

Supporting Information

DFT investigated Rh-catalyzed [4+1] annulation of N-methoxybenzamides with nitriles to synthesize different isoindolinones under solvent control.

Qian-Qian Li^{ab}, Meiju Wei, Yi-Li Zhao^{ab}, Fei-Wu Chen^{*ab}

*Corresponding authors

^aDepartment of Chemistry and Chemical Engineering, School of Chemistry and Biological Engineering, University of Science and Technology Beijing, Beijing 100083, P. R. China

E-mail: weimeiju@ustb.edu.cn

^bBeijing Key Laboratory for Science and Application of Functional Molecular and Crystalline Materials, Beijing 100083, P. R. China

Table of Content

1.Free energy profile of the entire amination reaction.....	3
2.Free energy profile of the entire allylation reaction.....	4
3.Free energy profile of other path for formation of 4 in TFE.....	5
4.Calculated electronic energies, and free energies of all structures at the M05-2X-D3/6-311++G(d,p)-SDD/SMD(2,2,2-trifluoroethanol)//B3LYP-D3/6-31G(d)-SDD/SMD(2,2,2-trifluoroethanol) level of theory.....	6
5.Calculated electronic energies, and free energies of all structures at the M05-2X-D3/6-311++G(d,p)-SDD/SMD(1,1,1,3,3,3-Hexafluoro-2-propanol)//B3LYP-D3/6-31G(d)-SDD/SMD(1,1,1,3,3,3-Hexafluoro-2-propanol) level of theory.....	9
6.Cartesian coordinates of the structures in TFE.....	12
7.Cartesian coordinates of the structures in HFIP.....	37

1. Free energy profile of the entire amination reaction

Because the free energy barrier of base-assisted ($(\text{CF}_3)_2\text{CHONa}$ and Na_2CO_3) hydrogen transfer, solvent-assisted hydrogen transfer ($\text{CF}_3\text{CH}_2\text{OH}$ and $(\text{CF}_3)_2\text{CHOH}$), Rh(III) catalyst-assisted hydrogen transfer and no external assistance process is too high, path A-a-2, path A-a-3, path A-b-1, path A-b-2, path A-c and path B all should be excluded. The correct route for this reaction is N-H deprotonation, the concerted metalation-deprotonation (CMD), the formation of a seven-membered rhodacycle by cyano group insertion and $\text{CF}_3\text{CH}_2\text{ONa}$ assisted hydrogen transfer to obtain 3-amino-2-methoxy-3-(phenoxymethyl)isoindolin-1-one **3** in TFE.

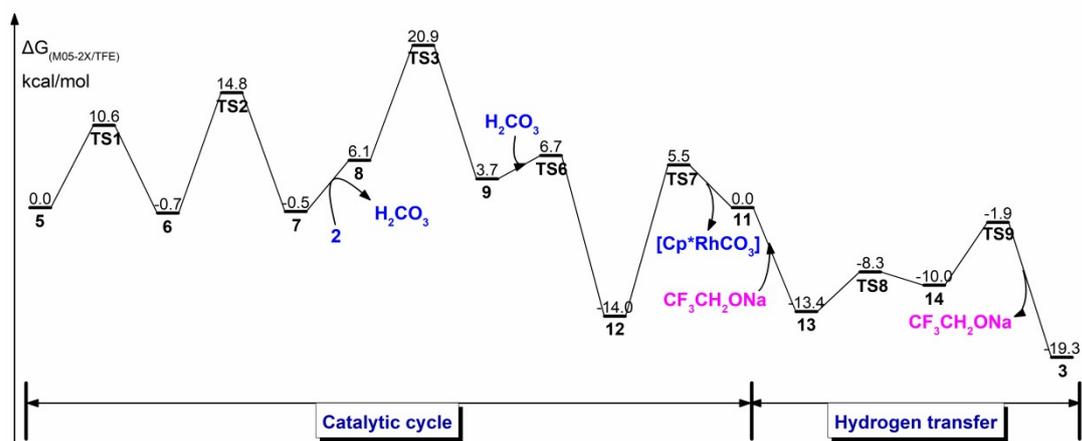


Figure S1. Calculated free energy profile for the entire amination reaction. The energy values (kcal/mol) are calculated using M05-2X method in TFE.

2. Free energy profile of other path in allylation reaction

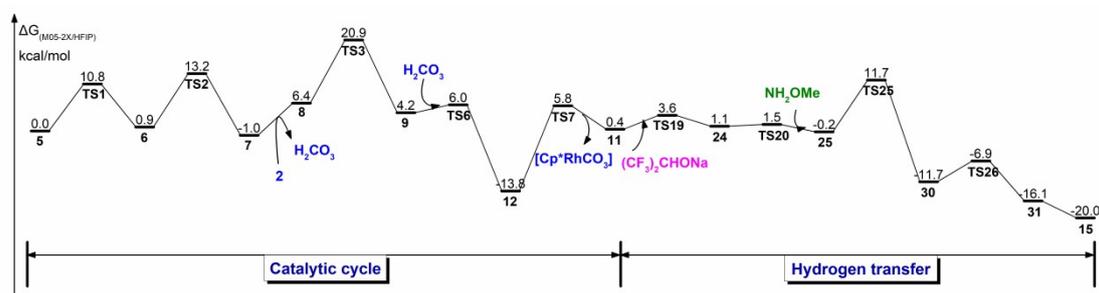


Figure S2. Calculated free energy profile for the entire allylation reaction. The energy values (kcal/mol) are calculated using M05-2X method in HFIP.

Due to the free energy barrier of base-assisted ($(\text{CF}_3)_2\text{CHONa}$ and Na_2CO_3) hydrogen transfer, solvent-assisted hydrogen transfer ($\text{CF}_3\text{CH}_2\text{OH}$ and $(\text{CF}_3)_2\text{CHOH}$), Rh(III) catalyst-assisted hydrogen transfer and no external assistance process is too high, path A-a'-2, path A-a'-3, path A-b'-1 and path A-b'-2 all should be excluded. The correct route for this reaction is N-H deprotonation, the concerted metalation-deprotonation (CMD), the formation of a seven-membered rhodacycle by cyano group insertion and $(\text{CF}_3)_2\text{CHONa}$ assisted hydrogen transfer to obtain (Z)-3-methyleneisindolineone **4** in HFIP.

3. Free energy profile of other path for formation of 4 in TFE.

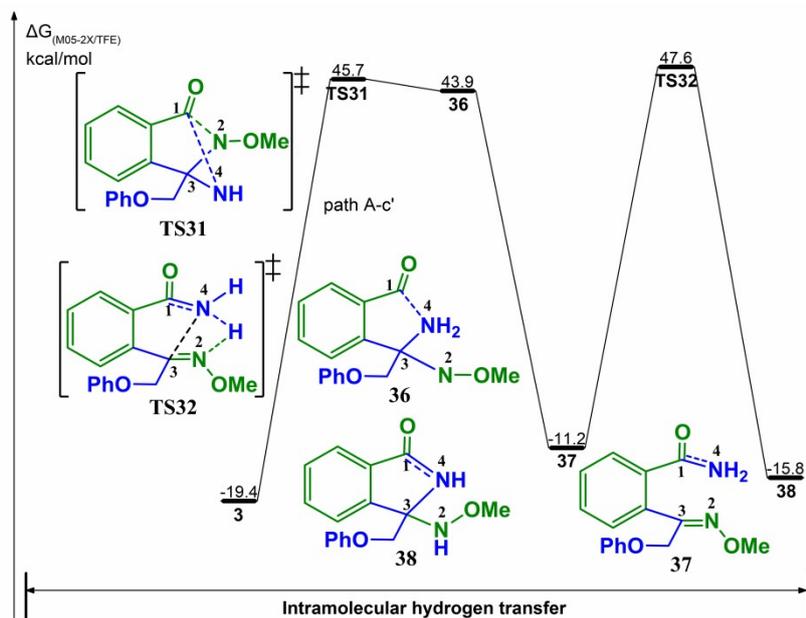


Figure S3. Free-energy profile for intramolecular hydrogen transfer to obtain alkenylation product 4. The energy values (in kcal/mol) are calculated using M05-2X method in trifluoroethanol.

3 can also be synthesized into the precursor of 4 through an intramolecular hydrogen transfer process, as shown in Figure S3. First, an amine exchange occurs through the transition state **TS31** with an energy barrier of 65.1 kcal/mol to form the intermediate **36**. Then, it undergoes isomerization to **37**, with an energy release of 55.1 kcal/mol. Proton transfer occurs to generate the precursor **38** of 4.

4. Calculated absolute energies and free energies of all involving acylation reaction structures at the M05-2X-D3/6-311++G(d,p)-SDD-SMD (2,2,2-trifluoroethanol) //B3LYP-D3/6-31G(d)-SDD-SMD (2,2,2-trifluoroethanol) level of theory

Geometry	$E_{(\text{elec-B3LYP-D3})}^1$	$G_{(\text{corr-B3LYP-D3})}^2$	$H_{(\text{corr-B3LYP-D3})}^3$	$E_{(\text{solv-M05-2X})}^4$
2	-439.013619	0.098189	0.141747	-439.083603
5	-1083.407674	0.215737	0.285569	-1083.440603
TS1	-1083.379360	0.209510	0.278979	-1083.417424
6	-1083.389421	0.210162	0.283422	-1083.436200
TS2	-1083.371725	0.210188	0.277034	-1083.411394
7	-1083.392167	0.212725	0.283865	-1083.438389
8	-1257.401826	0.299927	0.382065	-1257.44360
TS3	-1257.373498	0.298990	0.380366	-1257.419024
9	-1257.405597	0.303107	0.383200	-1257.450562
TS4	-1522.426649	0.335060	0.423933	-1522.532343
10	-1522.430627	0.334874	0.429125	-1522.537058
TS5	-1522.420697	0.332806	0.424498	-1522.526237
11	-954.458863	0.246614	0.316527	-954.613348
TS6	-1522.420050	0.334480	0.423995	-1522.534133
12	-1522.461170	0.341819	0.430586	-1522.574381
TS7	-1522.423872	0.425134	0.591794	-1522.537897
13	-1569.037158	0.282209	0.370881	-1569.273895
TS8	-1569.037023	0.367193	0.281238	-1569.273895
14	-1569.037148	0.282736	0.371241	-1569.278145
TS9	-1569.020631	0.280053	0.367023	-1569.262565
3	-954.484406	0.251131	0.317421	-954.644896

17	-1543.078781	0.254750	0.342479	-1543.244682
TS12	-1543.071374	0.253798	0.337864	-1543.237964
18	-1543.065713	0.253011	0.342074	-1543.24167
TS13	-1543.057747	0.251724	0.337547	-1543.22987
21	-1407.239834	0.297938	0.383476	-1407.511081
TS15	-1407.201722	0.292309	0.376073	-1407.476895
22	-1407.264103	0.299463	0.384775	-1407.539787
TS16	-954.393379	0.243236	0.311277	-954.550963
TS17	-1522.426263	0.340367	0.428568	-1522.539086
23	-1522.445994	0.338808	0.429873	-1522.5657521
TS18	-1522.438143	0.338632	0.424314	-1522.555347
TS21	-1569.002396	0.281701	0.369562	-1569.24712
26	-1569.029437	0.287315	0.372338	-1569.281023
TS22	-1569.015008	0.285370	0.370048	-1569.255059
27	-1397.973404	0.214264	0.295294	-1398.190891
TS23	-1543.039104	0.254693	0.339982	-1543.220576
28	-1543.067290	0.254020	0.341223	-1543.251852
TS24	-1543.059345	0.253035	0.337621	-1543.245174
29	-1372.021332	0.188456	0.266146	-1372.181185
TS29	-1407.196190	0.298194	0.378029	-1407.473825
34	-1236.200793	0.230981	0.306464	-1236.440865
TS30	-1236.146040	0.228644	0.300997	-1236.379713
35	-1236.219102	0.230596	0.307397	-1236.46209
TS31	-954.386783	0.248887	0.314834	-954.544802
36	-954.386831	0.246929	0.315859	-954.545800
37	-954.477451	0.246107	0.316417	-954.632841
TS32	-954.386783	0.244775	0.309242	-954.537776
38	-954.485129	0.25084	0.317424	-954.644896
H ₂ CO ₃	-264.997971	0.013094	0.043734	-265.069996
Na ₂ CO ₃	-588.577812	-0.016210	0.024320	-588.610746

CpRhCO₃	-567.947433	0.066478	0.110247	-567.907676
NH₂OMe	-171.017854	0.043650	0.073825	-171.046636
CF₃CH₂ONa	-614.528842	0.013095	0.053273	-614.623482
CF₃CH₂OH	-452.757233	0.026909	0.064093	-452.883983

¹The electronic energy calculated by B3LYP-D3(BJ) in 2,2,2-trifluoroethanol solvent.

²The thermal correction to Gibbs free energy calculated by B3LYP-D3(BJ) in 2,2,2-trifluoroethanol solvent.

³The thermal correction to enthalpy calculated by B3LYP-D3(BJ) in 2,2,2-trifluoroethanol solvent.

⁴The electronic energy calculated by M05-2X in 2,2,2-trifluoroethanol solvent.

5. Calculated absolute energies and free energies of all involving allylation reaction structures at the M05-2X-D3/6-311++G(d,p)-SDD-SMD (1,1,1,3,3,3-Hexafluoro-2-propanol) //B3LYP-D3/6-31G(d)-SDD-SMD (1,1,1,3,3,3-Hexafluoro-2-propanol) level of theory

Geometry	E _(elec-B3LYP-D3) ¹	G _(corr-B3LYP-D3) ²	H _(corr-B3LYP-D3) ³	E _(solv-M05-2X) ⁴
2	-439.013282	0.098182	0.141744	-439.083817
5	-1083.406563	0.215940	0.285609	-1083.434871
TS1	-1083.378234	0.209568	0.278995	-1083.41126
6	-1083.388220	0.212640	0.283571	-1083.430158
TS2	-1083.370683	0.207911	0.277958	-1083.405862
7	-1083.391298	0.212803	0.283862	-1083.433348
8	-1257.400535	0.299723	0.382040	-1257.441897
TS3	-1257.372337	0.298840	0.380352	-1257.417889
9	-1257.404330	0.303324	0.383193	-1257.448867
TS4	-1522.425556	0.335112	0.423963	-1522.528647
10	-1522.429391	0.335482	0.429139	-1522.532577
TS5	-1522.419346	0.333156	0.424539	-1522.520615
11	-954.458179	0.246652	0.316532	-954.612824
TS6	-1522.418757	0.334192	0.423978	-1522.529251
12	-1522.459572	0.342038	0.430603	-1522.568559
TS7	-1522.422187	0.336604	0.425158	-1522.531943
15	-1906.077917	0.282364	0.379929	-1906.411565
TS10	-1906.072728	0.279765	0.375679	-1906.406794
16	-1906.081272	0.282019	0.379583	-1906.412199
TS11	-1906.059021	0.280539	0.375561	-1906.393746
3	-954.483893	0.251168	0.317434	-954.644775
17	-1543.075598	0.253940	0.342504	-1543.244682
TS12	-1543.067576	0.254259	0.338243	-1543.237964

18	-1543.075599	0.257088	0.341575	-1543.24167
TS13	-1543.053979	0.251718	0.337568	-1543.22987
19	-1744.301698	0.301948	0.392922	-1744.665890
TS14	-1744.262828	0.294155	0.384958	-1744.626811
20	-1744.287895	0.299721	0.391193	-1744.641843
TS16	-954.392467	0.243290	0.311298	-954.550963
TS17	-1522.424636	0.340300	0.428561	-1522.533333
23	-1522.444369	0.341604	0.428954	-1522.560082
TS18	-1522.436237	0.336162	0.425287	-1522.549785
TS19	-1906.059998	0.284091	0.376281	-1906.402984
24	-1906.064150	0.285321	0.379850	-1906.407553
TS20	-1906.059557	0.283397	0.375760	-1906.402365
25	-1735.025786	0.215201	0.303606	-1735.333981
TS23	-1543.035674	0.256583	0.340189	-1543.217644
28	-1543.065410	0.253975	0.341264	-1543.250479
TS24	-1543.057437	0.252429	0.337674	-1543.243845
29	-1372.017357	0.185912	0.265797	-1372.181786
TS27	-1744.241399	0.298423	0.386296	-1744.61043
32	-1573.238001	0.231501	0.314293	-1573.566816
TS28	-1573.189498	0.229532	0.310280	-1573.519038
TS25	-1735.008128	0.211178	0.298506	-1735.311094
30	-1735.051507	0.217768	0.301755	-1735.354993
TS26	-1735.038458	0.216562	0.300748	-1735.345991
31	-2689.543207	0.486138	0.622586	-1735.360374
H ₂ CO ₃	-264.997599	0.013107	0.043734	-265.065357
Na ₂ CO ₃	-588.577812	-0.016042	0.024320	-588.607815
CpRhCO ₃	-567.946320	0.066603	0.110252	-567.901485
NH ₂ OMe	-171.017543	0.043644	0.073821	-171.046636
(CF ₃) ₂ CHONa	-951.577710	0.011868	0.061569	-951.763482
(CF ₃) ₂ CHOH	-789.792029	0.027042	0.072272	-790.007999

¹The electronic energy calculated by B3LYP-D3(BJ) in 1,1,1,3,3,3-Hexafluoro-2-propanol solvent.

²The thermal correction to Gibbs free energy calculated by B3LYP-D3(BJ) in 1,1,1,3,3,3-Hexafluoro-2-propanol solvent.

³The thermal correction to enthalpy calculated by B3LYP-D3(BJ) in 1,1,1,3,3,3-Hexafluoro-2-propanol solvent.

⁴The electronic energy calculated by M05-2X in 1,1,1,3,3,3-Hexafluoro-2-propanol solvent.

