.1356800	H	-3.0599490	0.2793650	3.0507470
H	3.6262190	5.3357420	-1.0629320	C	-2.9745670	2.7909890	1.8062010
H	3.8595090	6.1670150	0.4904400	H	-2.5420010	3.5113050	1.1059820
C	2.9011490	4.1558500	2.1377930	H	-3.5700900	2.0789570	1.2281590
H	2.0597490	3.6579100	2.6241100	H	-3.6524570	3.3317100	2.4760600
H	3.7843680	3.5270550	2.2768640	C	-1.1051080	3.1319400	3.4640730
H	3.0715760	5.1175360	2.6343910	H	-0.2979170	2.6552190	4.0246960
				H	-0.6708830	3.9088460	2.8263990
TS61				H	-1.7814460	3.6221080	4.1728400
C	2.6290960	-3.4845780	-0.6590880	C	1.1824950	0.7469350	-2.9890890
C	2.2284190	-2.2785100	-0.0464710	C	0.1427910	1.6934700	-2.7814580
C	3.1775990	-1.2386850	-0.0006730	C	-1.0982000	0.9512800	-2.6822560
C	4.4633810	-1.4401680	-0.5431560	C	-0.8167380	-0.4454780	-2.8535460
C	4.8138560	-2.6319200	-1.1569860	C	0.6137970	-0.5806790	-2.9666700
C	3.8877900	-3.6837800	-1.2252600	C	0.2609470	3.1901500	-2.7800650
H	1.9095190	-4.2974630	-0.7016820	H	1.2776210	3.5030420	-2.5351730
H	5.1801240	-0.6306650	-0.4615000	H	0.0057720	3.6082290	-3.7630140

H	-0.4159960	3.6402050	-2.0479750	C	0.7458670	-3.3546400	1.6638100
C	-2.4444930	1.5881630	-2.5118460	H	1.2995490	-4.2531840	1.3684200
H	-2.4551790	2.2403460	-1.6336330	H	-0.2831440	-3.6593990	1.8320920
H	-2.6840040	2.2004460	-3.3899280	C	-4.1235030	-1.7296430	0.6289970
H	-3.2378310	0.8492380	-2.3874970	H	-4.1384070	-2.7907390	0.3641350
C	-1.7856940	-1.5590810	-3.1367430	H	-4.1633810	-1.6752220	1.7212050
H	-1.6511210	-1.8934290	-4.1734970	C	-1.5714260	-1.8584210	0.6323500
H	-1.6277760	-2.4250500	-2.4887050	C	1.3369940	-2.8342550	2.9906020
H	-2.8241830	-1.2381920	-3.0359150	H	2.3776110	-2.5166670	2.8361770
C	2.6164880	1.0138080	-3.3265440	H	0.7778200	-1.9423730	3.2958280
H	2.8842650	2.0606560	-3.2073750	C	-5.8066400	-1.4013900	-1.2364920
H	3.2944710	0.4272440	-2.7027620	H	-5.3348620	-2.2273790	-1.7648520
H	2.7861740	0.7186530	-4.3707660	C	-6.8898320	-0.7391490	-1.8162770
C	1.3306770	-1.8345860	-3.3680210	H	-7.2513240	-1.0471710	-2.7937570
H	2.3789390	-1.8166120	-3.0672950	C	1.2914900	-3.8824790	4.1097370
H	0.8705430	-2.7178020	-2.9216640	H	0.2524360	-4.2074410	4.2568120
H	1.2961810	-1.9522420	-4.4606590	H	1.8486970	-4.7762970	3.7958480
F	-1.7877850	-3.1999510	0.2692370	C	-5.9667980	0.0173480	0.7000780
F	-1.6432560	-1.8474460	2.0259030	H	-5.6179440	0.3093010	1.6877620
C	0.8519330	-2.2915550	0.5601900	C	-7.0511270	0.6831860	0.1249570
C	-0.1596630	-1.4800930	0.1587750	H	-7.5367710	1.4906780	0.6660910