6. Cartesian coordinates of the structures in TFE

2				H	-1.86069000	-2.73408100	-2.81983100
C	2.69797400	0.34845700	-0.23956700	H	-0.97123600	-2.96968500	-1.28772500
N	3.16418000	1.10026400	-0.98997000	H	-2.33148100	-1.78643200	-1.37664200
C	2.09365800	-0.61827200	0.70445000	O	-2.57426000	0.63879600	-0.86187100
H	2.81128100	-1.42264500	0.88401800	C	-2.03524000	1.83312700	-1.08999200
H	1.89735700	-0.11537200	1.65962600	O	-2.50822700	2.69738300	-1.81588800
O	0.93651500	-1.23655300	0.17617200	N	0.04697600	-0.50595500	-1.37317200
C	-0.24011000	-0.51664500	0.11308600	H	0.18037900	0.41572800	-1.79395100
C	-0.37383700	0.82856500	0.47011600	O	-0.88509600	1.94730400	-0.41487800
C	-1.34605900	-1.24109100	-0.35004100	H	3.64149800	-1.91892400	-0.08202800
C	-1.62932000	1.43940000	0.36422300	TSI			
H	0.47005600	1.41282800	0.81866300	Rh	-0.87288100	-0.62746900	-0.11111900
C	-2.58738700	-0.61861200	-0.45033800	C	-0.37234700	-2.78052000	0.07415100
H	-1.21086300	-2.28343900	-0.62129100	H	-0.43707900	-3.31200800	1.01472700
C	-2.73715200	0.72666200	-0.09228900	C	-1.42265400	-2.62298000	-0.86635900
H	-1.72895100	2.48496600	0.64188300	H	-2.42791000	-3.01134200	-0.76847200
H	-3.44095000	-1.18719100	-0.80872100	C	-0.94248600	-1.78345700	-1.93626700
H	-3.70591000	1.21064400	-0.17159200	H	-1.50241600	-1.47454300	-2.80854900
5				C	0.43000200	-1.46831500	-1.65439200
Rh	-1.07154800	0.06947600	0.43783400	H	1.06832100	-0.83648000	-2.25754900
C	-0.46648600	0.38035200	2.55024100	C	0.78130700	-2.05695100	-0.40764700
H	0.05362800	1.27767200	2.85977500	H	1.73577900	-1.96883200	0.09319300
C	-1.89442400	0.23315400	2.44095400	O	-1.20776400	2.42784800	-0.53098500
H	-2.63582700	0.97004800	2.71899400	C	1.05161900	1.79505900	-0.53178400
C	-2.15717200	-1.10352000	1.96760300	C	2.13677100	0.97334600	0.09586500
H	-3.13492800	-1.52097800	1.76512700	C	2.12844700	0.60451300	1.44953500
C	-0.91469600	-1.73568400	1.71833400	C	3.20483500	0.57834100	-0.72313100
H	-0.77322300	-2.73231500	1.32232800	C	3.16333900	-0.17629700	1.96651300
C	0.14115100	-0.81158300	2.08344000	H	1.32562900	0.92526200	2.10383600
H	1.20408000	-0.99917600	2.01086600	C	4.22750000	-0.21782800	-0.20866900
O	-0.59789800	-1.24084100	-2.40726900	C	4.20570900	-0.60050200	1.13677400
C	1.32857200	-1.12334500	-1.01146500	H	3.15409300	-0.45374500	3.01640500
C	2.40216900	-0.21736500	-0.52749800	H	5.04058500	-0.53736300	-0.85372400
C	2.30483400	1.18626400	-0.51263400	H	5.00305400	-1.21864000	1.53898600
C	3.57759700	-0.83642500	-0.06515500	O	1.29408300	2.66856400	-1.35320900
C	3.37152500	1.94952900	-0.04086000	C	-1.66339300	2.21063200	-1.87309600
H	1.40383500	1.69699300	-0.83536400	H	-2.35829900	3.03021700	-2.07006200
C	4.63750800	-0.06758300	0.40579000	H	-0.83089500	2.24738400	-2.58011900
C	4.53607900	1.32755600	0.41836500	H	-2.19236400	1.25332800	-1.94514600
H	3.29065700	3.03211400	-0.03086500	O	-2.75762200	0.09342400	0.42076200
H	5.54081500	-0.55313000	0.76210800	C	-2.47528600	0.48998200	1.62772700
H	5.36297100	1.92860700	0.78519700	O	-3.22072300	0.92266400	2.48016000
O	1.43013100	-2.33008200	-1.07941800	N	-0.25540000	1.46650700	-0.11735400
C	-1.49755700	-2.24642000	-1.91273900	H	-0.58683400	1.12218600	1.16839800

O	-1.09049700	0.34308900	1.86297800	H	-0.82713400	-3.36132300	0.65488000
H	3.21575700	0.89030400	-1.76304100	C	-2.39001900	-1.99019100	-0.17618600
6				H	-3.16714700	-2.03213000	0.57703200
Rh	-0.81833600	-0.64243700	-0.11992000	C	-2.42815500	-1.17974100	-1.36097800
C	-0.35578400	-2.83001400	0.03035300	H	-3.25412800	-0.56246700	-1.68647000
H	-0.51811000	-3.40537000	0.93262700	C	-1.18067600	-1.36589600	-2.03946600
C	-1.29492900	-2.62291900	-1.00018000	H	-0.87571600	-0.89219500	-2.96279000
H	-2.30681100	-3.00476500	-1.02965100	O	-1.60512000	0.54583800	1.59463100
C	-0.70732500	-1.71542100	-1.96351100	O	0.38774200	0.80465200	2.62743300
H	-1.17585100	-1.35780300	-2.87075900	C	-0.87482700	0.95484400	2.53638200
C	0.63466300	-1.43213200	-1.53413400	O	-1.00938400	2.38607100	-1.07111000
H	1.33607800	-0.78219500	-2.03771100	C	1.20760200	1.66643600	-0.83893100
C	0.84289800	-2.07722100	-0.28471300	C	2.01845100	0.52237800	-0.30198700
H	1.73908400	-2.02451000	0.31704400	C	1.35593500	-0.42271600	0.52049200
O	-1.23164400	2.30227700	-0.35344100	C	3.36354300	0.37977100	-0.62988800
C	1.03231100	1.84541900	-0.36188100	C	2.08771300	-1.54147200	0.97131600
C	2.15950800	0.98165000	0.13541100	H	0.75370200	0.15910400	1.57309700
C	2.16135700	0.45919500	1.43649600	C	4.06902000	-0.73488200	-0.16489600
C	3.27047300	0.77033300	-0.69208800	C	3.43356000	-1.69492000	0.63309100
C	3.24932700	-0.28737800	1.89462200	H	1.60565100	-2.27118200	1.61697200
H	1.30996700	0.63990800	2.08466400	H	5.11703100	-0.85727200	-0.42434300
C	4.34593400	0.00186000	-0.24481700	H	3.99147100	-2.55428700	0.99475300
C	4.33683100	-0.52947200	1.04967900	O	1.69903800	2.68632200	-1.34470000
H	3.24622000	-0.68187900	2.90688600	C	-1.25896600	2.33490000	-2.48086400
H	5.19318500	-0.17674500	-0.90084000	H	-1.73269300	1.38438700	-2.75426300
H	5.17794700	-1.12051700	1.40084400	H	-1.94564100	3.15915200	-2.68977700
O	1.27443700	2.95318900	-0.85933300	H	-0.32784700	2.46900100	-3.04064900
C	-1.62515100	2.38740900	-1.72735200	O	-1.50921600	1.59941100	3.52668700
H	-2.39193100	3.16590700	-1.76310000	H	-0.84683800	1.86567400	4.18985300
H	-0.77417700	2.67077000	-2.35385400	H	3.83978700	1.12991300	-1.25468600
H	-2.05432300	1.43625600	-2.06408700	7			
O	-2.81636900	0.01939000	0.11235300	Rh	-0.86889100	-0.33296100	-0.08719600
C	-2.80625200	0.42121800	1.32999600	N	-0.06302400	1.53075400	0.15345700
O	-3.59283300	1.08729100	1.96761600	C	-2.08994300	-0.21858100	-1.85624300
N	-0.22179200	1.33856900	-0.15099700	H	-1.84033000	0.40458500	-2.70510300
H	-1.28630100	0.54205200	2.61381000	C	-1.71469000	-1.60092800	-1.68228000
O	-1.61597500	-0.08740700	1.94502400	H	-1.05152500	-2.15877600	-2.32936400
H	3.27857300	1.20546500	-1.68752500	C	-2.28509900	-2.05697300	-0.47280700
TS2				H	-2.16805800	-3.04109400	-0.03857400
Rh	-0.73631300	-0.46462400	-0.06411600	C	-3.12598600	-0.99054100	0.05212700
N	-0.11141500	1.38976300	-0.68142600	H	-3.68868500	-1.03677900	0.97587000
C	-0.38122800	-2.26382700	-1.26775700	C	-3.03867400	0.10970000	-0.80481300
H	0.61867900	-2.59277000	-1.51652800	H	-3.52826600	1.06471000	-0.66964400
C	-1.14523000	-2.67172300	-0.11456500	O	-0.40118700	-0.68693200	2.05033300

O	1.87134900	-0.54252600	2.17287800	H	-2.16982900	2.70377700	3.33636400
C	0.65540800	-0.64801600	2.68060600	H	-1.38788200	0.51026200	4.21028100
O	-0.82060100	2.60185000	0.64936000	O	0.02103700	3.21574800	-1.15662400
C	1.18956700	1.82115100	-0.28367500	C	2.95094400	2.37505900	-2.29272700
C	1.83213800	0.55512100	-0.76692800	H	3.76047500	2.01045000	-1.64834700
C	1.04551400	-0.61499400	-0.72568500	H	3.28316800	2.38618800	-3.33432300
C	3.16023300	0.52835200	-1.20153000	H	2.65423400	3.38262400	-1.98218300
C	1.63420400	-1.82588100	-1.12147900	C	-0.34451000	-1.50879900	-0.56289500
H	1.81607800	-0.49994400	1.18767000	N	0.04187400	-1.07031000	-1.59979400
C	3.72777900	-0.68105600	-1.60527700	C	-1.30619700	-2.27801200	0.28648500
C	2.96549200	-1.85400200	-1.55965400	H	-0.89606700	-3.28162400	0.42630000
H	1.06498000	-2.75130900	-1.08582400	H	-1.39303200	-1.80020400	1.26606700
H	4.75942900	-0.71473000	-1.94393900	O	-2.55034400	-2.43759500	-0.35890500
H	3.40805800	-2.79894900	-1.86513300	C	-3.39078600	-1.34427400	-0.46362300
O	1.74571500	2.92993700	-0.27738900	C	-3.14709000	-0.09858900	0.12215000
C	-1.33661400	3.40596200	-0.41885400	C	-4.55273500	-1.56227800	-1.21367600
H	-1.93568300	2.79586800	-1.10545900	C	-4.08038500	0.92916800	-0.05144100
H	-1.97122200	4.15937000	0.05525600	H	-2.25542900	0.09625300	0.70259000
H	-0.51938900	3.88930200	-0.96336200	C	-5.47405600	-0.52957500	-1.37317200
O	0.63143300	-0.72498700	4.00329100	H	-4.71351800	-2.53889000	-1.65958800
H	1.53999600	-0.69493900	4.35728200	C	-5.24306400	0.72387100	-0.79361300
H	3.72624500	1.45603100	-1.20889700	H	-3.87876900	1.89449600	0.40430500
8				H	-6.37409200	-0.70451600	-1.95601500
Rh	1.55665500	-0.48055600	-0.02864000	H	-5.96062200	1.52844900	-0.92374900
N	1.38184400	1.34893100	-0.93070200	H	-1.32516800	3.51482500	1.11143700
C	2.81676200	-1.35786700	1.59114000	TS3			
H	2.49040900	-1.32739100	2.62115000	Rh	-1.60672200	-0.40371700	-0.49824000
C	2.57904400	-2.40256200	0.66489400	N	-0.55915100	-0.99181200	1.18262700
H	2.05620600	-3.32792800	0.86785900	C	-3.74095700	0.30331100	-0.66428300
C	3.22741700	-2.05340500	-0.58454200	H	-4.03832900	1.28620200	-0.32256500
H	3.21656100	-2.65184700	-1.48611200	C	-3.25292900	-0.01801300	-1.97598100
C	3.81945700	-0.79262600	-0.43459900	H	-3.16870400	0.66448700	-2.81107000
H	4.35178500	-0.24339800	-1.19904500	C	-2.96788200	-1.42478900	-2.00121700
C	3.51640400	-0.30921000	0.89873300	H	-2.57034500	-1.97253600	-2.84612000
H	3.86410300	0.61827900	1.33382600	C	-3.21617000	-1.95642900	-0.71231000
O	1.82731600	1.48986500	-2.25086600	H	-3.08690700	-2.98637500	-0.40818300
C	0.40361700	2.21316500	-0.53871200	C	-3.69378500	-0.87199000	0.12678500
C	-0.10841400	1.77979900	0.79313000	H	-3.98470600	-0.95424700	1.16549800
C	0.32493000	0.53102600	1.26483200	O	-0.27999400	-2.34368200	1.43055700
C	-1.00210800	2.56401300	1.52699700	C	0.13528000	-0.10813000	1.93387600
C	-0.13820100	0.08325400	2.50768600	C	-0.15230000	1.28011200	1.44251900
C	-1.46915600	2.10660100	2.75995600	C	-0.65576800	1.41905600	0.12498200
C	-1.03030100	0.87147300	3.24934000	C	0.02714000	2.39659400	2.25385000
H	0.16849300	-0.88067700	2.90457100	C	-1.02229400	2.70074500	-0.33764100

C	-0.33855300	3.66136300	1.77995600	C	-0.66945000	1.76380000	0.01028100
C	-0.87639600	3.81109700	0.49439500	C	-2.01770600	1.81535000	2.05215500
H	-1.39475300	2.82028500	-1.35146600	C	-1.46464400	2.81274000	-0.51084700
H	-0.20784600	4.53355400	2.41382400	C	-2.78760500	2.83734300	1.51790200
H	-1.16552800	4.79563700	0.13848300	C	-2.51007700	3.33784700	0.23202600
O	0.89330700	-0.34959800	2.88848100	H	-1.23830800	3.20757300	-1.49713100
C	-1.18874900	-2.86138600	2.40592300	H	-3.60395500	3.25932400	2.09643600
H	-2.22578900	-2.76020500	2.06173300	H	-3.11135000	4.14495400	-0.17549400
H	-0.93841800	-3.91983200	2.51626400	O	0.79317900	0.46826000	2.79463400
H	-1.06159800	-2.34468900	3.36386500	C	-0.07960800	-3.20346800	1.88530700
C	0.50033300	0.60073900	-1.12208700	H	-0.75488200	-3.53401700	1.08603900
N	0.24573900	-0.52809100	-1.49673300	H	0.70987600	-3.94635800	2.02339200
C	1.60610400	1.61912500	-1.36002700	H	-0.64750700	-3.08098700	2.81599400
H	1.25093000	2.34592900	-2.09544300	C	0.49230500	1.20310700	-0.78074200
H	1.81510100	2.15035800	-0.42503000	N	0.42419200	-0.01024900	-1.14535500
O	2.75352200	1.01696600	-1.90555500	C	1.65717600	2.14009100	-1.07544200
C	3.52648900	0.21263300	-1.09233600	H	1.33763300	2.89941000	-1.79782800
C	3.28491300	-0.00826100	0.26799500	H	1.93344500	2.66987100	-0.15157800
C	4.61650600	-0.39789200	-1.72482500	O	2.77582600	1.50216900	-1.66109600
C	4.14069100	-0.84974500	0.98578600	C	3.57591900	0.71125600	-0.87260500
H	2.45011200	0.44435100	0.78667900	C	3.36233000	0.46288600	0.48882700
C	5.46338800	-1.22897000	-0.99472600	C	4.68013500	0.14363600	-1.52417200
H	4.78001400	-0.21061500	-2.78161200	C	4.25703500	-0.35832800	1.18251400
C	5.22984100	-1.46227200	0.36580700	H	2.50765200	0.86408200	1.01842000
H	3.93244600	-1.02369100	2.03772400	C	5.56340000	-0.67047200	-0.81844700
H	6.30701800	-1.69888500	-1.49269900	H	4.82576400	0.35225100	-2.57989700
H	5.88710600	-2.11648900	0.93079700	C	5.35822700	-0.92804000	0.54219000
H	0.43249300	2.26250400	3.25235100	H	4.07335000	-0.55400800	2.23562100
9				H	6.41522000	-1.10528800	-1.33467900
Rh	-1.39485100	-0.58561800	-0.41639600	H	6.04496000	-1.56607700	1.09078400
N	-0.35292300	-0.97006000	1.34106900	H	-2.21624500	1.43748100	3.05078500
C	-3.66113400	-1.03025200	-0.58721600	TS4			
H	-4.41176000	-0.56575100	0.03870600	N	-1.24872300	0.58515200	1.32283800
C	-3.14678500	-0.48434600	-1.83416800	C	-3.73880500	-1.48575900	-1.48340900
H	-3.47233500	0.43794300	-2.29773600	H	-3.69675200	-1.56324000	-2.56191600
C	-2.18100600	-1.37864800	-2.34595500	Rh	-2.09628500	-0.59080000	-0.27194900
H	-1.61225500	-1.25441000	-3.25787600	C	-3.28463000	-2.45466200	-0.55324000
C	-1.99675100	-2.42590800	-1.37369400	H	-2.76063000	-3.36858200	-0.79726100
H	-1.33887200	-3.27909600	-1.47501200	C	-3.46971700	-1.92598200	0.76335300
C	-2.97993900	-2.22450300	-0.32042000	H	-3.21857300	-2.41849200	1.69287300
H	-3.10656800	-2.85210200	0.55147300	C	-4.19511700	-0.67067000	0.63277200
O	0.58676700	-1.99579600	1.52700400	H	-4.47182600	-0.02384100	1.45337600
C	-0.04779000	0.20023700	1.92889100	C	-4.34521500	-0.39505300	-0.72991300
C	-0.95580100	1.25618600	1.31079300	H	-4.77733400	0.50014900	-1.15833700

O	-2.00616700	0.31767900	2.50639000	Rh	-0.28274300	1.80607300	-0.40200000
C	0.12787500	0.46815500	1.55787800	C	-0.33538000	3.72211000	0.65190500
C	0.95356400	0.96447500	0.40264700	H	-0.63778800	3.82527100	1.68557400
C	1.25018300	0.14816300	-0.69840900	C	0.98497100	3.46816600	0.17999400
C	1.46140500	2.26600800	0.47722000	H	1.86725900	3.30481800	0.78392700
C	2.06122300	0.66107600	-1.72032400	C	0.92004900	3.38214300	-1.25575600
C	2.25013400	2.77176600	-0.55555700	H	1.75104400	3.16755500	-1.91524700
C	2.54506000	1.96693900	-1.65974500	C	-0.42953600	3.68719200	-1.66588900
H	2.31041400	0.03589300	-2.57243200	H	-0.79553800	3.68658400	-2.68376400
H	2.63574000	3.78518300	-0.49649500	O	1.14540000	-2.97642000	-2.17517700
H	3.16015100	2.35278600	-2.46747800	C	2.62627900	-2.21462100	-0.51696000
O	0.62752300	0.10412600	2.61396400	C	3.04191100	-1.07257800	0.37130800
C	3.80882900	-1.48418700	0.27924800	C	2.16114800	-0.30357800	1.15390700
C	4.82991900	-1.61080900	-0.66890900	C	4.41628600	-0.79418300	0.41111400
C	3.90203200	-0.53418100	1.30094500	C	2.67299300	0.73999900	1.94080800
C	5.94022000	-0.76621100	-0.60081300	C	4.91463100	0.24782700	1.18925300
H	4.75468600	-2.36509700	-1.44666600	C	4.03833500	1.01939700	1.95842300
C	5.02059800	0.29838300	1.36447400	H	1.98705100	1.32209700	2.54918100
H	3.07929000	-0.43687100	2.00256500	H	5.98056400	0.45476400	1.19967100
C	6.04051900	0.19032400	0.41355300	H	4.41665700	1.82876000	2.57593800
H	6.73162000	-0.86328800	-1.33926600	O	3.29255500	-3.24838300	-0.58114500
H	5.08723000	1.04403700	2.15233300	C	-2.20506800	-1.78186000	1.36742700
H	6.90572100	0.84535100	0.46269700	C	-2.51702000	-0.81084000	2.32546900
C	-2.09950000	1.50044000	3.30633500	C	-3.19631700	-2.24518300	0.49002200
H	-2.69526900	1.21294500	4.17610400	C	-3.81546800	-0.29589000	2.38338000
H	-1.10989400	1.83721700	3.63454900	H	-1.75924700	-0.43118000	3.00047600
H	-2.60951000	2.30565600	2.76212300	C	-4.48742700	-1.72359100	0.55882000
C	-1.54865900	2.17624900	-1.28789700	H	-2.93076600	-2.99569400	-0.24692300
O	-1.47033100	0.97220400	-1.63869200	C	-4.80498400	-0.73979500	1.50353500
C	0.76515200	-1.26733400	-0.73114400	H	-4.04772200	0.46316700	3.12564500
N	-0.42037400	-1.69049100	-0.54325800	H	-5.24713500	-2.08829600	-0.12749400
C	1.86708000	-2.31940600	-0.89618500	H	-5.80978400	-0.33145000	1.55537400
H	2.46212100	-2.14535700	-1.80055000	C	0.20805500	-3.91045100	-1.61297000
H	1.40934100	-3.30801900	-0.95260300	H	-0.00110500	-4.61873800	-2.41879200
O	2.71096900	-2.32256900	0.27135900	H	0.65518700	-4.43501200	-0.76146700
O	-1.42750100	3.13894800	-2.20380100	H	-0.70622900	-3.39534300	-1.31285300
H	-1.31135000	2.71409600	-3.07362400	C	-1.43605200	-0.35802600	-1.98696900
O	-1.73290700	2.61076400	-0.09221300	O	-0.30844900	0.28037000	-1.87437500
H	-1.56543400	1.74500400	0.63551000	C	0.67735100	-0.53247900	1.20428800
H	1.23117000	2.88230300	1.34181400	N	-0.12369100	0.33895800	0.77305600
10				C	0.17279100	-1.83057700	1.84963300
N	1.48497700	-2.01632600	-1.23059200	H	0.01033400	-1.67555600	2.92504700
C	-1.19855400	3.88501800	-0.50430300	H	0.94113100	-2.59870900	1.74132100
H	-2.26584900	4.06186900	-0.46861400	O	-0.97482500	-2.36577200	1.21143200

O	-2.48611000	0.31127200	-1.40534600	H	1.25820000	-2.40993200	2.34819500
H	-3.23550500	-0.31004200	-1.35519000	C	0.95455500	0.52966600	2.39662100
O	-1.60878400	-1.43407400	-2.54747400	O	-0.34096500	0.50919400	2.20840200
H	1.00502800	-1.12348200	-1.37715800	C	-0.03717500	-0.85897900	-0.97919200
H	5.08458200	-1.40823900	-0.18382600	N	0.41926000	0.17452700	-0.40968200
TS5				C	0.87364200	-2.04355100	-1.29925500
N	-1.13471700	-2.13214100	1.36813800	H	1.00934400	-2.11944400	-2.38758000
C	-0.58785300	3.76504100	-0.41057500	H	0.37683100	-2.96162100	-0.97394800
H	0.27804600	4.29110400	-0.79141400	O	2.10578400	-2.01257400	-0.60859300
Rh	-0.44492500	1.76763100	0.52369900	O	1.58459200	1.23739500	1.36119000
C	-1.38398200	2.84041800	-1.13766500	H	1.45865200	0.55696100	0.45509200
H	-1.23557600	2.54737800	-2.16713300	O	1.58075500	0.02426900	3.30420300
C	-2.37895700	2.31436100	-0.24049300	H	-1.02281900	-1.12527300	1.50270400
H	-3.13878800	1.58543400	-0.48731500	H	-4.38575600	-2.55997800	-0.57805000
C	-2.22405200	2.99837900	1.02338000	11			
H	-2.80676200	2.80295100	1.91467700	N	0.23087800	1.76118100	0.45723300
C	-1.12521800	3.88055900	0.92893400	O	-0.70503800	2.75475500	0.18549700
H	-0.73131900	4.50386300	1.72016000	C	1.40329100	1.74057500	-0.25621900
O	-0.78384700	-2.85444200	2.50387300	C	2.26404700	0.53178300	0.03164800
C	-1.98658900	-2.70973000	0.47443900	C	1.88797100	-0.80204800	-0.24257900
C	-2.37348400	-1.82867800	-0.68758000	C	3.50977700	0.79325100	0.61247200
C	-1.47115200	-1.00453700	-1.38982000	C	2.76090200	-1.84063500	0.12024200
C	-3.70545100	-1.90867600	-1.11730500	C	4.37204200	-0.24781700	0.95609700
C	-1.91724500	-0.29474100	-2.51286200	C	3.99328200	-1.56970400	0.71323400
C	-4.14862500	-1.17239300	-2.21400000	H	2.49168700	-2.87113500	-0.09224400
C	-3.24874000	-0.36871700	-2.92047300	H	5.33174700	-0.02773700	1.41404300
H	-1.20808300	0.30954000	-3.07074600	H	4.65727700	-2.38781200	0.97545300
H	-5.18685800	-1.23557800	-2.52536600	O	1.79795600	2.67930500	-0.93786200
H	-3.57968200	0.19270100	-3.78904900	C	-2.22886800	-1.39887000	-0.03542100
O	-2.39568800	-3.86521700	0.56537600	C	-1.78969600	-0.88356200	1.19147000
C	3.10265500	-1.15707300	-1.01236000	C	-3.46800700	-1.00796900	-0.55657300
C	3.05281000	-0.34949900	-2.15454700	C	-2.59141100	0.03736600	1.87747900
C	4.23308100	-1.13451700	-0.18473500	H	-0.84813500	-1.19837400	1.62849000
C	4.14129300	0.47462500	-2.45822000	C	-4.25822300	-0.09573900	0.14085800
H	2.17802100	-0.33525100	-2.79395900	H	-3.78561500	-1.41872100	-1.50984700
C	5.30869000	-0.30655700	-0.49836500	C	-3.82158100	0.43966900	1.35801900
H	4.24252700	-1.76526900	0.69893900	H	-2.24011300	0.43732800	2.82440900
C	5.27083200	0.50438300	-1.63844100	H	-5.21467700	0.20681500	-0.27593800
H	4.09459200	1.10126300	-3.34491200	H	-4.43338900	1.15979800	1.89222700
H	6.17874400	-0.29421000	0.15240200	C	-1.47259000	2.43965200	-0.99277500
H	6.10869900	1.15106900	-1.88125300	H	-2.14310100	3.29163200	-1.12770900
C	0.58813700	-3.27442500	2.40050000	H	-0.81863600	2.32614700	-1.86172500
H	0.78112400	-3.84053200	3.31490400	H	-2.05954800	1.52659700	-0.84200200
H	0.73263200	-3.91645700	1.52448600	C	0.61899000	-1.12078800	-0.94872100

N	0.18078400	-0.32269500	-1.84545400	C	-0.23814900	-1.93316900	2.92765600
C	-0.11795800	-2.41021800	-0.55476800	H	0.45810900	-2.65137500	3.36784400
H	0.08637100	-2.68660100	0.48480100	H	-0.56542200	-1.21222300	3.68468100
H	0.21714900	-3.23847700	-1.18644100	H	-1.10339400	-2.46647600	2.51487800
O	-1.51478300	-2.29283200	-0.80320400	C	1.38414300	-2.81254000	-0.40854300
H	-0.71183700	-0.66533200	-2.21686500	O	1.09434500	-3.87138700	0.10210100
H	-0.19995800	0.89295400	0.76469100	O	0.52810300	-2.11565500	-1.17583000
H	3.79224300	1.82401300	0.80397700	H	0.67278700	-1.02183700	-1.50058300
TS6				C	0.09725500	1.40491400	-1.29796000
N	-0.31958900	-0.33821500	1.22426100	N	-0.04552900	0.14557500	-1.39550700
C	-3.21859900	-0.65254800	-1.54047000	C	1.26815500	2.08090100	-2.00073000
H	-3.22797900	0.01845800	-2.38946800	H	0.94570500	2.99017500	-2.51379000
Rh	-1.34080100	-1.03976400	-0.40794600	H	1.70615400	1.39335800	-2.73049400
C	-2.99038300	-2.04500100	-1.57868400	O	2.22683100	2.50377600	-1.02214700
H	-2.81504800	-2.64072400	-2.46479900	O	2.61847900	-2.29600800	-0.27924300
C	-3.03999100	-2.55007700	-0.21596900	H	2.71308400	-1.41957100	-0.69393300
H	-2.88992400	-3.58056100	0.07829900	H	-1.93207100	2.61702200	2.72994200
C	-3.27609900	-1.46581900	0.64607100	12			
H	-3.33860000	-1.50630600	1.72508000	N	-0.41944500	-0.47452600	1.35578700
C	-3.31931600	-0.25735400	-0.15558400	C	0.62467000	-2.77404200	-2.06504700
H	-3.50366000	0.74328700	0.21121200	H	0.42638400	-2.67854200	-3.12363400
O	0.49370500	-1.27265100	1.89221800	Rh	-0.02495500	-1.28727400	-0.53729300
C	-0.22723500	0.91897400	1.70174400	C	1.78030300	-2.29420700	-1.36736900
C	-0.97900400	1.97902600	0.92011400	H	2.59333700	-1.72606500	-1.80321400
C	-0.79571600	2.25220200	-0.45330000	C	1.64931700	-2.61191200	0.01410000
C	-1.82895900	2.80585800	1.66586500	H	2.34211200	-2.34367400	0.79820900
C	-1.46678500	3.33502700	-1.03973200	C	0.41033800	-3.33831600	0.17657400
C	-2.52990400	3.85101300	1.06462400	H	0.01494800	-3.71939600	1.10747800
C	-2.34882900	4.11743200	-0.29496900	C	-0.20699600	-3.43826500	-1.09753400
H	-1.31494400	3.55204100	-2.09346000	H	-1.17446400	-3.88123300	-1.29646800
H	-3.20317000	4.46333800	1.65743900	O	0.42212700	-1.07860000	2.33470600
H	-2.88185000	4.93509400	-0.77092200	C	-0.73979400	0.80763500	1.70040400
O	0.37578200	1.25012600	2.73847400	C	-1.64030700	1.55066000	0.74279700
C	3.08457000	1.53389800	-0.53518500	C	-1.22635500	2.06496600	-0.49885400
C	3.96484800	0.84689600	-1.38223000	C	-2.92156200	1.85861300	1.21515400
C	3.10512100	1.30833800	0.84301900	C	-2.09594200	2.88944700	-1.23255100
C	4.88361200	-0.05377200	-0.83405300	C	-3.79996700	2.62833600	0.45474100
H	3.95094600	1.03659600	-2.45093300	C	-3.38415800	3.14985300	-0.77335200
C	4.02995800	0.40875300	1.37883200	H	-1.77369400	3.29809300	-2.18611500
H	2.38828400	1.81829900	1.47673900	H	-4.79895400	2.83500600	0.82681800
C	4.92328100	-0.27134100	0.54728600	H	-4.05613600	3.76221000	-1.36657500
H	5.57034400	-0.58069200	-1.49031300	O	-0.45133200	1.33967900	2.77927500
H	4.03782000	0.23023600	2.45021200	C	2.77438600	2.19086800	-0.02448600
H	5.63490200	-0.97553700	0.96728500	C	3.81248600	1.87712200	-0.90867200

C	2.61298100	1.48544600	1.16915400	C	-1.38361100	3.34588800	-1.18169100
C	4.68556300	0.83247400	-0.59416400	C	-3.42612900	3.26172600	0.09493200
H	3.93105000	2.44361000	-1.82753800	C	-2.67721800	3.81133500	-0.94518000
C	3.49719400	0.44920400	1.47822700	H	-0.81045400	3.76408200	-2.00472200
H	1.78706100	1.72993800	1.82774400	H	-4.42982400	3.62355200	0.29814600
C	4.52845700	0.11390600	0.59637800	H	-3.08942200	4.59972900	-1.56742500
H	5.49279000	0.58615500	-1.27806000	O	0.12849200	0.86618200	2.07853700
H	3.35675600	-0.10928500	2.39867800	C	3.32795600	1.58314400	0.25044700
H	5.20799900	-0.69925000	0.83429900	C	4.27882600	1.36019600	-0.75309200
C	-0.37423400	-1.69396100	3.34824100	C	3.21564200	0.71111100	1.33658100
H	0.33704600	-2.14958600	4.04237800	C	5.12194000	0.24969500	-0.66161100
H	-0.98173900	-0.95073600	3.87516200	H	4.36949600	2.05221200	-1.58485200
H	-1.02117300	-2.47407500	2.92438300	C	4.08038000	-0.38231700	1.42787600
C	-3.06149200	-1.14106000	-0.63068400	H	2.43445200	0.88714900	2.06549500
O	-4.15075800	-1.13088500	-1.19263600	C	5.02985000	-0.62163700	0.42888600
O	-1.94268000	-0.79815300	-1.21043300	H	5.86167300	0.07624400	-1.43785400
H	1.50080000	0.55372100	-1.58805300	H	3.99675000	-1.05966400	2.27334400
C	0.09797700	1.77694500	-1.08149400	H	5.69334500	-1.47847300	0.49913900
N	0.56816000	0.58168300	-1.17809000	C	-1.63754300	-0.85011800	4.06417300
C	1.01561600	2.93719100	-1.45560500	H	-1.30697900	-1.68349600	4.69152200
H	0.45694800	3.85625800	-1.62790300	H	-1.05299900	0.04573000	4.30497000
H	1.60588900	2.70094400	-2.34877300	H	-2.70330300	-0.65415000	4.24118700
O	1.86444700	3.19952800	-0.32338900	C	-3.05755600	-1.06157900	-1.19773700
O	-2.99973200	-1.52686700	0.67844300	O	-3.75438600	-1.41488000	-2.14634000
H	-2.10771300	-1.30359400	1.03427800	O	-1.88130400	-0.42189400	-1.41809400
H	-3.22472800	1.48367400	2.18771900	H	1.72574400	0.47749400	-1.42793600
TS7				C	0.50211300	1.83384800	-0.81946000
N	-1.89210100	-0.26322000	1.81526900	N	0.75841600	0.60914200	-1.13182400
C	1.02314600	-3.05733200	-1.29693300	C	1.64652400	2.84919300	-0.90851700
H	1.45418200	-3.27963100	-2.26483100	H	1.26841000	3.86930500	-0.85754900
Rh	-0.16959700	-1.25545700	-0.93385200	H	2.19753000	2.72109700	-1.84780200
C	1.64129900	-2.30546400	-0.26163000	O	2.49975400	2.69485500	0.22957200
H	2.62182700	-1.84922700	-0.29904700	O	-3.39412900	-1.23033600	0.05739700
C	0.68854500	-2.16159300	0.79896700	H	-2.69588800	-0.75471800	0.83791400
H	0.79259700	-1.56463300	1.69594400	H	-3.44656700	1.83312100	1.71053300
C	-0.49877800	-2.91539700	0.43952300	H ₂ CO ₃			
H	-1.39844200	-2.96275900	1.03632800	O	0.69878400	-1.14910400	-0.00005500
C	-0.30204600	-3.45098900	-0.85396800	O	0.55828800	1.12327400	-0.00011800
H	-1.01760700	-4.02258100	-1.43016300	C	0.05273000	-0.12753800	0.00012800
O	-1.40919100	-1.25949500	2.71818600	H	1.52969200	1.05027000	0.00057300
C	-1.00992000	0.72670500	1.58969600	O	-1.28675800	-0.11086900	-0.00000200
C	-1.58599300	1.76654300	0.65570800	H	-1.60858800	0.80854900	0.00006000
C	-0.83578600	2.31382000	-0.40375700	CpRhCO ₃			
C	-2.87676400	2.25293700	0.88892600	C	1.78094800	0.02704900	1.25636500

H	1.66735300	0.04988800	2.33279700	C	-2.74594200	1.42669700	-0.22079900
Rh	0.07358800	-0.00035100	-0.04704900	O	-3.35367600	2.26480000	-0.89722700
C	1.87945200	-1.16253700	0.44663100	O	-0.83061400	0.65826300	0.91878900
H	1.83418100	-2.18096100	0.80785300	C	-0.63436400	0.88058500	2.31576600
C	1.94731700	-0.74855400	-0.90220100	H	-0.06790200	1.80164100	2.48847700
H	1.96817700	-1.39366300	-1.77084600	H	-1.59542700	0.92506500	2.84093000
C	1.94669400	0.70674900	-0.93301200	H	-0.05451500	0.02314400	2.66710300
H	1.96692500	1.31455500	-1.82824100	H	-2.93665400	-3.29103400	-0.44698000
C	1.88250800	1.17933400	0.39757300	O	0.34542400	2.94138700	-0.90889500
H	1.83920300	2.21258200	0.71408900	C	1.10718400	3.62678800	0.00553900
C	-2.39648600	0.00014900	0.01002300	H	0.58439500	3.83195000	0.96374000
O	-1.62084800	-1.09781100	-0.00206400	H	1.47610900	4.60636100	-0.35637400
O	-3.61203800	0.00001100	0.02997800	C	2.36250200	2.85685800	0.40546500
O	-1.62085400	1.09783100	-0.00175500	F	2.06028700	1.65060000	0.97166200
I3				F	3.13170500	3.52888800	1.28796100
N	-1.11525300	-0.35210100	-2.02609100	F	3.14413700	2.56443000	-0.67314300
C	-2.74460400	-1.14260200	-0.37020200	Na	0.94406200	0.89552800	-1.57265400
C	-3.35780200	0.06562500	0.02615800	TS8			
C	-3.39881800	-2.35911600	-0.13491600	N	1.47095400	-3.13850300	1.08738900
C	-4.62648100	0.03009900	0.61230200	C	2.81768500	-1.40810200	-0.02033900
C	-4.65722600	-2.38230600	0.46851000	C	3.01737200	-0.02330300	0.18275600
C	-5.27176500	-1.18595300	0.84307200	C	3.84613600	-2.17226300	-0.58604800
H	-5.10039400	0.96509900	0.89530600	C	4.24109700	0.55732400	-0.17033000
H	-5.15676600	-3.33153600	0.63748500	C	5.06168400	-1.58357800	-0.93959300
H	-6.25193300	-1.19789300	1.31051300	C	5.25964600	-0.21831200	-0.72765500
H	-1.93537900	0.17486000	-2.33851300	H	4.39364600	1.61578100	-0.00003800
N	-1.54978200	1.73775600	0.35153500	H	5.84828700	-2.19011800	-1.37890100
H	-0.83891900	2.37287600	-0.19202600	H	6.20602600	0.24455200	-0.99170900
C	-1.41022500	-1.10705900	-1.03432900	H	2.40034900	-3.36094900	1.45837500
C	-0.35174900	-1.98403900	-0.40091300	N	1.57176100	1.97455400	0.53104600
H	-0.38614500	-1.82293200	0.68183400	H	0.53052900	2.38767500	0.93564000
H	-0.58141200	-3.04201800	-0.59379700	C	1.53942400	-2.10038300	0.34579000
O	0.92743200	-1.65262700	-0.92088200	C	0.27998900	-1.62108000	-0.36301000
C	2.02965100	-2.27257300	-0.37443100	H	0.37306200	-0.58663000	-0.70545100
C	1.97430300	-3.20121400	0.67078400	H	0.15430600	-2.25703800	-1.25049000
C	3.26413200	-1.91489200	-0.93551300	O	-0.84548000	-1.74846700	0.50134300
C	3.16498400	-3.75571200	1.15564400	C	-2.10486500	-1.80524900	-0.04807400
H	1.03063400	-3.49952700	1.11129100	C	-2.40045800	-1.53620700	-1.38835800
C	4.43901600	-2.47459700	-0.44034800	C	-3.13074100	-2.13655400	0.84769300
H	3.28761600	-1.20984500	-1.76148500	C	-3.72887700	-1.60495400	-1.82152100
C	4.39758300	-3.39804500	0.61110400	H	-1.62365600	-1.24519800	-2.08459400
H	3.11581700	-4.47475400	1.96870300	C	-4.44918000	-2.19453700	0.40330800
H	5.39042900	-2.18986500	-0.88094000	H	-2.87321400	-2.34595700	1.88217100
H	5.31504200	-3.83308200	0.99585100	C	-4.75715400	-1.93138200	-0.93678600

H	-3.95374200	-1.39134400	-2.86301300	C	4.54776600	-2.61249400	-0.42615200
H	-5.23774900	-2.45224000	1.10512400	H	3.41123300	-1.25279500	-1.66610000
H	-5.78517000	-1.97930600	-1.28347300	C	4.49362100	-3.59180200	0.57289500
C	1.93150700	0.73791200	0.88565500	H	3.19977800	-4.71337600	1.88195200
O	1.31593100	0.16222000	1.82367900	H	5.50201400	-2.32390700	-0.85794900
O	2.24048300	2.60535900	-0.53764100	H	5.40425300	-4.06680300	0.92520700
C	1.60984300	2.30914200	-1.78875000	C	-2.77154700	1.32353800	-0.23372600
H	1.66897900	1.23667200	-2.01450500	O	-3.51444100	2.11714700	-0.85385300
H	0.56089000	2.62182800	-1.78925100	O	-0.80173800	0.64513300	0.81451100
H	2.17000300	2.87356900	-2.53850500	C	-0.70814100	0.80943700	2.22321500
H	3.68257300	-3.23224600	-0.75900500	H	-0.27383700	1.78349400	2.47679900
O	-0.65763300	2.63356700	1.46123800	H	-1.69566500	0.71265600	2.69296500
C	-1.51147000	3.15819900	0.51017200	H	-0.04951200	0.01116200	2.58027700
H	-1.00752600	3.80102200	-0.23643400	H	-2.74886000	-3.42830700	-0.45876000
C	-2.19192400	2.05775700	-0.29331800	O	0.22647300	3.00334200	-1.05384500
F	-3.02457800	2.53442500	-1.24141900	C	0.86525100	3.91943100	-0.20299900
F	-2.92508800	1.23036100	0.50694600	H	0.22762600	4.22057500	0.63835700
F	-1.27861400	1.26304400	-0.91527300	H	1.16528200	4.82046100	-0.74996700
Na	-0.89376100	0.47886800	2.23162400	C	2.12931800	3.31271800	0.38320200
H	-2.32540600	3.76154900	0.94636800	F	1.85172000	2.21908200	1.14623800
14				F	2.80240400	4.18718200	1.15017900
N	-0.98675200	-0.44613800	-2.00813400	F	2.96874300	2.87864300	-0.59355700
C	-2.64091200	-1.27187400	-0.38453800	Na	1.00649400	0.77833100	-1.18207500
C	-3.29923400	-0.08480900	0.00155000	TS9			
C	-3.24895300	-2.51470900	-0.14985400	N	-0.27569200	-0.07772400	1.56125700
C	-4.56757300	-0.17961200	0.58686800	C	1.77219700	0.96212700	0.74419300
C	-4.50579100	-2.59076400	0.44995600	C	2.11548900	2.17020800	0.11291300
C	-5.16573700	-1.41760700	0.82241400	C	2.73183000	0.26333700	1.48783000
H	-5.08059400	0.73760300	0.85934700	C	3.42783200	2.64242800	0.17583400
H	-4.96709900	-3.55934800	0.61897600	C	4.03839100	0.74952700	1.55981400
H	-6.14517400	-1.46596500	1.28996000	C	4.38819900	1.93441400	0.89914300
H	-1.80556700	0.07643500	-2.33055700	H	3.67339500	3.56711600	-0.33797600
N	-1.58385400	1.72729600	0.24672300	H	4.78894000	0.19536700	2.11648300
H	-0.59199500	2.59278900	-0.54100200	H	5.40937100	2.30221400	0.95231900
C	-1.29706900	-1.20429000	-1.02369000	H	0.08549200	0.14892000	2.48404400
C	-0.23998400	-2.06989400	-0.36845800	N	-0.14746700	2.48918700	-0.09412000
H	-0.31176000	-1.93282900	0.71623600	H	-1.31493200	-0.77012400	1.42108500
H	-0.43475600	-3.12831300	-0.59176800	C	0.39507600	0.42702700	0.55849100
O	1.05021000	-1.69839000	-0.83699300	C	-0.03639700	-0.02853900	-0.83125200
C	2.14413900	-2.36777800	-0.33107500	H	-1.07108000	0.25066700	-1.01685000
C	2.07557000	-3.34835500	0.66423200	H	0.60160400	0.41272700	-1.59854200
C	3.38126900	-2.00297300	-0.88088300	O	-0.00046700	-1.47707600	-0.93413200
C	3.25782100	-3.95288800	1.10816700	C	1.25534900	-2.05283600	-0.76799500
H	1.12872200	-3.64697000	1.09767300	C	2.27629900	-1.81952000	-1.69211100