C	-2.7996590	-1.1078670	0.1328100	C	-7.5153380	0.3087120	-1.1370790
H	-2.7850210	-1.1190130	-0.9541000	H	-8.3614570	0.8228260	-1.5839640
H	-2.7333530	-0.0651410	0.4358810	C	1.8580030	-3.3662180	5.4365110
C	-5.3246490	-1.0321300	0.0284140	H	1.8114400	-4.1317030	6.2185960

H	1.2981810	-2.4930120	5.7900510	H	4.0732030	3.4934560	2.3710580
H	2.9058540	-3.0633440	5.3284490	H	3.3769370	5.0940250	2.6990530
C	4.2551300	-4.9975270	-1.8725090				
H	3.3820240	-5.6441850	-1.9944570	62			
H	4.7051290	-4.8437120	-2.8593580	C	2.6789590	-3.4730900	-0.5827130
H	4.9899180	-5.5419080	-1.2670760	C	2.2744190	-2.2551190	0.0033040
H	0.9728790	0.4856190	1.4069790	C	3.2210300	-1.2109950	0.0186280
C	3.0018640	0.1113470	0.6124520	C	4.5065760	-1.4197530	-0.5244810
O	3.9326150	0.7009830	1.1286800	C	4.8589700	-2.6237730	-1.1106490
Rh	0.1386900	0.2535370	-0.9870570	C	3.9350240	-3.6796850	-1.1514580
N	1.7077870	0.7215190	0.4866470	H	1.9636970	-4.2904950	-0.5996350
C	2.6589110	2.9065120	0.1049500	H	5.2208040	-0.6061580	-0.4643460
O	1.8223260	2.1260950	0.8413000	H	5.8542980	-2.7521440	-1.5281980
O	3.1846590	2.5573460	-0.9261140	C	-0.9259890	1.3811400	1.6898280
C	2.8158620	4.2866450	0.7644530	O	-0.0483330	0.7589340	2.3343790
C	1.4856640	5.0618110	0.6293810	O	-1.0284130	1.3814610	0.4061630
H	0.6634650	4.5294790	1.1131800	C	-1.9631030	2.2019800	2.4959490
H	1.5840730	6.0444810	1.1029470	C	-2.6778960	1.2310720	3.4619390
H	1.2216070	5.2205380	-0.4213900	H	-1.9549260	0.7341710	4.1123860
C	3.9376810	5.0421130	0.0320950	H	-3.3923970	1.7826400	4.0835230
H	4.8907960	4.5132080	0.1174170	H	-3.2273860	0.4552990	2.9202830
H	3.7144750	5.1561930	-1.0317230	C	-2.9881980	2.9004760	1.5901180
H	4.0546220	6.0380950	0.4713290	H	-2.5007630	3.5820940	0.8869100
C	3.1790520	4.1123540	2.2553410	H	-3.5730310	2.1821840	1.0085250
H	2.3679110	3.6370850	2.8106580	H	-3.6846460	3.4849940	2.2021880

C	-1.1952750	3.2515190	3.3286040	C	1.3776280	-1.9004890	-3.3274130
H	-0.4300320	2.7704690	3.9419700	H	2.4292820	-1.8532620	-3.0416540
H	-0.7075770	3.9928690	2.6869760	H	0.9410960	-2.7797380	-2.8504150
H	-1.8883090	3.7867510	3.9872980	H	1.3319600	-2.0500470	-4.4157170
C	1.1842440	0.6860660	-3.0039030	F	-1.7205100	-3.2212610	0.3440720
C	0.1266330	1.6196770	-2.8203430	F	-1.5963580	-1.8427850	2.0801190
C	-1.0984160	0.8590320	-2.6972080	C	0.9028150	-2.2656630	0.6211240
C	-0.7901650	-0.5384490	-2.8307770	C	-0.1222690	-1.4784300	0.2050450
C	0.6411420	-0.6500970	-2.9513650	C	-2.7661940	-1.1475590	0.1770060
C	0.2141210	3.1177560	-2.8583290	H	-2.7602810	-1.1985510	-0.9090590
H	1.2286010	3.4582300	-2.6437620	H	-2.7053240	-0.0938560	0.4403970
H	-0.0719940	3.5055340	-3.8451780	C	-5.2921710	-1.1147960	0.0746490
H	-0.4560290	3.5711680	-2.1220680	C	0.8165970	-3.3009910	1.7530230
C	-2.4552340	1.4753470	-2.5387600	H	1.3868570	-4.1969520	1.4820280
H	-2.4730120	2.1493110	-1.6772540	H	-0.2071150	-3.6197430	1.9276720
H	-2.7086960	2.0594410	-3.4320140	C	-4.0796180	-1.7645510	0.7054840
H	-3.2343110	0.7256060	-2.3914700	H	-4.0792120	-2.8371370	0.4910810
C	-1.7419550	-1.6739430	-3.0833160	H	-4.1176040	-1.6586740	1.7939160
H	-1.6039590	-2.0318010	-4.1117700	C	-1.5272800	-1.8700870	0.6901140
H	-1.5701900	-2.5205100	-2.4140180	C	1.3959580	-2.7338290	3.0656460
H	-2.7849310	-1.3662900	-2.9882690	H	2.4334720	-2.4082360	2.9049460
C	2.6138050	0.9737420	-3.3446850	H	0.8243690	-1.8406170	3.3423930
H	2.8616010	2.0271950	-3.2416310	C	-5.7877120	-1.5704380	-1.1563540
H	3.3019660	0.4087180	-2.7117600	H	-5.3173930	-2.4274020	-1.6342510
H	2.7910930	0.6659210	-4.3839080	C	-6.8817410	-0.9537450	-1.7656160

H	-7.2536070	-1.3287040	-2.7154520	O	3.0755890	2.5980020	-0.9640110
C	1.3607180	-3.7484950	4.2156330	C	2.7105830	4.3425370	0.7121220
H	0.3246450	-4.0778330	4.3728930	C	1.3898670	5.1056150	0.4566080
H	1.9258600	-4.6464860	3.9287650	H	0.5348880	4.5815950	0.8907520
C	-5.9314460	-0.0250600	0.6820940	H	1.4489480	6.1008120	0.9097080
H	-5.5722350	0.3348450	1.6431530	H	1.2066280	5.2337200	-0.6150910
C	-7.0261140	0.5956660	0.0771050	C	3.8751980	5.0717910	0.0196750
H	-7.5091340	1.4358070	0.5686320	H	4.8240330	4.5572010	0.1961660
C	-7.5042090	0.1347070	-1.1507580	H	3.7222640	5.1298700	-1.0605460
H	-8.3585890	0.6137300	-1.6204040	H	3.9563560	6.0888770	0.4163280
C	1.9227650	-3.1871680	5.5258930	C	2.9792140	4.2339340	2.2278310
H	1.8813980	-3.9283660	6.3313060	H	2.1378520	3.7798850	2.7548600
H	1.3564300	-2.3075020	5.8518000	H	3.8672190	3.6265520	2.4249890
H	2.9685540	-2.8802990	5.4088700	H	3.1472890	5.2350340	2.6391670
C	4.2948400	-4.9970600	-1.7947860				
H	5.2318290	-5.3932610	-1.3880530	TS63			
H	3.5149800	-5.7470430	-1.6389370	C	3.1099640	3.1540770	0.5635470
H	4.4386950	-4.8831930	-2.8760170	C	2.3444120	2.1606230	-0.1009510
H	1.0611550	0.4652550	1.3392870	C	3.0376110	1.0172360	-0.5459000
C	3.0434320	0.1458700	0.6042540	C	4.4367940	0.9639450	-0.4102100
O	3.9700890	0.7760290	1.0682700	C	5.1554230	1.9628920	0.2277340