C	1.46331000	-2.88216500	0.33566800	C	-3.32313200	1.00520400	0.44857000
C	3.52205000	-2.41945600	-1.49863500	C	-4.41555900	-0.32040200	-1.74762900
H	2.09529100	-1.17573600	-2.54722000	H	-2.47626100	-1.21731800	-2.00719900
C	2.70952800	-3.48819400	0.51338100	C	-4.65462000	1.21153600	0.09966500
H	0.66127700	-3.01887700	1.05419400	H	-2.87551900	1.50833500	1.30037900
C	3.74258000	-3.25374200	-0.39832200	C	-5.21108200	0.54902600	-1.00193200
H	4.31997400	-2.23672100	-2.21276700	H	-4.83332000	-0.84140500	-2.60495800
H	2.87475500	-4.13183100	1.37284600	H	-5.26156000	1.89143500	0.69146800
H	4.71352300	-3.71824100	-0.25334700	H	-6.25053600	0.71037300	-1.27179900
C	1.02766500	2.90446000	-0.61189000	C	3.01873100	-1.09171400	-1.11138300
O	1.26314300	3.72737200	-1.52168300	O	3.91932600	-1.57427500	-1.78776200
O	-1.24271000	2.83947100	-0.92710300	O	0.30693800	-0.70170700	2.40995100
C	-2.36023300	3.15010200	-0.10898400	C	-0.88864400	-1.28088100	2.92366300
H	-2.60452900	2.32503500	0.56946600	H	-1.63497000	-1.42573700	2.13539800
H	-2.18328500	4.05844600	0.48420100	H	-0.68629600	-2.23636200	3.42386500
H	-3.20086200	3.31379900	-0.79011900	H	-1.26841500	-0.55826200	3.65230200
H	2.46916300	-0.68016300	1.95594500	H	0.39982300	1.69791700	1.26609200
O	-2.33853800	-1.42664100	1.26739700	N	1.89687000	-1.75408500	-0.66184500
C	-3.41884700	-0.58040400	1.46645400	H	1.73226900	-2.73324800	-0.85273500
H	-3.11598000	0.41277100	1.84111600	H	1.85997900	-1.69577400	1.79286500
C	-4.17628500	-0.33446100	0.17043800	17			
F	-3.38747300	0.22119400	-0.78851300	N	-0.55645300	0.34367200	-2.52937800
F	-5.23628500	0.47957300	0.34183500	C	-1.68400800	-1.26196900	-1.01335800
F	-4.63823900	-1.50219400	-0.36261500	C	-2.83456900	-0.55311000	-0.60345500
Na	-2.03805200	-2.66467100	-0.58395600	C	-1.63477500	-2.64857700	-0.78783500
H	-4.15906800	-0.98227900	2.17666100	C	-3.88580400	-1.22766700	0.02509300
3				C	-2.69520900	-3.31832900	-0.17480300
C	1.68896500	0.40576500	0.12075800	C	-3.82145000	-2.60547600	0.24265700
C	2.87927100	0.29870800	-0.60206900	H	-4.75911500	-0.66643500	0.34528600
C	1.32164800	1.61406400	0.70563800	H	-2.64029100	-4.39289600	-0.02698300
C	3.74030300	1.37907900	-0.76859400	H	-4.64767100	-3.11792100	0.72676500
C	2.18349800	2.70651700	0.54494000	H	-1.52576800	0.52068200	-2.80693200
C	3.37835800	2.59472700	-0.18229600	N	-2.65233900	1.69640500	0.16486200
H	4.65852000	1.27042200	-1.33804100	H	-2.14913000	1.35120100	1.02811500
H	1.92055800	3.66125200	0.99194800	C	-0.50792600	-0.55642100	-1.62404700
H	4.02373700	3.46164300	-0.29030800	C	0.82707300	-0.97369200	-1.03408900
N	0.89801800	-1.60310300	1.46026400	H	0.77125100	-0.88715400	0.06060700
C	0.98389600	-0.94466500	0.13355700	H	1.02467700	-2.02799500	-1.27827200
C	-0.38850100	-0.92038700	-0.55666500	O	1.86758200	-0.15365300	-1.54688400
H	-0.24415000	-0.61677200	-1.60113500	C	3.12343100	-0.31743100	-1.03769400
H	-0.81416500	-1.93230900	-0.53169800	C	3.48840200	-1.30565800	-0.10966800
O	-1.23531900	-0.00292900	0.11849500	C	4.08416600	0.60303300	-1.49152300
C	-2.52916400	0.12945100	-0.30723300	C	4.80859400	-1.35613700	0.35855100
C	-3.07421200	-0.53812600	-1.41079800	H	2.76534100	-2.02647800	0.25227700

C	5.39069800	0.53890900	-1.01513300	C	5.33394700	0.78152100	-0.84970800
H	3.78033200	1.35693200	-2.21133900	H	3.67478400	1.77166300	-1.83018100
C	5.76275600	-0.44021700	-0.08386900	C	5.76147000	-0.36711000	-0.17018400
H	5.08192100	-2.12589200	1.07532700	H	5.17751900	-2.31156900	0.55540600
H	6.12355100	1.25649400	-1.37381500	H	6.02566200	1.60107900	-1.02449100
H	6.78326300	-0.48866500	0.28383600	H	6.78466100	-0.44634200	0.18458800
C	-2.99060500	0.92606400	-0.88197700	C	-3.04022100	0.99255900	-0.71210600
O	-3.40197000	1.33491700	-1.97614600	O	-3.47702900	1.46386100	-1.78839200
O	-2.68215800	3.08209000	0.00767900	O	-2.84836500	3.04561700	0.33650300
C	-1.43378200	3.52780100	-0.56248900	C	-1.70091200	3.62385400	-0.28993900
H	-0.60205400	3.22203700	0.08141400	H	-0.78617100	3.33293900	0.23977900
H	-1.30783600	3.11952100	-1.57177300	H	-1.62968400	3.31663300	-1.34108900
H	-1.51211000	4.61750500	-0.60794700	H	-1.84340600	4.70873200	-0.23486100
H	-0.76884800	-3.21892300	-1.10839500	H	-0.71645900	-3.07230000	-1.33940200
C	-0.05408400	0.85821900	2.09263900	C	0.04945400	0.62257600	1.98572500
O	0.44995800	1.99302700	1.77910900	O	0.51305200	1.72067100	1.57444800
Na	2.52607700	1.11453600	1.73298800	Na	2.65300900	0.93294200	1.95193000
O	0.71531500	-0.19853000	2.21641700	O	0.77738700	-0.38614500	2.32157100
O	-1.33751500	0.71194600	2.28643600	O	-1.27844300	0.43793400	2.09929600
Na	-1.11726900	-1.50244300	2.60851700	Na	-1.03284600	-1.80896200	2.52198700
TS12				18			
N	-0.60539900	0.64329300	-2.38962300	N	1.01251400	0.26070500	2.17214500
C	-1.67997800	-1.15341800	-1.06342700	C	2.86017200	-0.47724200	0.73762100
C	-2.84585500	-0.51000200	-0.59148200	C	3.48991200	-0.12344000	-0.47605000
C	-1.59585200	-2.55462700	-0.96910700	C	3.57486400	-1.21726300	1.69648600
C	-3.87846800	-1.27339200	-0.03651800	C	4.79592300	-0.56572700	-0.71821400
C	-2.63914000	-3.30751000	-0.42798400	C	4.88535100	-1.62519000	1.45216400
C	-3.78358200	-2.66381000	0.04924100	C	5.49622900	-1.30242900	0.23547800
H	-4.76503200	-0.76619500	0.33442100	H	5.24920400	-0.30934000	-1.67101900
H	-2.55761900	-4.38983700	-0.38397900	H	5.41873800	-2.20865100	2.19739800
H	-4.59922600	-3.23993400	0.47732400	H	6.51367000	-1.62718200	0.03375700
H	-1.58667100	0.86336300	-2.58932000	H	1.79164800	0.43318300	2.81140300
N	-2.69152400	1.62729800	0.40361500	N	1.99680000	1.59519900	-0.93285200
H	-1.87979900	1.06477600	1.38705000	H	-1.65546300	3.75747600	1.06444800
C	-0.52649000	-0.36971500	-1.61578200	C	1.43591800	-0.14195000	1.02499900
C	0.83739500	-0.86712500	-1.16154200	C	0.37461700	-0.45831900	-0.02489700
H	0.83277900	-0.98756700	-0.06991900	H	-0.13476500	0.45436200	-0.34358100
H	1.03381000	-1.85536100	-1.60280700	H	0.82408000	-0.93683800	-0.89815300
O	1.84899000	0.04812900	-1.55235500	O	-0.58147100	-1.35260000	0.58390700
C	3.11452100	-0.16413800	-1.08817300	C	-1.61377200	-1.79333800	-0.20388300
C	3.53675800	-1.32209400	-0.41617700	C	-1.77212500	-1.46375000	-1.55745100
C	4.02279100	0.88613900	-1.30710700	C	-2.55024900	-2.62620300	0.42841600
C	4.85934600	-1.41072500	0.03743900	C	-2.86861400	-1.97516100	-2.26423500
H	2.85569100	-2.14643700	-0.24113400	H	-1.06398700	-0.82171500	-2.06657400

C	-3.63838400	-3.12075900	-0.28590700	C	3.66544900	-2.24381100	1.91841900
H	-2.40553800	-2.87536900	1.47566700	H	2.33172400	-2.98257600	0.38230400
C	-3.80573300	-2.79989100	-1.63999700	C	3.92938200	-1.21326300	2.82931900
H	-2.98015700	-1.72076800	-3.31473800	H	3.23684500	0.67472400	3.60831100
H	-4.35498000	-3.76628700	0.21455100	H	4.32414300	-3.10634000	1.86425000
H	-4.64924100	-3.19482500	-2.19820400	H	4.79264200	-1.26701200	3.48571700
C	2.79684800	0.71134900	-1.52853900	C	-3.39276000	1.20686700	0.76920000
O	3.03117100	0.50597300	-2.74942800	O	-4.19681400	1.68018900	1.61281400
O	1.19557300	2.27149100	-1.91907700	O	-2.21822200	3.14881700	0.52673600
C	0.56379600	3.36209000	-1.28168800	C	-0.86769800	3.51628900	0.32422200
H	-0.05906600	3.03615600	-0.43661400	H	-0.19984400	3.05024800	1.06724300
H	1.29266300	4.09937100	-0.91063100	H	-0.50466000	3.23695700	-0.67324500
H	-0.07463700	3.83572200	-2.03556600	H	-0.82281800	4.60449600	0.44411800
H	3.08299500	-1.51059500	2.62048100	H	-2.00410600	-2.63893900	-1.57683700
C	-2.66873800	2.15315100	0.89571300	C	2.28584800	0.95067000	-1.87734200
O	-3.16459400	2.59513000	-0.16527100	O	1.83114600	1.96720500	-1.26303900
Na	-4.37745200	0.58918800	-0.34967400	Na	3.73181100	1.94018600	0.05666300
O	-2.90629500	1.03444400	1.44026400	O	3.49361500	0.51978100	-1.71819600
O	-1.75515100	2.93389200	1.57259700	O	1.50746200	0.25148000	-2.70201000
Na	-1.30894000	0.06915600	2.68951700	Na	2.85907200	-1.58073200	-2.40754800
TS13				Na ₂ CO ₃			
N	-0.85639200	-0.08882700	-2.03580600	C	-0.00000600	0.57359000	0.00184700
C	-2.55199200	-0.86054700	-0.48726700	O	-1.12893400	1.19627500	-0.00082900
C	-3.52749100	-0.22867300	0.31092600	O	0.00001800	-0.75321800	0.00636700
C	-2.76453900	-2.16258500	-0.96370500	O	1.12891900	1.19628100	-0.00011100
C	-4.68284500	-0.94041200	0.64671200	Na	-2.24151600	-0.75256100	-0.00234500
C	-3.92620800	-2.85753200	-0.62092000	Na	2.24151800	-0.75255200	-0.00260800
C	-4.88308000	-2.24494800	0.19268600	(CF ₃) ₂ CHONa			
H	-5.41968600	-0.43697800	1.26456100	O	0.00299800	1.18527600	1.18944200
H	-4.07632000	-3.87117200	-0.98116700	C	-0.00103300	-0.11152100	0.84548000
H	-5.78737900	-2.78198900	0.46662700	H	-0.00371200	-0.84315100	1.68859200
H	-1.53525600	-0.33259100	-2.75465100	C	-1.26694500	-0.47860200	0.03509500
N	-2.38809700	1.78592800	0.11465000	F	-2.37309100	-0.23204300	0.76887000
H	0.29383100	0.19566700	-2.35871400	F	-1.32850400	-1.77416700	-0.35371100
C	-1.26308300	-0.20098900	-0.81471900	F	-1.37650900	0.27483100	-1.09938900
C	-0.24130200	0.04749500	0.27813300	Na	0.01323000	2.66493000	-0.40005300
H	0.31560600	0.95960100	0.05821300	C	1.26270600	-0.48752800	0.03573500
H	-0.73266300	0.11526000	1.24938200	F	2.37068900	-0.24041400	0.76634100
O	0.65249300	-1.08472700	0.24731300	F	1.31907400	-1.78555000	-0.34529100
C	1.69505400	-1.07194600	1.13090600	F	1.37343300	0.25874500	-1.10364300
C	1.93942200	-0.04468100	2.05493500	CF ₃ CH ₂ ONa			
C	2.55490700	-2.18094000	1.08080800	O	-1.20634900	1.24683000	0.00007800
C	3.05773900	-0.12569500	2.89517400	C	0.14392200	1.32136300	-0.00006700
H	1.28138700	0.81318900	2.12783800	H	0.60051800	1.83323600	0.88429600

H	0.60040800	1.83308100	-0.88456400	C	1.84044600	1.76234400	-0.83932400
C	0.81305700	-0.05532100	-0.00001000	H	1.95526900	1.02153000	-0.04159800
F	0.44646800	-0.80024200	1.08587900	C	2.20232900	3.12044700	-0.27468500
F	2.16631500	-0.00076600	0.00012000	F	2.23651100	4.07065400	-1.23468500
F	0.44669300	-0.80018000	-1.08593800	F	1.32909600	3.53273500	0.66484700
Na	-2.25702600	-0.62059300	-0.00004100	F	3.42876100	3.06884600	0.29364700
21				O	0.51530500	1.83804100	-1.32316900
N	-1.12053100	-0.09395500	-2.43544600	H	0.32250100	1.03536400	-1.85719100
C	-2.86156800	-0.49408300	-0.77028100	H	2.56205800	1.53814800	-1.63403300
C	-3.07016400	-0.02452900	0.54729200	TS15			
C	-3.97135800	-0.76819900	-1.58564500	N	1.09370200	-0.09617200	-2.14091700
C	-4.38496000	0.13446600	1.00930900	C	2.90022500	0.59077600	-0.73565400
C	-5.27068400	-0.59887700	-1.11196300	C	3.13301500	-0.17092600	0.43069100
C	-5.47762800	-0.14541100	0.19269200	C	3.95649400	1.13973600	-1.47057500
H	-4.53205100	0.48594100	2.02468500	C	4.46342700	-0.34936100	0.83311500
H	-6.11461100	-0.82598400	-1.75627500	C	5.27038700	0.94192700	-1.04740000
H	-6.48564100	-0.01088200	0.57312500	C	5.52079900	0.19093000	0.10355500
H	-1.84527000	0.54859800	-2.76997600	H	4.64711500	-0.91325200	1.74072100
N	-0.80703900	0.77086100	1.04528400	H	6.09014200	1.37194700	-1.61439500
H	-0.66399700	1.23527100	0.14522300	H	6.54187100	0.03074200	0.43661700
C	-1.50916700	-0.69050500	-1.37095800	H	1.77386200	-0.77073500	-2.48764200
C	-0.58958900	-1.70536500	-0.72115000	N	0.81649100	-0.92978600	0.83570000
H	-0.79637600	-1.78382200	0.34989600	H	0.28686500	-1.35516800	-0.18802800
H	-0.80426800	-2.68561400	-1.17442700	C	1.50624300	0.70291400	-1.21445800
O	0.75699300	-1.32689400	-0.95710000	C	0.59640800	1.72653700	-0.61171000
C	1.75199800	-2.14549900	-0.48471700	H	0.74694300	1.73084400	0.47205800
C	1.53480800	-3.29060400	0.29083100	H	0.92660000	2.70602500	-0.99957000
C	3.05854100	-1.75494000	-0.81305800	O	-0.73449000	1.44592600	-0.97233400
C	2.63472300	-4.03403100	0.73498600	C	-1.73720600	2.20842900	-0.41649200
H	0.53387600	-3.60951600	0.55643700	C	-1.52086300	3.26717100	0.47125700
C	4.14146000	-2.50426200	-0.36204300	C	-3.03840800	1.85239200	-0.79400700
H	3.20180400	-0.87016600	-1.42450200	C	-2.62360200	3.95985500	0.98566500
C	3.93678200	-3.64979300	0.41662200	H	-0.52118000	3.56357300	0.76669000
H	2.45986200	-4.92121800	1.33739200	C	-4.12349800	2.55219600	-0.27385800
H	5.14937200	-2.19272300	-0.62190700	H	-3.17619500	1.03206700	-1.49013800
H	4.78271000	-4.23285300	0.76806900	C	-3.92313600	3.60955600	0.62185500
C	-1.99682300	0.32287300	1.54925900	H	-2.45225300	4.78061500	1.67643800
O	-2.17940500	0.15926600	2.75537000	H	-5.12992700	2.26930800	-0.56927300
O	0.16857500	1.17884300	1.95607200	H	-4.77135000	4.15241500	1.02777500
C	0.90369000	0.04565700	2.44831600	C	2.06273900	-0.73787300	1.35309500
H	0.24493900	-0.62993700	3.00169300	O	2.35893800	-0.91033400	2.54382700
H	1.39428600	-0.49134500	1.63019000	O	-0.12192000	-1.32832600	1.83077800
H	1.65402300	0.46920200	3.11967400	C	-0.64016100	-0.18255800	2.50488300
H	-3.80356300	-1.14062200	-2.59190200	H	0.15242000	0.35422200	3.03898100

H	-1.14531000	0.49762400	1.80658900	O	0.80075200	-0.57070400	0.76532500
H	-1.36794400	-0.56937300	3.22410600	C	0.25514600	-1.32504400	1.86281900
H	3.74568100	1.72024700	-2.36347000	H	0.53393300	-0.86370700	2.81424100
C	-1.81546400	-1.59007000	-0.80138700	H	-0.83037900	-1.39421500	1.76333200
H	-1.98730300	-0.89989200	0.03635400	H	0.71587200	-2.30956400	1.77062900
C	-2.37030900	-2.94253500	-0.38559200	H	-1.39777100	3.42994500	-2.03413100
F	-2.34844800	-3.83289600	-1.40693800	C	2.99021100	-1.55929900	-1.25107900
F	-1.68444600	-3.49895800	0.63429800	H	1.94302500	-1.84104300	-1.42085700
F	-3.66480500	-2.82611500	0.01271100	C	3.61216800	-2.64440700	-0.38794800
O	-0.47903500	-1.69949200	-1.17359700	F	4.93329300	-2.45754900	-0.20002200
H	0.10343900	-0.52314800	-2.04773800	F	3.03621600	-2.67458900	0.84205900
H	-2.44604300	-1.25139200	-1.63748300	F	3.44108700	-3.86092400	-0.94918000
22				O	3.12425400	-0.29006500	-0.65400300
N	0.09728200	0.56635700	-1.70419100	H	-0.10736300	-0.43145400	-1.68730600
C	-0.16629400	2.65829600	-0.43299400	H	3.51275300	-1.54704700	-2.21045300
C	0.74563600	2.96687800	0.57941200	TS16			
C	-0.70138600	3.66026400	-1.23405300	N	0.75417600	0.14820000	2.00453700
C	1.15637400	4.27468100	0.82360300	C	2.16458400	-0.98298700	0.45315400
C	-0.29980100	4.98004300	-0.99179900	C	2.66763000	0.19424200	-0.17864800
C	0.61708500	5.28606600	0.02519600	C	2.83856200	-2.20333400	0.39175200
H	1.87345300	4.49029600	1.60961300	C	3.88986900	0.06435500	-0.84646600
H	-0.69977100	5.78038600	-1.60747300	C	4.06779800	-2.28489100	-0.26520500
H	0.91207900	6.31842000	0.18749400	C	4.58819900	-1.14670700	-0.87989900
H	1.11249400	0.66261100	-1.73447400	H	4.27676300	0.93749600	-1.35835100
N	0.31678100	0.73713500	0.75716800	H	4.60600100	-3.22706100	-0.29712600
H	2.56332700	-0.30834300	0.14780800	H	5.53908200	-1.19920600	-1.40237700
C	-0.41388700	1.15944500	-0.48914300	H	1.65837200	0.46653200	2.35353500
C	-1.90260300	0.83591200	-0.34180700	N	0.70170800	1.72026700	0.12504700
H	-2.28278200	1.27949900	0.58534400	H	0.26042100	1.01029300	1.48995900
H	-2.45133200	1.25037700	-1.19630500	C	0.85965700	-0.78100100	1.09099600
O	-2.02118100	-0.58176500	-0.31094000	C	-0.36978000	-1.31585700	0.42685800
C	-3.26204100	-1.13901100	-0.14281400	H	-0.30075400	-1.07967400	-0.64364600
C	-4.45003900	-0.40598700	-0.04312000	H	-0.36222200	-2.41570700	0.51675000
C	-3.28699200	-2.53917500	-0.06813400	O	-1.51205600	-0.73643600	1.01424200
C	-5.65997100	-1.08817500	0.13130500	C	-2.68876000	-0.74765300	0.30324900
H	-4.44832700	0.67643100	-0.09832000	C	-2.94707700	-1.60279500	-0.77285400
C	-4.49872000	-3.20222800	0.10522200	C	-3.66174300	0.16186200	0.73751700
H	-2.34992600	-3.08164500	-0.14954800	C	-4.18842200	-1.53302600	-1.41581100
C	-5.69458400	-2.48045200	0.20649300	H	-2.20792000	-2.32233700	-1.10705800
H	-6.58005200	-0.51518000	0.20836300	C	-4.89377000	0.21558000	0.09044900
H	-4.50917900	-4.28727100	0.16231000	H	-3.42942400	0.81514200	1.57266400
H	-6.63873900	-2.99939100	0.34258600	C	-5.16364400	-0.63002500	-0.99235500
C	1.18922500	1.71337200	1.23113300	H	-4.38645600	-2.19769200	-2.25212400
O	2.11588900	1.51714900	2.00547200	H	-5.64327500	0.92542400	0.42921700

H	-6.12341800	-0.58304700	-1.49811000	H	-5.92616300	-2.47858900	-1.46153800
C	1.97409200	1.58326100	-0.32643200	C	1.37393100	-0.24911400	3.79023400
O	2.61697700	2.45835500	-0.93677700	H	1.96758300	-0.87051500	4.46446900
O	0.20776000	3.01118000	-0.19897300	H	1.51613000	0.80554100	4.04247800
C	-1.19050900	3.00076500	0.03377400	H	0.31781600	-0.52428900	3.87779200
H	-1.69955000	2.23836900	-0.57174400	C	0.93838900	0.97710000	-2.62780900
H	-1.42461800	2.81443800	1.09362500	O	1.28565900	1.76346200	-3.50233700
H	-1.55002800	3.99581500	-0.24383200	O	1.62486300	0.75751200	-1.53676400
H	2.41427400	-3.07359200	0.88310600	H	-1.07877000	-1.51375800	0.17933800
TS17				C	-0.71863300	0.33346600	0.75005800
N	1.27288000	0.23155300	1.46713700	N	-0.65411600	-0.65023400	-0.15393200
C	3.05641900	-2.30001600	0.35514000	C	-1.60766000	0.19437700	1.98146000
H	3.61515400	-2.05491800	1.24794900	H	-1.29836200	0.90893300	2.74371300
Rh	1.44380500	-0.95437500	-0.36393400	H	-1.54277500	-0.81776700	2.39273400
C	1.80589200	-3.00640600	0.32810000	O	-2.94706900	0.55728100	1.63865700
H	1.30751300	-3.45650400	1.17535300	O	-0.23278500	0.29342200	-2.78683100
C	1.37137600	-3.04872800	-1.04244200	H	-0.47715900	-0.14311400	-1.93453800
H	0.45088700	-3.49031700	-1.40332300	H	1.85537100	4.19341200	0.69679700
C	2.31285400	-2.33672400	-1.83603800	23			
H	2.24368600	-2.16146900	-2.90128500	N	-0.94618400	1.42853200	-1.65507600
C	3.36840400	-1.87276400	-0.96219100	C	-2.93141000	-1.50412700	-1.04007300
H	4.22719300	-1.28499600	-1.25680000	H	-3.41126800	-0.63110800	-1.46377300
O	1.87703600	-0.54847400	2.48120500	Rh	-1.20605200	-1.32555600	0.30078000
C	1.65589600	1.58197800	1.50526100	C	-1.82551100	-2.19176200	-1.58986100
C	0.69770800	2.38788500	0.71745300	H	-1.30945600	-1.93456900	-2.50387400
C	-0.46548400	1.73518200	0.29227700	C	-1.43471900	-3.20997400	-0.64387000
C	0.94438000	3.71256600	0.35480100	H	-0.60509400	-3.89650700	-0.75553600
C	-1.37168800	2.39265000	-0.54140700	C	-2.40617800	-3.21996200	0.43670200
C	0.02609300	4.38019800	-0.45392100	H	-2.37938900	-3.86837000	1.30224000
C	-1.12296800	3.71864100	-0.90521000	C	-3.29635500	-2.15981400	0.21123600
H	-2.25794100	1.87784700	-0.89541400	H	-4.08942000	-1.83941500	0.87475300
H	0.20647200	5.41065600	-0.74485600	O	-1.01793800	0.57852900	-2.75454600
H	-1.83156200	4.23920500	-1.54261500	C	-2.12496200	1.83161600	-1.04624400
O	2.59800200	2.03460200	2.14865800	C	-1.71398300	2.24846100	0.31591800
C	-3.68409300	-0.29716500	0.83880600	C	-0.38246500	1.87609000	0.53268600
C	-3.65769100	-1.69113600	0.96289200	C	-2.46992600	2.87642400	1.30295300
C	-4.52681900	0.31267900	-0.09567900	C	0.24117000	2.14561600	1.74550500
C	-4.46515900	-2.46788100	0.12695700	C	-1.85222100	3.13517600	2.52908400
H	-3.03239200	-2.17440100	1.70648700	C	-0.51243200	2.77635800	2.74315200
C	-5.33583000	-0.47333200	-0.91695100	H	1.26945000	1.85248000	1.91759800
H	-4.53835900	1.39602200	-0.16072000	H	-2.41036700	3.62151600	3.32357500
C	-5.30287200	-1.86734000	-0.81592000	H	-0.05157500	2.98681200	3.70387800
H	-4.44063500	-3.54958700	0.22465800	O	-3.23839700	1.82455800	-1.55973500
H	-5.98660000	0.00707100	-1.64202600	C	3.45674300	0.69307000	-0.59881400

C	3.44967000	-0.24051100	-1.64184100	C	2.88708600	2.93842500	0.28240200
C	4.46488800	0.64153100	0.37407700	C	0.13969900	3.18994500	-0.39317800
C	4.44804700	-1.21964500	-1.69618500	C	2.42062800	4.07163900	-0.37854900
H	2.68880700	-0.22526000	-2.41268300	C	1.05993300	4.19356000	-0.70936800
C	5.45121500	-0.33839400	0.30878300	H	-0.90695400	3.28557500	-0.65583400
H	4.44812700	1.37298700	1.17587100	H	3.11036900	4.86623800	-0.64498500
C	5.45003600	-1.27933300	-0.72782100	H	0.71651200	5.08578800	-1.22439800
H	4.43189800	-1.93964000	-2.51006600	O	3.22275300	0.22143900	1.76943000
H	6.22335700	-0.36809100	1.07280100	C	-3.38268200	1.13495500	0.45203600
H	6.21850000	-2.04495800	-0.77754500	C	-4.06736400	0.11229000	1.11861300
C	-1.00511300	1.33731400	-3.97782300	C	-3.75526900	1.51295800	-0.84192900
H	-1.03271100	0.58910200	-4.77270400	C	-5.11568300	-0.54440700	0.46807400
H	-1.88778600	1.98047300	-4.03339700	H	-3.79880500	-0.16213100	2.13356900
H	-0.09243800	1.93731400	-4.05559300	C	-4.81206000	0.85775800	-1.47546600
C	0.75819100	-0.95241300	2.66186000	H	-3.20616000	2.30762500	-1.33674800
O	0.97884500	-0.94345800	3.86820100	C	-5.49149600	-0.17794200	-0.82676700
O	-0.43790800	-1.25408000	2.17668100	H	-5.64581100	-1.33875900	0.98582500
H	0.67588000	-0.68008300	-1.31720300	H	-5.09605200	1.15207800	-2.48175000
C	0.16686700	1.16288100	-0.69324400	H	-6.30820700	-0.69218900	-1.32432400
N	0.39852000	-0.24640000	-0.43694400	C	0.98939400	0.01607900	3.73168800
C	1.42407500	1.84759400	-1.28219500	H	0.43892300	-0.50204500	4.51827300
H	1.22824500	2.91958800	-1.36369300	H	2.06382100	-0.04923700	3.90900300
H	1.61325400	1.46220200	-2.28839300	H	0.67698200	1.06313600	3.69179900
O	2.55236300	1.71378300	-0.43278200	C	1.64526500	0.40407700	-2.44047300
O	1.73838800	-0.67958300	1.78722300	O	2.54758100	0.81478600	-3.18354900
H	1.34422600	-0.52787700	0.85336700	O	1.98952000	-0.36369200	-1.38987300
H	-3.50282700	3.15330800	1.11518000	H	-1.61288700	-0.21758200	-0.38545300
TS18				C	-0.17881400	0.84111100	0.70596200
N	0.92754000	-0.03971700	1.31171500	N	-0.63562700	0.05694900	-0.44979000
C	-0.09070300	-3.33530100	0.73245000	C	-1.31607700	1.13130900	1.70281700
H	-0.64018300	-3.30340900	1.66294900	H	-0.96066500	1.77410200	2.50835400
Rh	0.69736100	-1.52780700	-0.27928100	H	-1.66923300	0.19038100	2.13048300
C	-0.63852200	-3.25094900	-0.57699300	O	-2.35153400	1.85019800	1.03966300
H	-1.68441100	-3.10984300	-0.81952200	O	0.37706800	0.69144800	-2.61189100
C	0.43999200	-3.29264900	-1.52580400	H	-0.25461100	0.44081300	-1.54641700
H	0.34485300	-3.24421300	-2.60206600	H	3.93380300	2.81615900	0.54104300
C	1.66421300	-3.47773200	-0.78269900	TS21			
H	2.65908800	-3.52596900	-1.20481200	N	-1.74163600	-1.80932700	1.68573600
C	1.34308100	-3.48048400	0.59370600	O	-2.32211800	-2.63789200	0.68621400
H	2.05028500	-3.53900600	1.41092900	C	-1.85023700	-0.41885100	1.37036100
O	0.62172700	-0.70086200	2.52815100	C	-2.87699300	0.02151300	0.33594700
C	2.21468800	0.67941400	1.28297900	C	-2.41436800	0.46120500	-0.91543700
C	1.95796200	1.94645100	0.60611000	C	-4.23466500	0.07498000	0.63310100
C	0.60469600	2.06726800	0.28318900	C	-3.30613900	0.95911400	-1.86769900

C	-5.13188400	0.56512600	-0.32518000	C	-2.88390400	0.66546900	-0.45245400
C	-4.67144200	1.00468500	-1.56909100	C	-4.17149500	-0.65570500	1.11163800
H	-2.95074800	1.29650000	-2.83704600	C	-4.02954800	1.27449900	-0.96122000
H	-6.19288900	0.60602200	-0.09585400	C	-5.33478300	-0.05213600	0.60736200
H	-5.37337100	1.38192900	-2.30671900	C	-5.26586300	0.89977100	-0.41794600
O	-1.48764100	0.37334100	2.26933700	H	-3.97666900	2.01690900	-1.75323900
C	1.51918300	2.04686600	-0.85445300	H	-6.30327900	-0.32340600	1.01943800
C	0.62782700	2.94999400	-0.26408500	H	-6.17876800	1.35478600	-0.79187000
C	2.85045400	1.98695800	-0.42354700	O	-1.13321000	-0.57775500	2.17384400
C	1.08270800	3.79534300	0.75609900	C	1.20828000	2.37348200	-0.80779900
H	-0.41095100	3.00167600	-0.56991300	C	0.67762300	3.10471000	0.26331100
C	3.29147900	2.83990800	0.58354700	C	2.58230700	2.09911000	-0.85510100
H	3.50039900	1.23913900	-0.86302200	C	1.52896100	3.55073000	1.28035200
C	2.41006900	3.74935800	1.18389800	H	-0.38415500	3.31238000	0.32758400
H	0.38547200	4.49455100	1.21007100	C	3.41784700	2.54601500	0.16620000
H	4.32596400	2.78627200	0.91235300	H	2.96564800	1.50931600	-1.68084000
H	2.75655400	4.41273700	1.97106700	C	2.89782100	3.27413100	1.24307900
C	-1.31191300	-3.49323400	0.14450900	H	1.10884800	4.11554800	2.10833300
H	-1.81858400	-4.08368800	-0.62473700	H	4.47895300	2.31621900	0.12387200
H	-0.49665300	-2.91795700	-0.30548100	H	3.55056700	3.62270400	2.03795600
H	-0.90792900	-4.16425500	0.91375900	C	-0.72630100	-2.78501600	-1.67923900
C	-0.94486800	0.33022100	-1.05263600	H	-1.18038800	-2.88513800	-2.66977500
N	-0.41640000	-0.33114000	-0.10732000	H	0.02945400	-1.99334200	-1.69781400
C	-0.17657100	0.99028000	-2.18437700	H	-0.25297800	-3.73887600	-1.40292700
H	-0.65109500	1.93726700	-2.47198700	C	-1.44250700	0.83808700	-0.75185200
H	-0.19083400	0.33748400	-3.06290800	N	-0.67335600	0.08994700	-0.05083600
O	1.19175200	1.17107000	-1.86398600	C	-0.93807100	1.83910200	-1.76090400
H	0.61803500	-0.44532400	0.06619900	H	-1.36669500	2.82998600	-1.55183400
H	-2.24073200	-1.99658400	2.55612400	H	-1.28849000	1.55116000	-2.75783300
O	1.98035600	-0.68596600	1.07562100	O	0.47662400	1.89119300	-1.86237000
C	2.46786400	-1.93984800	0.87279400	H	0.43885900	-2.36704000	0.86796800
H	3.40513200	-2.17060400	1.42603000	H	-1.81391100	-2.73987000	1.14579600
C	2.82204200	-2.18698500	-0.59167700	O	1.36238100	-2.31356700	1.27520800
F	3.75556200	-1.32142600	-1.06254300	C	2.34437500	-2.86008500	0.43136500
F	3.31620700	-3.43894200	-0.79017300	H	1.93595200	-3.56505300	-0.30190500
F	1.73697900	-2.06527000	-1.40637000	C	3.07526000	-1.76844400	-0.33655200
Na	0.82600800	0.50422100	2.48292800	F	2.28109400	-1.16140900	-1.24745300
H	1.76709500	-2.77129300	1.12200600	F	4.14419600	-2.26519100	-0.99015500
H	-4.59750300	-0.26053400	1.60077200	F	3.52021100	-0.79306000	0.50065500
26				Na	1.02029000	0.00125600	1.70215700
N	-1.25312500	-2.17004200	0.50802300	H	-4.23134300	-1.38982300	1.91152800
O	-1.79214900	-2.45994700	-0.79464000	H	3.09571000	-3.38347400	1.03146100
C	-1.52011200	-0.72759900	0.91991600	TS22			
C	-2.95052300	-0.28922100	0.56755900	N	-1.23418200	-2.12859600	0.36123600

O	-1.54544200	-2.22910300	-1.01533500	H	3.03009900	-3.38601800	1.10685400
C	-1.61186900	-0.46976500	1.20693500	27			
C	-3.03388000	-0.26953500	0.73521600	C	2.16241100	-1.15487500	-1.17559800
C	-2.97375100	0.52771600	-0.41476800	C	3.48264600	-0.91632800	-0.51921600
C	-4.24325000	-0.72755900	1.23185100	C	3.21558700	-0.14454200	0.61970100
C	-4.12777100	0.88477300	-1.10837500	C	4.76690200	-1.30573900	-0.85293500
C	-5.41210300	-0.36946700	0.54249800	C	4.23405600	0.26710700	1.46649800
C	-5.35415800	0.42243700	-0.61239500	C	5.80746000	-0.89591300	0.00113600
H	-4.08869700	1.50061500	-2.00240600	C	5.54468000	-0.12486600	1.13716600
H	-6.37709600	-0.70797900	0.90919900	H	4.04171600	0.86765600	2.34986800
H	-6.27363200	0.68431000	-1.12786400	H	6.82995100	-1.18150200	-0.22555600
O	-1.24053600	-0.58995000	2.39952200	H	6.36662600	0.17852000	1.77809900
C	1.11520000	2.33641000	-0.81818700	O	1.90522400	-1.77411000	-2.18599500
C	0.57246500	3.25352500	0.08980100	C	-0.72191900	1.98621700	0.49329800
C	2.47519000	2.00625000	-0.75470400	C	0.17792700	2.79681900	-0.20734500
C	1.39702700	3.82251900	1.06511900	C	-2.10228300	2.11841200	0.28768000
H	-0.48015000	3.51130000	0.06385300	C	-0.31774100	3.74560500	-1.10894500
C	3.28501300	2.57863000	0.22500300	H	1.24959300	2.70173100	-0.07573400
H	2.86366300	1.26832800	-1.44648100	C	-2.57818200	3.06295500	-0.61918500
C	2.75175100	3.49012600	1.14352000	H	-2.77304400	1.45667800	0.82327900
H	0.96803300	4.53000800	1.76973700	C	-1.68965200	3.88580500	-1.32103600
H	4.33462000	2.30205300	0.27423100	H	0.38520000	4.37350300	-1.64937800
H	3.38307500	3.93547700	1.90675200	H	-3.64931500	3.15539100	-0.77616300
C	-0.36265300	-2.17591100	-1.82197600	H	-2.06315800	4.62295200	-2.02539100
H	-0.72866600	-2.12819100	-2.84995100	C	1.74535900	0.06178100	0.62171000
H	0.23510900	-1.29140400	-1.59357000	N	1.14658000	-0.49879000	-0.38343400
H	0.24629200	-3.07866300	-1.68753300	C	1.00884100	0.81711000	1.68778000
C	-1.53973000	0.83741800	-0.61814200	H	1.52597700	1.76176000	1.90515400
N	-0.77255600	0.31930600	0.27483400	H	1.04424600	0.22105200	2.60760500
C	-1.01136100	1.67564100	-1.75131300	O	-0.36032600	1.01318200	1.40178300
H	-1.44682100	2.68432700	-1.70936300	O	-2.17503400	-2.76381100	-0.72075200
H	-1.33340900	1.23467800	-2.70041900	C	-3.35222500	-2.83211200	-0.05932400
O	0.40551800	1.70907200	-1.81488800	H	-3.36154300	-3.48981700	0.84603200
H	-0.17646700	-2.29365500	0.56954400	C	-3.80644300	-1.47423600	0.48324600
H	-1.81738800	-2.82520700	0.82902800	F	-2.89721300	-0.93912400	1.35170100
O	1.28810700	-2.24221400	1.08383400	F	-4.99251700	-1.52069900	1.13587200
C	2.33953700	-2.83018700	0.43893900	F	-3.93992100	-0.54477900	-0.51139800
H	2.05334300	-3.54862900	-0.35814200	Na	-1.11937800	-0.92883000	-1.07513800
C	3.23368400	-1.81154300	-0.26652000	H	4.96378600	-1.90263200	-1.73786500
F	2.59254400	-1.16382900	-1.27637300	H	-4.22955500	-3.17650100	-0.66304400
F	4.33976500	-2.37938700	-0.80324000	TS23			
F	3.66333000	-0.83610500	0.58691600	N	2.34357700	2.03224500	1.18156400
Na	1.12025200	-0.11289800	1.69102200	O	2.74165900	2.34233300	-0.16612700
H	-4.28547600	-1.34184800	2.12699900	C	2.28851100	0.57080800	1.38740700