Rh	0.1464620	0.2264730	-0.9872370	C	4.4866630	3.0731670	0.7590070
N	1.7194570	0.7440630	0.5054680	H	2.6053290	4.0203870	0.9742680
C	2.5873290	2.9442040	0.0860580	H	4.9457190	0.0948040	-0.8112690
O	1.8195810	2.1408230	0.8717530	H	6.2349370	1.8760100	0.3245080

Rh	0.1939910	-0.3851550	1.0160160	H	0.4874100	-3.7720100	2.0196230
C	-1.1297120	-1.2358060	-1.5326980	C	-1.8913880	-2.2794880	2.7552170
O	-0.5870380	-0.2212690	-2.0612480	H	-1.7967780	-2.9655360	1.9095310
O	-1.0654410	-1.4923490	-0.2855230	H	-1.9381570	-2.8766550	3.6742520
C	-1.9415480	-2.1726970	-2.4518590	H	-2.8393530	-1.7489820	2.6479890
C	-3.0928350	-1.3524890	-3.0767390	C	-1.9877680	0.8947700	3.3626610
H	-2.7066130	-0.4756240	-3.6024630	H	-1.9966710	1.8659830	2.8661890
H	-3.6373380	-1.9753860	-3.7946760	H	-2.9189730	0.3795090	3.1174250
H	-3.8088030	-1.0219620	-2.3172300	H	-1.9877200	1.0700330	4.4466380
C	-2.5182970	-3.3647770	-1.6737580	C	2.9591780	-0.5200480	2.8227160
H	-1.7307010	-3.9587200	-1.2034870	H	3.3623850	-1.1555630	2.0304320
H	-3.2029960	-3.0326940	-0.8882080	H	3.3486240	0.4892490	2.6796110
H	-3.0743550	-4.0152440	-2.3578450	H	3.3261060	-0.8913120	3.7886190
C	-1.0067990	-2.6589560	-3.5808340	C	0.9677680	1.9926170	3.2770720
H	-0.5850990	-1.8124180	-4.1272950	H	1.9664240	2.2269240	2.9070240
H	-0.1777660	-3.2506980	-3.1856020	H	0.2631680	2.6998190	2.8342460
H	-1.5700630	-3.2857620	-4.2807480	H	0.9648680	2.1497910	4.3639890
C	1.4613120	-0.5393710	2.8127340	F	-1.6552220	3.0182300	0.8964390
C	0.6493720	-1.7335940	2.6898330	F	-1.8060090	2.8520560	-1.3105820
C	-0.7271540	-1.3375650	2.8118530	C	0.8865350	2.4525310	-0.2922420
C	-0.7851760	0.0825640	2.9796180	C	-0.1383910	1.5239860	-0.1732630
C	0.5798750	0.5765610	2.9731540	C	-2.7672860	1.1641620	-0.0446410
C	1.1543600	-3.1429960	2.6148610	H	-2.6179210	0.4678450	0.7794130
H	2.1491860	-3.1825320	2.1699080	H	-2.8104400	0.5757210	-0.9604780
H	1.2141640	-3.5804890	3.6206430	C	-5.2859740	1.0002600	0.1994880

C	0.6376520	3.8990840	-0.7150820	H	0.2063560	5.0310160	-4.7928880
H	1.3235770	4.5787150	-0.2078860	H	1.9135460	5.3837750	-4.5023860
H	-0.3673280	4.2304400	-0.4791100	C	5.2391230	4.1604670	1.4896750
C	-4.0962950	1.9332290	0.1267080	H	5.9343500	4.6796080	0.8193760
H	-4.0479970	2.5438670	1.0328880	H	4.5601780	4.9092240	1.9074770
H	-4.2125720	2.6237320	-0.7144680	H	5.8352660	3.7502140	2.3125380
C	-1.5670190	2.0959950	-0.1636930	H	-0.1509920	0.5795400	-1.0373350
C	0.8772280	4.0520650	-2.2382410	C	2.5044060	-0.2640840	-1.1471400