C	3.22676100	-0.25628300	0.49816900	C	2.27847500	1.69242900	-0.33464400
C	2.61933000	-0.88354400	-0.59541300	C	1.01323100	2.27652500	-0.26352500
C	4.57687400	-0.45976600	0.75161700	C	3.41785700	2.48027400	-0.38378700
C	3.34570100	-1.70427900	-1.45991400	C	0.84365600	3.65968800	-0.23094800
C	5.31812700	-1.27622800	-0.11369300	C	3.26497100	3.87532000	-0.35215100
C	4.70945200	-1.89305000	-1.21301200	C	1.99355900	4.45907100	-0.27400500
H	2.87094000	-2.19058300	-2.30750900	H	-0.14242500	4.11311100	-0.17347700
H	6.37679000	-1.43586300	0.07257000	H	4.14371500	4.51384600	-0.39083200
H	5.29567400	-2.52541500	-1.87320300	H	1.89892200	5.54104900	-0.25056400
O	2.12999800	0.22843100	2.58417400	O	2.72019800	-0.46336600	-1.35408100
C	-1.87696000	-1.54270400	-0.72778400	C	-3.51558200	0.24981200	-0.15305400
C	-1.38284900	-2.41417100	0.25022400	C	-4.32268200	0.09192600	-1.27935900
C	-3.25954600	-1.40710400	-0.91406500	C	-4.06905600	0.45762700	1.11195500
C	-2.28160300	-3.14341800	1.03707700	C	-5.71194700	0.13907500	-1.13395000
H	-0.31805800	-2.51806900	0.42233000	H	-3.85717700	-0.06660400	-2.24758700
C	-4.14368000	-2.13894400	-0.12369700	C	-5.45807900	0.51036600	1.24550600
H	-3.61891200	-0.72880900	-1.68026300	H	-3.41485300	0.56649200	1.97200400
C	-3.66056000	-3.01373600	0.85878200	C	-6.28051600	0.35118100	0.12526100
H	-1.89071600	-3.81733700	1.79438300	H	-6.34750300	0.01313200	-2.00583000
H	-5.21352100	-2.02988700	-0.27982700	H	-5.89705100	0.66865300	2.22643400
H	-4.35024900	-3.58885600	1.46931600	H	-7.36040600	0.38894500	0.23472400
C	1.77059700	3.21393500	-0.74263900	C	1.43047700	-0.54585700	2.97250100
H	2.08383300	3.34846900	-1.78432100	H	0.96410500	0.10292700	3.72086400
H	0.76056700	2.78866800	-0.70824100	H	0.67177800	-1.13331900	2.44622000
H	1.76825700	4.19379500	-0.24227900	H	2.12707200	-1.23331900	3.47527600
C	1.17906800	-0.55137200	-0.62781400	C	0.05275600	1.15014200	-0.26847200
N	0.84053700	0.21875500	0.32739100	N	0.59732300	-0.01137600	-0.32594100
C	0.27483400	-1.10335600	-1.70374800	C	-1.42917600	1.38694600	-0.23294200
H	0.41584300	-2.19069200	-1.77688500	H	-1.72511800	2.03010600	-1.07474600
H	0.58498100	-0.67161500	-2.66170900	H	-1.68509400	1.92255200	0.69218000
O	-1.09449600	-0.77551600	-1.55459400	O	-2.13544500	0.14480800	-0.30006700
H	-0.12549300	0.61287900	0.52324000	H	2.41913000	-2.18764200	0.92831100
H	3.12093700	2.35769000	1.76140200	H	3.61285300	-0.25980700	0.95581000
H	5.05111800	0.01053200	1.60913600	Na	2.78404600	-2.61618600	-1.76938000
C	-2.18056800	1.86933400	0.22331400	H	4.40669800	2.03203400	-0.44615900
O	-1.62530600	2.47291700	-0.76232300	C	1.01502400	-3.31354700	0.21446300
Na	-3.60018300	2.44873100	-1.86341600	O	0.79638800	-3.65978700	-0.98474000
O	-3.48717400	1.80297000	0.31002000	Na	-0.98071100	-1.89038800	-0.54693900
O	-1.47055000	1.28841600	1.15133200	O	0.15447800	-3.08571100	1.09845300
Na	-3.29025100	0.32899100	2.03527600	O	2.35466400	-3.11573300	0.53327700
28				TS24			
N	2.60402500	-0.43379000	0.95952500	N	2.49203400	-0.58705000	0.97330600
O	2.11860800	0.32743600	2.08095000	O	2.06343100	0.08711700	2.15712300
C	2.12171700	0.16154500	-0.36427400	C	2.13642200	0.08649800	-0.41924300

C	2.38257000	1.59286200	-0.28521900	C	4.43396700	-1.29904500	-0.16752500
C	1.14740500	2.24296100	-0.27706200	C	2.34480600	-3.24147500	-0.20816500
C	3.56554300	2.30982900	-0.21147000	C	4.71540800	-2.66370100	-0.36615400
C	1.05236600	3.63016600	-0.18218400	C	3.69083500	-3.61391600	-0.38525000
C	3.48581800	3.70792300	-0.11486700	H	1.55756800	-3.98831500	-0.22969900
C	2.24547900	4.35957400	-0.09786500	H	5.74312800	-2.98307000	-0.50792700
H	0.09198600	4.13812000	-0.17327900	H	3.93573000	-4.65979300	-0.54174400
H	4.39794700	4.29540500	-0.05521900	O	2.96431800	1.47483300	0.26902400
H	2.20923600	5.44253800	-0.02295400	C	-2.82689600	-1.07440800	0.08124300
O	2.78655200	-0.56582000	-1.33627300	C	-3.31833100	-2.37596700	0.20830900
C	-3.44347000	0.37142900	-0.29534400	C	-3.67299100	-0.01474100	-0.27010100
C	-4.36746800	0.46146500	-1.33543500	C	-4.68056500	-2.61004800	-0.01342900
C	-3.85381900	0.32414100	1.03861000	H	-2.66736400	-3.19921900	0.48044400
C	-5.73121000	0.50240800	-1.03134600	C	-5.02759500	-0.26648600	-0.47916100
H	-4.01223100	0.49450200	-2.36092700	H	-3.24888700	0.97940800	-0.39010900
C	-5.21819100	0.37183900	1.33205600	C	-5.53876700	-1.56387500	-0.35243500
H	-3.10818600	0.24435300	1.82464100	H	-5.06446700	-3.62157000	0.08525000
C	-6.15745600	0.46086500	0.29931900	H	-5.68482900	0.55417100	-0.75319000
H	-6.45847400	0.56916700	-1.83544700	H	-6.59428800	-1.75537700	-0.52109900
H	-5.54657200	0.33271600	2.36674800	C	0.83092800	-1.11979300	0.20366200
H	-7.21793700	0.49412300	0.53135700	N	1.02806400	0.15562300	0.35388200
C	0.78757800	-0.37971800	2.63271000	C	-0.52443500	-1.74460400	0.24391100
H	0.79709900	-0.17792000	3.70730500	H	-0.57326700	-2.41343000	1.11722000
H	-0.03370700	0.17286400	2.16412100	H	-0.65793600	-2.36931400	-0.65123800
H	0.64869700	-1.44656500	2.43749100	O	-1.50706800	-0.72779800	0.30432900
C	0.13079900	1.17417300	-0.40127200	Na	2.12163900	3.73762300	-0.15478100
N	0.61766300	-0.01350100	-0.47606100	H	5.22453800	-0.55535600	-0.15444800
C	-1.33850100	1.47241600	-0.40197900	C	-0.43980200	3.45846200	-0.33452200
H	-1.57733700	2.20333400	-1.18762900	O	0.10805300	3.51847200	0.86866300
H	-1.60239700	1.93139600	0.56184400	Na	-0.89111000	1.52224100	1.26398400
O	-2.08850500	0.27226400	-0.60224000	O	-1.56134300	2.83358900	-0.47686500
H	2.25048400	-1.79134900	0.92858200	O	0.19169000	3.98101700	-1.33275300
H	3.51140100	-0.51154500	1.01996500	TS29			
Na	2.77121400	-2.78084700	-1.57961800	N	-1.24635900	-1.52194900	1.36940200
H	4.52939400	1.80732900	-0.22909000	O	-1.34874000	-0.26208100	2.00434000
C	0.87464300	-3.26483400	0.27855200	C	-1.96950200	-1.59499700	-0.14813700
O	0.67916300	-3.56367200	-0.95977600	C	-3.16102500	-0.64879300	-0.15588700
Na	-1.02777100	-1.88066900	-0.65683300	C	-2.82199900	0.55108500	-0.79306600
O	-0.08014900	-3.08740300	1.10029800	C	-4.45017800	-0.87446700	0.29499000
O	2.13748000	-3.05022400	0.67524000	C	-3.75628900	1.57144500	-0.97598800
29				C	-5.39681200	0.14562600	0.11969900
C	2.44681500	0.37432100	0.22560500	C	-5.05473900	1.35288000	-0.50585200
C	3.10908700	-0.94545100	0.01146000	H	-3.49467900	2.50278400	-1.46848200
C	2.07963400	-1.89542400	-0.00929200	H	-6.41358100	-0.00132600	0.47208300

H	-5.80796500	2.12441800	-0.63126200	H	-6.38921400	0.06348300	0.17295500
O	-2.04459500	-2.79247600	-0.48830300	H	-5.57567600	0.73094200	-2.05683700
C	1.42781900	1.80230500	-0.63067700	O	-1.78507000	-0.81276100	2.69745700
C	0.80838300	2.04352600	0.59950400	C	1.62388900	1.62818100	-0.58825700
C	2.81606900	1.92337800	-0.76101100	C	0.87593700	2.77361700	-0.30007500
C	1.59616500	2.40764800	1.69801200	C	2.96836900	1.54282600	-0.20322700
H	-0.25991200	1.92000800	0.73331600	C	1.49371500	3.84298200	0.35980600
C	3.58711600	2.27143500	0.34387600	H	-0.17186000	2.84857900	-0.56856100
H	3.26847700	1.71009200	-1.72263500	C	3.56785100	2.61448900	0.45109600
C	2.98112800	2.52102300	1.58092300	H	3.49942900	0.61971500	-0.40571600
H	1.11290300	2.59361000	2.65274100	C	2.83546500	3.77495500	0.73344400
H	4.66547800	2.34704500	0.23800000	H	0.90968500	4.73215200	0.58144500
H	3.58320500	2.79625500	2.44159800	H	4.61063500	2.54199700	0.74826300
C	-0.41724100	-0.16911900	3.09350400	H	3.30522900	4.60950100	1.24561600
H	-0.59872600	0.81256200	3.53494500	C	-1.12465700	0.15973000	-0.45274900
H	-0.60829700	-0.95049100	3.83917600	N	-0.69520100	-0.19995400	0.71665800
H	0.61537000	-0.22836800	2.73550400	C	-0.21312600	0.45559000	-1.60625300
C	-1.40478000	0.47395900	-1.16680800	H	-0.55694700	1.35594400	-2.13411300
N	-0.90695400	-0.67607900	-0.87095200	H	-0.29781500	-0.37757000	-2.31379100
C	-0.63809500	1.58785900	-1.82316400	O	1.14853500	0.52359100	-1.25493000
H	-0.94536500	2.54952100	-1.39290600	C	1.90877600	-2.35004000	1.16419500
H	-0.91498600	1.60194100	-2.88393500	H	1.01347300	-2.89550200	1.49839500
O	0.76226700	1.41667500	-1.77616400	C	2.04804900	-2.61540600	-0.32975300
H	0.11754700	-1.00121800	-0.72475900	F	0.93152500	-2.27573300	-1.01971800
H	-0.18319800	-1.75632100	1.12090300	F	2.25848800	-3.93668000	-0.55133800
H	-1.72110000	-2.23329200	1.93642200	F	3.08204900	-1.94362800	-0.87874900
O	1.02388800	-1.84005800	0.25037300	H	-4.77197700	-0.52510900	1.99770900
C	2.25835400	-1.37813600	0.65251800	O	1.88506900	-0.98789500	1.47947600
H	2.28523800	-0.31497900	0.94845100	H	1.01021300	-0.62409600	1.19581800
C	3.26416000	-1.51976500	-0.48019200	H	2.78132200	-2.80297200	1.64552300
F	2.83523300	-0.92836100	-1.62283100	TS30			
F	4.45882400	-0.95501900	-0.16255600	C	-1.14831300	0.81718600	1.72040000
F	3.51154500	-2.81668000	-0.78838000	C	-1.12399300	1.94458000	0.75107400
H	-4.71750900	-1.81239800	0.77239200	C	-0.40813400	1.52216300	-0.38516400
H	2.68611400	-1.95094000	1.49777500	C	-1.65612500	3.21789100	0.84139800
34				C	-0.20738500	2.37211700	-1.46931500
C	-1.85536600	-0.44326300	1.54612700	C	-1.46903100	4.07515200	-0.25707500
C	-3.07127400	-0.16766500	0.72071300	C	-0.75937000	3.65853200	-1.39037200
C	-2.60596200	0.21090800	-0.54455600	H	0.34922800	2.05728000	-2.34591700
C	-4.42128800	-0.23151000	1.01324700	H	-1.88088200	5.07881400	-0.22649400
C	-3.48348000	0.54211500	-1.56660000	H	-0.63128400	4.34463700	-2.22121300
C	-5.32088000	0.10054600	-0.01644200	O	-1.68124000	0.71074700	2.79959400
C	-4.85953600	0.47939900	-1.28070800	C	2.93248800	-0.92298400	-0.20138300
H	-3.13581600	0.83877500	-2.55114400	C	3.20189400	0.40950800	-0.53121100

C	3.93740800	-1.72715700	0.35531100	C	-5.32344600	-2.03479400	0.11234700
C	4.48016700	0.92939500	-0.29390700	H	-4.36199300	-3.87636100	0.69572100
H	2.44232800	1.04747000	-0.96602500	H	-5.98385800	-0.06170300	-0.46786000
C	5.20292500	-1.19554300	0.58656600	H	-6.32389600	-2.45656800	0.12521200
H	3.70183100	-2.75802000	0.60097700	C	0.81858700	-0.80190600	0.15266600
C	5.48370700	0.13796700	0.26304500	N	1.18247200	0.21824900	1.04302800
H	4.68143500	1.96558300	-0.55168800	C	-0.41666800	-1.09955500	-0.28368200
H	5.97357100	-1.82557000	1.02229500	H	-0.60082600	-1.90960000	-0.98046000
H	6.47175800	0.55043400	0.44405900	H	-1.42806700	1.37184900	0.85716900
C	0.04238500	0.16449300	-0.12640500	O	-1.51104200	-0.34559600	0.07109700
N	-0.36145600	-0.20704700	1.09659800	C	-0.98673200	3.23832300	0.45401400
C	0.65992100	-0.82351200	-0.98623200	H	-0.66763200	4.10937200	1.03024400
H	0.90684200	-0.46385100	-1.98734500	C	0.00481500	3.03535700	-0.68144100
H	-0.18387800	-1.68064400	-0.92553200	F	1.27229700	2.91676700	-0.23132100
O	1.71978200	-1.55061300	-0.37522400	F	-0.03320400	4.07707600	-1.53787800
C	-2.16439600	-2.93575700	-0.39794000	F	-0.27884200	1.91049000	-1.37984200
H	-2.68719400	-3.64433300	0.27520500	H	5.23808300	-0.69899800	0.80485300
C	-3.01856600	-1.67327600	-0.38266600	O	-1.01899800	2.12607300	1.32668000
F	-3.10710100	-1.12681400	0.85816600	H	0.55416300	0.95974900	1.34774000
F	-4.28226500	-1.90081400	-0.80769300	H	-1.96650100	3.44823600	0.00879700
F	-2.49435500	-0.70490600	-1.18777600				
H	-2.19968000	3.53902400	1.72382100	TS31			
O	-0.86637500	-2.71386500	-0.01278600	C	-1.85829900	-0.73830000	0.18699800
H	-0.47563200	-1.21873700	1.27071800	C	-2.87278900	0.08608500	0.68879100
H	-2.27558900	-3.34461400	-1.42272400	C	-2.12313100	-2.03250100	-0.21330400
35				C	-4.18679700	-0.35260000	0.79178800
C	2.55415400	0.29906800	1.22638300	C	-3.45365700	-2.49026100	-0.11977200
C	3.11790300	-0.82183400	0.43302400	C	-4.46684500	-1.66320800	0.37116800
C	2.06568700	-1.48185100	-0.22201300	H	-4.96177300	0.29010800	1.19786600
C	4.44152900	-1.22680000	0.28877000	H	-3.69488000	-3.49721700	-0.44772200
C	2.32614500	-2.57994900	-1.04407100	H	-5.48341500	-2.04019200	0.43552800
C	4.70371300	-2.32332200	-0.53501700	N	-0.86483900	1.23172900	-0.84584600
C	3.65414100	-2.98884100	-1.19174800	C	-0.62078500	0.15276700	0.08498400
H	1.52766600	-3.10544300	-1.55944900	C	0.71657800	-0.57347300	0.00492100
H	5.72450600	-2.66757700	-0.67221800	H	0.78819300	-1.37967700	0.74729400
H	3.87975300	-3.83930500	-1.82882700	H	0.79026900	-1.00935200	-0.99947800
O	3.13737700	1.13393300	1.91135200	O	1.72816400	0.40057200	0.22521000
C	-2.76107500	-0.95659000	0.07620400	C	3.03910700	0.00812500	0.19020100
C	-2.93031300	-2.29858200	0.41993800	C	3.46980800	-1.29087400	-0.10578800
C	-3.84946200	-0.14370800	-0.24350100	C	3.97648600	1.01308500	0.47212600
C	-4.22177700	-2.83283500	0.42904600	C	4.84123100	-1.57145600	-0.11553300
H	-2.07404900	-2.90712200	0.69169300	H	2.76049900	-2.07971700	-0.32767700
C	-5.13300100	-0.68912700	-0.21895900	C	5.33672200	0.71791300	0.45797200
H	-3.68079800	0.89311600	-0.51722400	H	3.61543800	2.01202000	0.69742400

C	5.77928800	-0.57802700	0.16420000	O	-1.15376800	-0.41148900	2.15070200
H	5.16932100	-2.58151900	-0.34599400	C	-1.29342100	-1.30902800	3.22972900
H	6.05477800	1.50341700	0.67754900	H	-2.11570400	-2.02036200	3.05659100
H	6.84089200	-0.80652400	0.15411200	H	-0.36898500	-1.88164400	3.39784700
C	-2.29320200	1.38622300	1.06910700	H	-1.51762900	-0.70463200	4.11435600
O	-2.75583300	2.42264600	1.48476600	H	-1.36640300	2.65128400	0.56423500
O	-1.21480100	0.56517000	-2.07043100	N	-0.77675800	-1.12052100	-1.21495200
C	-1.32764300	1.54311900	-3.08267700	H	-0.52499600	-0.73123800	-2.13189600
H	-2.12232900	2.26899700	-2.85279400	H	-0.21356600	-1.95856100	-1.03185200
H	-0.38350600	2.09076600	-3.21809500	37			
H	-1.58031600	1.01024100	-4.00462100				
H	-1.34355800	-2.67653200	-0.60902900	C	1.93738700	0.23618300	-0.47564400
N	-0.77469700	1.01088700	1.31409200	C	2.57259600	-0.88847700	0.09761800
H	-0.59022700	0.54991000	2.21273500	C	2.38048100	0.70158200	-1.72313100
H	-0.17930400	1.84014400	1.21772000	C	3.59035000	-1.54133800	-0.60890800
36				C	3.41757200	0.06253100	-2.40211000
C	-1.86659300	0.69963700	-0.20592500	C	4.01866600	-1.07026500	-1.84863300
C	-2.87403300	-0.13007100	-0.71486100	H	4.05193900	-2.41420300	-0.15890100
C	-2.13837900	2.00236400	0.16199000	H	3.74255800	0.43951500	-3.36746100
C	-4.18436200	0.31294400	-0.86076200	H	4.81653500	-1.58265300	-2.37791300
C	-3.46429600	2.46304200	0.02803000	N	0.85541100	2.19463000	0.27559500
C	-4.46928900	1.63147900	-0.47314500	C	0.77550800	0.91506100	0.16032200
H	-4.95029500	-0.33419900	-1.27659400	C	-0.45899500	0.12211100	0.53812200
H	-3.70924800	3.47642900	0.33261100	H	-0.22380100	-0.94261100	0.62821200
H	-5.48187800	2.01173500	-0.57096800	H	-0.85902300	0.48346100	1.49143600
N	-0.84247200	-1.18219600	0.97227400	O	-1.40525100	0.32857400	-0.51502800
C	-0.62881800	-0.18150100	-0.04224900	C	-2.64014100	-0.24695700	-0.38791500
C	0.70501300	0.56473800	-0.04041500	C	-3.03601900	-1.05254400	0.68746000
H	0.75769900	1.31849100	-0.83789900	C	-3.53700200	0.01506100	-1.43545100
H	0.79158400	1.06881800	0.93024700	C	-4.32969600	-1.58767100	0.70330200
O	1.72083700	-0.41507500	-0.21115300	H	-2.35856300	-1.27002600	1.50509000
C	3.03024700	-0.01736800	-0.20496300	C	-4.81940000	-0.52487000	-1.40492800
C	3.45771000	1.29941200	0.00430900	H	-3.20591600	0.64266500	-2.25731300
C	3.97024200	-1.03599800	-0.42229300	C	-5.22583300	-1.33089700	-0.33381200
C	4.82836100	1.58376500	-0.00645400	H	-4.62976600	-2.21188800	1.54079500
H	2.74619600	2.09892400	0.17490000	H	-5.50550900	-0.31484800	-2.22111800
C	5.32966200	-0.73683400	-0.42973500	H	-6.22700200	-1.75108600	-0.31180200
H	3.61166700	-2.04857700	-0.58074900	C	2.25235800	-1.44082300	1.46153600
C	5.76893900	0.57669900	-0.22172200	O	2.29996000	-2.64835900	1.69608700
H	5.15401800	2.60760400	0.15690800	O	-0.31187300	2.75520400	0.78271300
H	6.04962500	-1.53312700	-0.59838700	C	-0.10288700	4.15125800	1.01139400
H	6.82992900	0.80819800	-0.22789300	H	0.67236000	4.31496200	1.76853500
C	-2.30166300	-1.43423900	-1.06894400	H	0.17518000	4.66143400	0.08264600
O	-2.76373600	-2.47898200	-1.46057900	H	-1.06069800	4.53092600	1.37313900

H	1.88268000	1.55893300	-2.16436900	38			
N	1.91278800	-0.52794700	2.41773600	C	1.68896500	0.40576500	0.12075800
H	1.79977800	-0.86961600	3.36386400	C	2.87927100	0.29870800	-0.60206900
H	2.11948300	0.45522700	2.30632700	C	1.32164800	1.61406400	0.70563800
TS32				C	3.74030300	1.37907900	-0.76859400
C	1.58217500	-0.63738700	-0.34205900	C	2.18349800	2.70651700	0.54494000
C	2.71609700	-0.76232500	0.46725400	C	3.37835800	2.59472700	-0.18229600
C	1.19056900	-1.68970600	-1.16387400	H	4.65852000	1.27042200	-1.33804100
C	3.47146500	-1.93826600	0.50779700	H	1.92055800	3.66125200	0.99194800
C	1.93723900	-2.87135500	-1.12555800	H	4.02373700	3.46164300	-0.29030800
C	3.06563500	-2.99942800	-0.29718800	N	0.89801800	-1.60310300	1.46026400
H	4.34670400	-2.00671600	1.14594200	C	0.98389600	-0.94466500	0.13355700
H	1.64063800	-3.70834300	-1.75100100	C	-0.38850100	-0.92038700	-0.55666500
H	3.62626100	-3.92894800	-0.29333300	H	-0.24415000	-0.61677200	-1.60113500
N	1.06944800	1.46866500	-1.43654000	H	-0.81416500	-1.93230900	-0.53169800
C	0.90897000	0.71663200	-0.22146700	O	-1.23531900	-0.00292900	0.11849500
C	-0.44350800	0.68239300	0.48694600	C	-2.52916400	0.12945100	-0.30723300
H	-0.33943900	0.20990500	1.47226700	C	-3.07421200	-0.53812600	-1.41079800
H	-0.81945200	1.70301100	0.60784900	C	-3.32313200	1.00520400	0.44857000
O	-1.30533400	-0.07523200	-0.34769700	C	-4.41555900	-0.32040200	-1.74762900
C	-2.60139600	-0.26286900	0.05015300	H	-2.47626100	-1.21731800	-2.00719900
C	-3.14840800	0.24183700	1.23599700	C	-4.65462000	1.21153600	0.09966500
C	-3.39509900	-1.01933100	-0.82505700	H	-2.87551900	1.50833500	1.30037900
C	-4.49130800	-0.01791600	1.53477000	C	-5.21108200	0.54902600	-1.00193200
H	-2.55140500	0.82863800	1.92447600	H	-4.83332000	-0.84140500	-2.60495800
C	-4.72855100	-1.26841200	-0.51351300	H	-5.26156000	1.89143500	0.69146800
H	-2.94638100	-1.39748800	-1.73865400	H	-6.25053600	0.71037300	-1.27179900
C	-5.28683000	-0.76897400	0.67005300	C	3.01873100	-1.09171400	-1.11138300
H	-4.91025000	0.37636300	2.45673500	O	3.91932600	-1.57427500	-1.78776200
H	-5.33508800	-1.85505900	-1.19820500	O	0.30693800	-0.70170700	2.40995100
H	-6.32749700	-0.96431000	0.91125200	C	-0.88864400	-1.28088100	2.92366300
C	2.98552900	0.48263400	1.19135300	H	-1.63497000	-1.42573700	2.13539800
O	3.84118300	0.76456300	1.99830000	H	-0.68629600	-2.23636200	3.42386500
O	0.03931900	2.51440300	-1.48918800	H	-1.26841500	-0.55826200	3.65230200
C	0.50411600	3.76643200	-1.01920800	H	0.39982300	1.69791700	1.26609200
H	0.61976200	3.80282000	0.07812000	N	1.89687000	-1.75408500	-0.66184500
H	1.46622100	4.03584600	-1.47926400	H	1.73226900	-2.73324800	-0.85273500
H	-0.25030000	4.50936900	-1.30289700	H	1.85997900	-1.69577400	1.79286500
H	0.32181600	-1.59166700	-1.80353200				
N	1.98831700	1.44328600	0.70054400				
H	1.68545500	2.12718000	1.39950600				
H	2.16708700	1.92210400	-0.38700100				

7. Cartesian coordinates of the structures in HFIP

2				H	-1.85926000	-2.70466200	-2.84914100
C	2.69933200	0.34771400	-0.23799200	H	-0.97744100	-2.95292800	-1.31463400
N	3.16909500	1.09943800	-0.98626800	H	-2.33486900	-1.76571600	-1.40188200
C	2.09259300	-0.61941800	0.70396800	O	-2.57520200	0.64577800	-0.85409300
H	2.80924300	-1.42462800	0.88389400	C	-2.03737700	1.84297400	-1.07105200
H	1.89508300	-0.11736400	1.65939000	O	-2.51060000	2.71382400	-1.78798700
O	0.93568800	-1.23654800	0.17383900	N	0.04683500	-0.49122900	-1.37846300
C	-0.24086800	-0.51638300	0.11165300	H	0.18099800	0.43416800	-1.79086100
C	-0.37363400	0.82930700	0.46727500	O	-0.88655200	1.95028400	-0.39520800
C	-1.34759100	-1.24104700	-0.34907200	H	3.64421100	-1.91767800	-0.10973100
C	-1.62900000	1.44035300	0.36253700	TS1			
H	0.47132400	1.41375300	0.81297000	Rh	-0.87430800	-0.62589300	-0.11214800
C	-2.58886100	-0.61830600	-0.44822600	C	-0.37883600	-2.78031300	0.07190900
H	-1.21290500	-2.28368500	-0.61938700	H	-0.44801000	-3.31271300	1.01165900
C	-2.73768500	0.72733100	-0.09144400	C	-1.42544000	-2.61976900	-0.87229700
H	-1.72807700	2.48634300	0.63879900	H	-2.43197000	-3.00577400	-0.77804900
H	-3.44314600	-1.18694400	-0.80481700	C	-0.94000500	-1.78042000	-1.93985100
H	-3.70641000	1.21153500	-0.16987900	H	-1.49627300	-1.47014500	-2.81399200
5				C	0.43188300	-1.46790600	-1.65257000
Rh	-1.07183600	0.06515500	0.43788800	H	1.07377000	-0.83679300	-2.25270000
C	-0.46734600	0.35644900	2.55342700	C	0.77783800	-2.05833300	-0.40505100
H	0.05033500	1.25211300	2.87172500	H	1.73077700	-1.97217100	0.09906700
C	-1.89491500	0.20669700	2.44254200	O	-1.20576600	2.43026600	-0.52344800
H	-2.63819600	0.93906100	2.72746100	C	1.05237800	1.79160900	-0.53384200
C	-2.15431500	-1.12605100	1.95620000	C	2.13802600	0.97113800	0.09488000
H	-3.13109500	-1.54374000	1.74952300	C	2.12906500	0.60211100	1.44848000
C	-0.91018700	-1.75232400	1.70058900	C	3.20751200	0.57779300	-0.72302200
H	-0.76576600	-2.74423700	1.29377200	C	3.16454800	-0.17731800	1.96632100
C	0.14335600	-0.82920300	2.07499600	H	1.32538400	0.92172700	2.10223400
H	1.20674300	-1.01331400	2.00039700	C	4.23089800	-0.21687200	-0.20775100
O	-0.59533000	-1.21736800	-2.42030600	C	4.20835100	-0.59986300	1.13758200
C	1.32680800	-1.11275700	-1.01858100	H	3.15473600	-0.45464300	3.01625300
C	2.40206800	-0.21161400	-0.52879200	H	5.04543700	-0.53458900	-0.85190800
C	2.30370300	1.19165300	-0.49596800	H	5.00643500	-1.21656700	1.54058900
C	3.57968600	-0.83551500	-0.07872600	O	1.29389900	2.66096200	-1.35966500
C	3.37170300	1.94966500	-0.01866100	C	-1.66668700	2.21813400	-1.86435400
H	1.40088100	1.70575300	-0.80819500	H	-2.36281300	3.03817400	-2.05488200
C	4.64096500	-0.07185500	0.39750400	H	-0.83721500	2.25853900	-2.57473300
C	4.53853600	1.32291900	0.42804400	H	-2.19595900	1.26107600	-1.93771200
H	3.28989200	3.03195600	0.00548200	O	-2.75795000	0.09500300	0.41993900
H	5.54616100	-0.56116200	0.74382700	C	-2.47462700	0.48751700	1.62815800
H	5.36647000	1.91996100	0.79910600	O	-3.21711500	0.91892800	2.48293200
O	1.42594900	-2.31935100	-1.09239200	N	-0.25433200	1.46644400	-0.11463400
C	-1.49941700	-2.22408300	-1.93696700	H	-0.58458000	1.11931300	1.17109600

O	-1.08858200	0.33593100	1.86064100	H	-0.97499700	-3.36420900	0.59701800
H	3.21917300	0.89086500	-1.76259600	C	-2.44030900	-1.92259500	-0.29839400
6				H	-3.25779500	-1.94336300	0.41182600
Rh	-0.83167000	-0.63969300	-0.12070500	C	-2.38484800	-1.09996500	-1.46969400
C	-0.50439000	-2.85199300	0.00746200	H	-3.16867600	-0.44740200	-1.82860400
H	-0.76241400	-3.43945800	0.87894700	C	-1.10571900	-1.31988700	-2.08111600
C	-1.35166700	-2.56534300	-1.08162500	H	-0.73401200	-0.84709600	-2.98016500
H	-2.38119900	-2.88036500	-1.19018900	O	-1.60910900	0.48823000	1.61378600
C	-0.64593000	-1.67271300	-1.97785800	O	0.38194800	0.72134600	2.65646500
H	-1.02604200	-1.27167000	-2.90793400	C	-0.88048200	0.87186100	2.56751800
C	0.67840200	-1.48408400	-1.44964000	O	-1.00524900	2.41571000	-1.00329000
H	1.45383800	-0.86925500	-1.88370700	C	1.21175000	1.68856700	-0.77763300
C	0.75617900	-2.16584800	-0.20670700	C	2.01800600	0.52551500	-0.27569600
H	1.60743400	-2.17418600	0.45947400	C	1.35129400	-0.44303400	0.51517000
O	-1.20018600	2.30627700	-0.32570000	C	3.36278200	0.38811100	-0.60714600
C	1.05859600	1.82953300	-0.35335400	C	2.07821900	-1.57859500	0.93091900
C	2.18554100	0.95961900	0.13369100	H	0.75079900	0.10643900	1.58184500
C	2.17231600	0.38690000	1.41325000	C	4.06320700	-0.74382300	-0.17769100
C	3.31683800	0.80025100	-0.67860300	C	3.42357500	-1.72651100	0.58901200
C	3.26485000	-0.35824600	1.86355000	H	1.59168600	-2.32658900	1.55196300
H	1.30807800	0.53121200	2.05343600	H	5.11086400	-0.86214900	-0.44051600
C	4.39743900	0.03453200	-0.23989300	H	3.97803700	-2.59912800	0.92325600
C	4.37291700	-0.54746600	1.03240300	O	1.70758100	2.71925800	-1.25571100
H	3.25016100	-0.79004400	2.86046300	C	-1.20689500	2.42526200	-2.42210800
H	5.26118200	-0.10197600	-0.88450200	H	-1.64110700	1.47526700	-2.75685700
H	5.21834000	-1.13583900	1.37780300	H	-1.91198700	3.23792500	-2.61433800
O	1.30430800	2.94095200	-0.84032800	H	-0.26260600	2.61441000	-2.94212100
C	-1.60181100	2.41868900	-1.69523500	O	-1.51749300	1.48637200	3.57544700
H	-2.36810000	3.19826300	-1.71091000	H	-0.85544000	1.73543700	4.24550900
H	-0.75390500	2.71374500	-2.32043600	H	3.84226300	1.15610200	-1.20728900
H	-2.03396500	1.47454800	-2.04747100	7			
O	-2.81860300	0.05138600	0.09076300	Rh	-0.86832800	-0.33510500	-0.08234300
C	-2.81760800	0.45712400	1.30759400	N	-0.06094000	1.53014400	0.13681600
O	-3.60381100	1.13336300	1.93397300	C	-2.08726100	-0.24097000	-1.85420300
N	-0.19965200	1.32853300	-0.14676900	H	-1.83512100	0.37053500	-2.71076400
H	-1.30853600	0.56787700	2.60353600	C	-1.71539400	-1.62187800	-1.66205400
O	-1.64020200	-0.06421600	1.93822900	H	-1.05245500	-2.18929400	-2.30101100
H	3.33575800	1.27578900	-1.65508600	C	-2.28866600	-2.06119800	-0.44781300
TS2				H	-2.17444500	-3.03988000	-0.00071000
Rh	-0.73895400	-0.46114700	-0.07925000	C	-3.12761300	-0.98620500	0.06241600
N	-0.10872800	1.41372000	-0.62610000	H	-3.69083900	-1.01889500	0.98640300
C	-0.38821600	-2.26388300	-1.28365800	C	-3.03675900	0.10270400	-0.80847000
H	0.61276300	-2.62341000	-1.48044800	H	-3.52346000	1.06081300	-0.68548200
C	-1.22355700	-2.65168500	-0.17709600	O	-0.40282700	-0.66355500	2.05929900

O	1.86886400	-0.50550200	2.18230800	H	-2.16664200	2.70709600	3.33530300
C	0.65259000	-0.60772600	2.68999700	H	-1.38907900	0.51195700	4.20882000
O	-0.82075900	2.60758700	0.61414100	O	0.03062200	3.21882800	-1.15485500
C	1.19007000	1.81545300	-0.30943300	C	2.94952100	2.37166800	-2.29603300
C	1.83270500	0.54233700	-0.77391900	H	3.75984900	2.01080400	-1.65033000
C	1.04592800	-0.62687100	-0.71590500	H	3.28187400	2.38044400	-3.33762200
C	3.16078800	0.50903100	-1.20794500	H	2.65023300	3.37935700	-1.98861300
C	1.63429200	-1.84342200	-1.09431200	C	-0.34577800	-1.50941800	-0.56369300
H	1.81506600	-0.47827500	1.19646400	N	0.04473800	-1.07488900	-1.60063000
C	3.72819600	-0.70623000	-1.59392200	C	-1.30953400	-2.27508200	0.28661100
C	2.96566600	-1.87823300	-1.53164000	H	-0.90032600	-3.27878000	0.42924800
H	1.06458000	-2.76803500	-1.04589800	H	-1.39636800	-1.79433900	1.26482800
H	4.75992100	-0.74499300	-1.93184300	O	-2.55341000	-2.43546300	-0.35832900
H	3.40809500	-2.82759300	-1.82340700	C	-3.39424100	-1.34217000	-0.46343400
O	1.74451700	2.92460500	-0.32283100	C	-3.14679900	-0.09402300	0.11522100
C	-1.33182600	3.39780700	-0.46669700	C	-4.56015700	-1.56329000	-1.20623300
H	-1.92637400	2.77835200	-1.14900500	C	-4.08043800	0.93335300	-0.05832200
H	-1.97003600	4.15597000	-0.00516900	H	-2.25153000	0.10363000	0.68910600
H	-0.51236100	3.87554700	-1.01263900	C	-5.48174800	-0.53088400	-1.36573000
O	0.62770600	-0.66196500	4.01399800	H	-4.72353100	-2.54188100	-1.64681200
H	1.53582300	-0.61906500	4.36766000	C	-5.24707300	0.72511400	-0.79332100
H	3.72665200	1.43657300	-1.22879400	H	-3.87556700	1.90088400	0.39121400
s				H	-6.38486100	-0.70802000	-1.94314700
Rh	1.55627200	-0.48233800	-0.02833300	H	-5.96474600	1.52954800	-0.92374800
N	1.38260700	1.34554600	-0.93192600	H	-1.31875400	3.51773400	1.11098800
C	2.81845100	-1.35613900	1.59247400	TS3			
H	2.49212000	-1.32429100	2.62248200	Rh	-1.60845200	-0.40161100	-0.50008100
C	2.58244100	-2.40267100	0.66791600	N	-0.56311300	-0.99361700	1.17960500
H	2.06139100	-3.32874300	0.87236600	C	-3.74448100	0.30312300	-0.66680300
C	3.22968900	-2.05406500	-0.58217500	H	-4.04358200	1.28542100	-0.32483500
H	3.21907600	-2.65325500	-1.48325700	C	-3.25573300	-0.01717700	-1.97845600
C	3.81967500	-0.79206400	-0.43417200	H	-3.17282900	0.66540300	-2.81362900
H	4.35004400	-0.24282700	-1.19996000	C	-2.96830600	-1.42346400	-2.00382900
C	3.51618100	-0.30725900	0.89837100	H	-2.56898600	-1.97036700	-2.84842100
H	3.86178800	0.62166900	1.33203600	C	-3.21611800	-1.95564300	-0.71510200
O	1.82803600	1.48412500	-2.25190600	H	-3.08389000	-2.98513700	-0.41073100
C	0.40797000	2.21377700	-0.53872300	C	-3.69584700	-0.87222300	0.12402100
C	-0.10536800	1.78073100	0.79285600	H	-3.98664100	-0.95507400	1.16271700
C	0.32525000	0.53103500	1.26418800	O	-0.28701200	-2.34629900	1.42414400
C	-0.99797900	2.56616800	1.52660200	C	0.13250300	-0.11229700	1.93270700
C	-0.13915400	0.08353000	2.50662200	C	-0.15407300	1.27733200	1.44412800
C	-1.46667500	2.10894000	2.75903100	C	-0.65512200	1.41929600	0.12600200
C	-1.03033700	0.87288000	3.24817600	C	0.02461800	2.39189900	2.25823000
H	0.16602800	-0.88106100	2.90327700	C	-1.01992000	2.70236800	-0.33444500