H	1.8956160	3.7263860	-2.4843540	O	2.9758300	-0.6961700	-2.1990800
H	0.1924410	3.3863680	-2.7736820	N	1.7399120	-0.9740340	-0.2674400
C	-5.7602400	0.5327910	1.4331560	C	2.7213340	-3.0838770	-0.5176200
H	-5.2925910	0.8838980	2.3504950	O	1.6065890	-2.3308300	-0.7476040
C	-6.8338670	-0.3570650	1.5022140	O	3.6445090	-2.7391370	0.1901630
H	-7.1887060	-0.7016540	2.4698100	C	2.6706110	-4.4154460	-1.2818620
C	0.6689340	5.4957950	-2.7126850	C	1.3153550	-5.1193270	-1.0700450
H	-0.3494670	5.8163130	-2.4548990	H	0.4840890	-4.5008190	-1.4106820
H	1.3484660	6.1627780	-2.1640850	H	1.2978250	-6.0604600	-1.6301040
C	-5.9294730	0.5609010	-0.9665380	H	1.1523050	-5.3570970	-0.0129040
H	-5.5894250	0.9270710	-1.9323790	C	3.8094170	-5.3150790	-0.7732830
C	-7.0034320	-0.3285010	-0.9034710	H	4.7795180	-4.8283620	-0.8943600
H	-7.4896220	-0.6526700	-1.8194430	H	3.6876490	-5.5533270	0.2879820
C	-7.4575040	-0.7938650	0.3322030	H	3.8156660	-6.2541950	-1.3366410
H	-8.2953340	-1.4832270	0.3830640	C	2.8836150	-4.0997910	-2.7817390
C	0.8926900	5.6636480	-4.2190830	H	2.1240120	-3.4120000	-3.1567400
H	0.7319470	6.7003960	-4.5331220	H	3.8572710	-3.6298050	-2.9454950

H	2.8450410	-5.0298080	-3.3599420	C	-3.5388900	-2.5565620	-1.6378380
				H	-4.0647340	-1.9007900	-0.9369050
64				H	-3.3823640	-2.0096290	-2.5707600
C	2.9197590	3.0847790	-1.4363820	H	-4.1923180	-3.4118670	-1.8441830
C	2.1223130	1.9387960	-1.1993140	C	1.5509690	0.7965880	2.8367650
C	2.4736370	0.7570350	-1.8991750	C	1.8119410	-0.6115910	2.7823750
C	3.4790130	0.8190860	-2.8765420	C	0.5583990	-1.2954180	2.8486800
C	4.1916610	1.9806670	-3.1342850	C	-0.4874630	-0.2938200	3.0357090
C	3.9416320	3.1337270	-2.3836760	C	0.1250270	0.9795890	3.0719360
H	2.7201290	3.9981290	-0.8953670	C	3.1781760	-1.2174100	2.6990320
H	3.7022670	-0.0996540	-3.4052010	H	3.6288760	-1.0673390	1.7131960
H	4.9661610	1.9817320	-3.8972880	H	3.8323280	-0.7626730	3.4516150
Rh	0.4907340	-0.0695690	1.0254060	H	3.1484340	-2.2920540	2.8872860
C	-1.2631530	-1.7992360	-0.9237550	C	0.3222070	-2.7687840	2.9126960
O	-0.9307940	-1.2027440	-1.9495900	H	-0.4871260	-3.0497030	2.2365450
O	-0.9536060	-1.4560280	0.2989040	H	1.2101170	-3.3316160	2.6281190
C	-2.1914680	-3.0484980	-1.0661370	H	0.0375770	-3.0612950	3.9318090
C	-2.4389900	-3.7932390	0.2525170	C	-1.9330110	-0.6151620	3.2512660
H	-2.9124710	-3.1487660	0.9990280	H	-2.5533340	0.2829690	3.2230790
H	-3.1051560	-4.6461180	0.0765290	H	-2.2838150	-1.3047760	2.4784290
H	-1.5087550	-4.1824010	0.6761390	H	-2.0777880	-1.0982840	4.2259310
C	-1.5362800	-3.9991080	-2.0893690	C	2.6287870	1.8331310	2.9684350
H	-1.3254490	-3.4689340	-3.0200240	H	3.3951080	1.7154480	2.1974930
H	-0.5933780	-4.4051860	-1.7113480	H	2.2356380	2.8477220	2.9080970
H	-2.2053100	-4.8412840	-2.3016880	H	3.1248050	1.7312880	3.9428590

C	-0.5465370	2.2378810	3.5391770	H	-7.5378130	-1.0353330	1.1877000
H	0.0388900	3.1309040	3.3191460	C	0.7480790	5.9368130	0.5581160
H	-1.5380230	2.3658830	3.1050500	H	0.3704010	5.8483870	1.5867110
H	-0.6589050	2.1886730	4.6302190	H	1.8421900	6.0051020	0.6429580
F	-1.8201420	2.5925990	0.7976220	C	-5.8971190	0.5258690	-1.9528200
F	-1.7859000	2.9355870	-1.3808870	H	-5.4413110	0.9671610	-2.8360440
C	0.8996160	2.1211920	-0.3639050	C	-6.9832900	-0.3388760	-2.0931590
C	-0.2595530	1.3648570	-0.5952820	H	-7.3678460	-0.5655830	-3.0836660
C	-2.8459250	0.9973350	-0.5941970	C	-7.5772450	-0.9077200	-0.9647730
H	-2.7984270	0.2333440	0.1844630	H	-8.4245780	-1.5788100	-1.0722260
H	-2.7295660	0.4818020	-1.5497710	C	0.2037720	7.2217050	-0.0741020
C	-5.3829790	0.8376800	-0.6867320	H	0.4888050	8.1048370	0.5068920
C	0.8640780	3.3894790	0.4844780	H	-0.8898920	7.1990560	-0.1336410
H	1.8655650	3.5724000	0.8796360	H	0.5864880	7.3545310	-1.0922780
H	0.2080130	3.2330130	1.3314690	C	4.7355700	4.3983720	-2.6092470
C	-4.1893150	1.7561570	-0.5394940	H	5.8116820	4.2117540	-2.5219840
H	-4.2560950	2.2962780	0.4106030	H	4.5606570	4.8023800	-3.6133750
H	-4.2001890	2.5091580	-1.3330010	H	4.4698640	5.1756170	-1.8872980
C	-1.6618870	1.9305600	-0.4191280	H	-0.2492020	0.6455140	-1.4119120
C	0.3678130	4.6771560	-0.2315390	C	2.0582280	-0.6662090	-1.6175780
H	0.7714970	4.7445690	-1.2472420	O	2.1985190	-1.5259810	-2.4828410
H	-0.7160230	4.6283130	-0.3406630	N	1.8457390	-0.9422390	-0.2795940
C	-5.9912780	0.2623660	0.4374680	C	3.0300090	-2.9784280	-0.2578010
H	-5.6140850	0.5035710	1.4290920	O	1.7992650	-2.3821190	-0.1278950
C	-7.0778780	-0.6036170	0.3028900	O	4.0804330	-2.3791680	-0.2255370

C	2.9134090	-4.4946200	-0.4878620
C	4.2614500	-5.1425060	-0.1257680
H	4.4915490	-5.0195420	0.9379610
H	4.2254600	-6.2150900	-0.3440760
H	5.0772430	-4.6945270	-0.6961900
C	2.6273450	-4.6942990	-1.9969050
H	1.7041570	-4.1952890	-2.2950320
H	3.4348850	-4.2763740	-2.6036430
H	2.5478850	-5.7662100	-2.2109810
C	1.7877030	-5.1334370	0.3454200
H	1.9989100	-5.0688170	1.4185690
H	0.8243200	-4.6584170	0.1548620
H	1.7046830	-6.1958920	0.0920760