C	-0.33969200	3.65783800	1.78648800	C	0.56230400	1.76096500	-0.03006800
C	-0.87501000	3.81082000	0.50019400	C	0.56440100	1.86655100	2.38827800
H	-1.39000600	2.82421200	-1.34893800	C	0.70690900	3.15550200	-0.06890500
H	-0.20976800	4.52857500	2.42256300	C	0.66356200	3.25610800	2.34158600
H	-1.16279800	4.79640200	0.14597600	C	0.73693900	3.90505400	1.10611500
O	0.88992800	-0.35609100	2.88677400	H	0.78520000	3.65818400	-1.02881600
C	-1.18716300	-2.86095100	2.40880800	H	0.69913700	3.82874800	3.26401400
H	-2.22761400	-2.75542700	2.07595500	H	0.82855600	4.98628500	1.05699800
H	-0.93977500	-3.92047700	2.51544300	O	1.25833700	-0.91555000	2.22377800
H	-1.04739900	-2.34582400	3.36577100	C	3.33590800	-0.02048600	-1.10141500
C	0.50076100	0.60306500	-1.11955100	C	2.71751900	-1.26174100	-1.29746200
N	0.24317600	-0.52369900	-1.49853700	C	4.47722800	0.07562000	-0.29319200
C	1.60935100	1.61965500	-1.35261600	C	3.25365600	-2.39767700	-0.68130300
H	1.25539100	2.35091500	-2.08429300	H	1.82348000	-1.35460700	-1.90113700
H	1.81898200	2.14570500	-0.41472400	C	4.99771800	-1.06402800	0.31403600
O	2.75565100	1.01879400	-1.90083400	H	4.93345600	1.05073600	-0.15223000
C	3.52998500	0.21280700	-1.09020300	C	4.38947700	-2.31026000	0.12311200
C	3.28587900	-0.01704100	0.26806000	H	2.76479300	-3.35634600	-0.83261300
C	4.62425200	-0.38906300	-1.72350000	H	5.88067000	-0.97770800	0.94164700
C	4.14352500	-0.85875900	0.98319500	H	4.79375600	-3.19763400	0.60120500
H	2.44730300	0.42777400	0.78731700	C	-1.07043100	-2.90795200	2.07787400
C	5.47298700	-1.22048000	-0.99603100	H	-0.97930700	-3.99751400	2.08784400
H	4.78940700	-0.19493100	-2.77879100	H	-0.56636900	-2.48062900	2.94959800
C	5.23706500	-1.46257700	0.36252200	H	-2.13117400	-2.62996500	2.07498100
H	3.93268900	-1.03997900	2.03336900	C	0.49837500	0.99604200	-1.31467100
H	6.31997300	-1.68378800	-1.49454600	N	-0.43961700	0.19444100	-1.60228300
H	5.89573900	-2.11724200	0.92537800	C	1.64489900	1.19987600	-2.30598200
H	0.42837300	2.25514900	3.25701600	H	1.58865500	2.20052200	-2.74467800
9				H	1.56743800	0.46518700	-3.11549400
N	-0.48923700	-1.07135200	0.73553900	O	2.91776800	1.16027100	-1.66690500
C	-3.49232800	1.10826400	-0.89367900	H	0.55381300	1.34818600	3.34206300
H	-3.26945800	2.01521900	-1.43990800	TS4			
Rh	-1.92771500	-0.44148500	-0.57362700	N	-1.24858800	0.58586500	1.32125800
C	-3.99877900	-0.09404300	-1.43269600	C	-3.73970300	-1.48739600	-1.48195200
H	-4.25491500	-0.26959900	-2.46961400	H	-3.69793600	-1.56665900	-2.56034300
C	-4.15115700	-1.05631200	-0.35188000	Rh	-2.09630800	-0.58971100	-0.27223800
H	-4.51581100	-2.06936200	-0.45926300	C	-3.28456200	-2.45437600	-0.55037000
C	-3.70059800	-0.45644000	0.83140600	H	-2.75926700	-3.36793800	-0.79289600
H	-3.66417100	-0.91007600	1.81209300	C	-3.46912900	-1.92347500	0.76540800
C	-3.21574100	0.87426300	0.50350900	H	-3.21600500	-2.41361300	1.69562400
H	-2.82396600	1.59755700	1.20699300	C	-4.19554900	-0.66894000	0.63303900
O	-0.42991900	-2.47896000	0.87107400	H	-4.47207800	-0.02091600	1.45275000
C	0.46810500	-0.40228500	1.41342300	C	-4.34636500	-0.39571500	-0.73000000
C	0.48967800	1.10163800	1.21577600	H	-4.77930200	0.49849900	-1.15971900

O	-2.00717600	0.32016500	2.50464900	Rh	-0.28130500	1.81011100	-0.39906300
C	0.12807500	0.47168200	1.55843800	C	-0.32886600	3.72961200	0.64961400
C	0.95445600	0.96416300	0.40194700	H	-0.62852000	3.83638900	1.68372000
C	1.25052200	0.14561000	-0.69751500	C	0.98989900	3.47203200	0.17492700
C	1.46441700	2.26500200	0.47446900	H	1.87353900	3.30861500	0.77690900
C	2.06296300	0.65562500	-1.71975500	C	0.92118000	3.38195300	-1.26042000
C	2.25432800	2.76794600	-0.55867100	H	1.75000600	3.16381400	-1.92146800
C	2.54882700	1.96074000	-1.66118400	C	-0.42907400	3.68765000	-1.66784500
H	2.31208400	0.02834700	-2.57034800	H	-0.79791600	3.68386700	-2.68467800
H	2.64151300	3.78085200	-0.50103000	O	1.13638000	-2.97793100	-2.17742900
H	3.16542900	2.34407300	-2.46898800	C	2.61854500	-2.22245300	-0.51741000
O	0.62709000	0.11570200	2.61730000	C	3.04038100	-1.07990100	0.36765000
C	3.80643000	-1.48611000	0.28141500	C	2.16453100	-0.30505200	1.14976900
C	4.82776300	-1.61314900	-0.66638600	C	4.41596700	-0.80717100	0.40384700
C	3.89820800	-0.53410700	1.30133400	C	2.68232600	0.73919600	1.93203400
C	5.93687100	-0.76692400	-0.59995900	C	4.92021700	0.23523100	1.17762300
H	4.75360400	-2.36941400	-1.44236300	C	4.04878200	1.01312200	1.94589600
C	5.01552600	0.30016800	1.36309600	H	1.99995500	1.32580200	2.54015500
H	3.07544800	-0.43697500	2.00299000	H	5.98709500	0.43751500	1.18547000
C	6.03555400	0.19184800	0.41236800	H	4.43189400	1.82275800	2.56015200
H	6.72862200	-0.86446200	-1.33801800	O	3.27899000	-3.25999300	-0.57759700
H	5.08104100	1.04743100	2.14952700	C	-2.20393900	-1.78024800	1.36224600
H	6.89982700	0.84822500	0.46031400	C	-2.51888700	-0.80114600	2.31094800
C	-2.09665900	1.50223100	3.30569700	C	-3.19376800	-2.25438700	0.48896500
H	-2.69497900	1.21620100	4.17423600	C	-3.81847000	-0.28869000	2.36339200
H	-1.10628000	1.83429100	3.63617600	H	-1.76231000	-0.41303700	2.98240100
H	-2.60241800	2.31042700	2.76172100	C	-4.48608000	-1.73489500	0.55201700
C	-1.54578500	2.17614000	-1.29078300	H	-2.92621200	-3.01104400	-0.24079400
O	-1.46893100	0.97192500	-1.64068200	C	-4.80637400	-0.74271900	1.48703200
C	0.76410400	-1.26936100	-0.72866100	H	-4.05285600	0.47685600	3.09829400
N	-0.42196200	-1.69117200	-0.54199500	H	-5.24453300	-2.10804300	-0.13112100
C	1.86471900	-2.32324600	-0.89180700	H	-5.81207200	-0.33604400	1.53427700
H	2.45917700	-2.15189000	-1.79722100	C	0.20260900	-3.91459600	-1.61412100
H	1.40514800	-3.31111600	-0.94584400	H	-0.00951900	-4.62019500	-2.42152500
O	2.70969600	-2.32583900	0.27446400	H	0.65448200	-4.44181300	-0.76675900
O	-1.42178200	3.13819500	-2.20705600	H	-0.71072700	-3.40127700	-1.30810300
H	-1.30299000	2.71204400	-3.07582600	C	-1.44034500	-0.35552400	-1.96603300
O	-1.73171400	2.61182500	-0.09561400	O	-0.31083600	0.28280300	-1.86768500
H	-1.56547200	1.74794600	0.63147500	C	0.68023600	-0.52884000	1.20568400
H	1.23502000	2.88288600	1.33813100	N	-0.11990500	0.34558300	0.77882800
10				C	0.17279200	-1.82528000	1.85246200
N	1.47874300	-2.01958800	-1.23218200	H	0.00540300	-1.66746300	2.92679000
C	-1.19473200	3.89006600	-0.50478400	H	0.94134400	-2.59390000	1.74929500
H	-2.26175600	4.06811700	-0.46696100	O	-0.97233500	-2.36214100	1.21131000

O	-2.48270900	0.31788800	-1.37459100	H	1.26173400	-2.40462600	2.35898900
H	-3.23022000	-0.30425400	-1.30602900	C	0.94243700	0.53295200	2.39853400
O	-1.62010400	-1.43316200	-2.52022000	O	-0.35255500	0.50615700	2.20534000
H	1.00279500	-1.12482200	-1.37969900	C	-0.03277700	-0.85855300	-0.97761900
H	5.08030600	-1.42626500	-0.19026000	N	0.42119900	0.17684400	-0.40941300
TS5				C	0.88008200	-2.04233400	-1.29485900
N	-1.12797800	-2.14166400	1.36535700	H	1.01625400	-2.12030500	-2.38304100
C	-0.59088800	3.76497700	-0.40889100	H	0.38440500	-2.96044500	-0.96802400
H	0.27594500	4.29126700	-0.78726100	O	2.11147400	-2.00789900	-0.60370700
Rh	-0.45054600	1.76669500	0.52345300	O	1.57036900	1.24687100	1.36480400
C	-1.38649400	2.84196100	-1.13871600	H	1.45539100	0.56263300	0.45773600
H	-1.23612600	2.55005400	-2.16824100	O	1.56912700	0.02947200	3.30603800
C	-2.38405400	2.31553000	-0.24467800	H	-1.02163600	-1.13476000	1.50527400
H	-3.14373600	1.58740800	-0.49427600	H	-4.37772200	-2.56965700	-0.58305300
C	-2.23098300	2.99724500	1.02038300	11			
H	-2.81520600	2.80071600	1.91045700	N	-2.12650200	3.88244900	-0.76557100
C	-1.13081800	3.87843800	0.92971800	C	2.09236300	-2.78481700	1.16413500
H	-0.73782900	4.49974100	1.72298900	H	2.41419900	-3.44152600	0.36734000
O	-0.77742000	-2.86761700	2.49883100	Rh	0.57649300	-1.23628700	0.80284300
C	-1.97892400	-2.71803400	0.46978000	C	2.66429100	-1.51566200	1.48306700
C	-2.36719000	-1.83376100	-0.68966300	H	3.48045800	-1.04737700	0.94545600
C	-1.46613200	-1.00632000	-1.38951700	C	1.93273800	-0.94818700	2.57581600
C	-3.69877900	-1.91525600	-1.12025000	H	2.13718600	-0.00408700	3.06003000
C	-1.91313400	-0.29476100	-2.51116100	C	0.91038300	-1.89284600	2.93437700
C	-4.14288300	-1.17731300	-2.21542100	H	0.16055500	-1.75199000	3.70040300
C	-3.24419100	-0.37036300	-2.91972400	C	1.00615800	-3.02271800	2.08096800
H	-1.20475900	0.31224100	-3.06715700	H	0.35173000	-3.88345200	2.08700800
H	-5.18080200	-1.24199000	-2.52759000	O	-3.07993200	3.80832600	-1.77053600
H	-3.57578500	0.19203500	-3.78746600	C	-1.27632900	2.83126700	-0.60622800
O	-2.38575800	-3.87442800	0.55566400	C	-0.19094600	3.02572700	0.40619900
C	3.10694600	-1.15113200	-1.00853100	C	0.97898900	2.24925100	0.31014100
C	3.05876000	-0.35055100	-2.15562800	C	-0.34421700	3.90138500	1.49126500
C	4.23418700	-1.12017500	-0.17696700	C	1.98303900	2.38573500	1.27497200
C	4.14585100	0.47494700	-2.46044100	C	0.65603900	4.02437500	2.45416300
H	2.18631800	-0.34305000	-2.79838300	C	1.82482800	3.26850100	2.34416000
C	5.30834200	-0.29091400	-0.49175300	H	2.89175600	1.79938900	1.17906700
H	4.24190100	-1.74512000	0.71079100	H	0.51700800	4.70036100	3.29195300
C	5.27231100	0.51284800	-1.63691200	H	2.60881000	3.35860700	3.08987700
H	4.10057400	1.09607100	-3.35110700	O	-1.42232800	1.77113000	-1.22712600
H	6.17584000	-0.27178200	0.16223400	C	3.70007400	0.44338200	-2.09034000
H	6.10915500	1.16054000	-1.88059400	C	4.46582800	1.21408100	-1.20899200
C	0.59857100	-3.27500900	2.40085200	C	3.99708100	-0.90766400	-2.29297100
H	0.79066300	-3.84585700	3.31249000	C	5.52734900	0.61733000	-0.52052900
H	0.75411100	-3.90960900	1.52127400	H	4.24675000	2.26481400	-1.05241400

C	5.06335900	-1.48857000	-1.60640700	N	-0.31897900	-0.33849800	1.22641800
H	3.34927600	-1.49073000	-2.93696000	C	-3.20739600	-0.68481500	-1.54387700
C	5.83053800	-0.73266600	-0.71253700	H	-3.22527800	-0.01078600	-2.39036400
H	6.11820700	1.21810800	0.16537000	Rh	-1.32472900	-1.05018800	-0.41055100
H	5.28267200	-2.54200200	-1.75714500	C	-2.95937000	-2.07383600	-1.58722900
H	6.65357800	-1.19106100	-0.17237600	H	-2.77459200	-2.66377200	-2.47528900
C	-4.33323000	3.35044600	-1.22933300	C	-3.00245400	-2.58432300	-0.22650400
H	-5.01275500	3.32265300	-2.08377800	H	-2.83654700	-3.61336300	0.06426500
H	-4.22988700	2.34774700	-0.80318500	C	-3.25503500	-1.50657900	0.63934200
H	-4.70824500	4.04674800	-0.47099200	H	-3.31620400	-1.55179000	1.71825400
C	-0.11313500	-2.50630300	-1.88864100	C	-3.31546000	-0.29613900	-0.15784000
O	-0.53721000	-2.21735600	-0.61708000	H	-3.51325800	0.70067400	0.21241000
C	1.23045300	1.30250300	-0.81627800	O	0.51669400	-1.25901300	1.88493200
N	1.09594700	0.04568900	-0.69088000	C	-0.24244000	0.92020700	1.70366400
C	1.79166500	1.88086300	-2.11534100	C	-1.01173300	1.96895100	0.92374700
H	2.31655300	2.81959000	-1.90263200	C	-0.82916400	2.24767200	-0.44854100
H	0.96446900	2.10809200	-2.79432900	C	-1.87713700	2.78008100	1.66875100
O	2.61656900	0.94454900	-2.79348100	C	-1.51703600	3.31959400	-1.03535100
O	0.98933400	-2.00090500	-2.30255300	C	-2.59435300	3.81391700	1.06706000
H	1.25462700	-0.60295000	-1.51821600	C	-2.41454200	4.08537600	-0.29174000
O	-0.87426100	-3.25442600	-2.53467500	H	-1.36570300	3.54097000	-2.08830700
H	-1.85571900	4.83555600	-0.55198600	H	-3.27928000	4.41405700	1.65900500
H	-1.26749300	4.45897000	1.60978900	H	-2.96032600	4.89457800	-0.76772500
O	-1.78853200	0.82466600	1.64763500	O	0.35899200	1.26010800	2.73797400
C	-2.44065700	-1.31936000	1.08088300	C	3.06939300	1.56387600	-0.52685400
C	-3.58105400	-1.38759500	0.14205500	C	3.95581500	0.89868700	-1.38475900
C	-3.73937800	-0.52529200	-0.95669500	C	3.09470700	1.31953300	0.84807600
C	-4.55655200	-2.36883400	0.39837500	C	4.88534900	0.00064000	-0.85070800
C	-4.85820700	-0.64771000	-1.77990800	H	3.93825400	1.10325200	-2.45068600
H	-3.01242000	0.24497100	-1.18603400	C	4.03070100	0.42320300	1.36975700
C	-5.66724100	-2.48909600	-0.42998300	H	2.37295600	1.81220800	1.48988700
C	-5.82081600	-1.62670700	-1.52140200	C	4.93016700	-0.23521600	0.52748600
H	-4.97465000	0.02310000	-2.62571100	H	5.57687600	-0.50943000	-1.51523800
H	-6.41284400	-3.25219300	-0.22785000	H	4.04171500	0.22938300	2.43836600
H	-6.68835800	-1.71932300	-2.16847200	H	5.64998800	-0.93751500	0.93650000
O	-2.34575200	-1.98643300	2.09102800	C	-0.19685100	-1.94555000	2.91578200
C	-1.22615800	0.82024900	2.96072800	H	0.51514100	-2.65619000	3.34270400
H	-1.62357700	1.72615300	3.42223100	H	-0.53283300	-1.24030800	3.68386900
H	-1.54535700	-0.06015600	3.52522800	H	-1.05437700	-2.48993600	2.50121900
H	-0.13585100	0.88016400	2.91002000	C	1.41033000	-2.79598100	-0.40086400
N	-1.38021500	-0.30451400	0.84429900	O	1.11916600	-3.85408300	0.10968000
H	-1.42955500	0.10503200	-0.09367400	O	0.55405700	-2.09743600	-1.16780900
H	-4.42455600	-3.02847300	1.24911000	H	0.69236300	-1.00183700	-1.49198300
TS6				C	0.08107700	1.41656700	-1.29073000

N	-0.04185100	0.15532400	-1.39107500	C	-0.36899900	-1.69173700	3.35021400
C	1.24651100	2.11139900	-1.98432900	H	0.34380000	-2.14637100	4.04349600
H	0.91651600	3.02382300	-2.48691600	H	-0.97516800	-0.94781400	3.87758900
H	1.69148700	1.43628100	-2.72149500	H	-1.01700400	-2.47234500	2.92873700
O	2.19992200	2.53063700	-0.99945000	C	-3.05837700	-1.14475200	-0.63327600
O	2.64578300	-2.28148800	-0.27610800	O	-4.14593000	-1.13682900	-1.19735200
H	2.73715800	-1.40135600	-0.68333300	O	-1.93892900	-0.79736000	-1.21062100
H	-1.97883800	2.58834400	2.73246000	H	1.50092700	0.55668500	-1.58478200
12				C	0.09551800	1.77785300	-1.08004700
N	-0.41862200	-0.47506200	1.35634500	N	0.56775500	0.58326100	-1.17602700
C	0.62775600	-2.77286600	-2.06466500	C	1.01162400	2.93896800	-1.45558100
H	0.42977500	-2.67670600	-3.12324500	H	0.45161200	3.85738300	-1.62710700
Rh	-0.02335200	-1.28613700	-0.53635600	H	1.60039500	2.70299600	-2.34998500
C	1.78293400	-2.29328600	-1.36583900	O	1.86269000	3.20283700	-0.32571900
H	2.59634000	-1.72484700	-1.80071200	O	-2.99714600	-1.53228600	0.67561300
C	1.65126600	-2.61192200	0.01522800	H	-2.10673400	-1.30585900	1.03314000
H	2.34322600	-2.34363800	0.80003700	H	-3.22674400	1.47801000	2.18833800
C	0.41180600	-3.33768600	0.17658300	TS7			
H	0.01549400	-3.71877500	1.10710800	N	-1.89189000	-0.26800000	1.81841600
C	-0.20471600	-3.43708200	-1.09804900	C	1.03612300	-3.04931000	-1.29586600
H	-1.17235800	-3.87932400	-1.29777900	H	1.46632600	-3.27127500	-2.26423700
O	0.42517600	-1.07785600	2.33419100	Rh	-0.16388100	-1.25242300	-0.93154100
C	-0.74007000	0.80717300	1.70108800	C	1.65351300	-2.29463900	-0.26198400
C	-1.64219600	1.54867900	0.74387100	H	2.63242400	-1.83490600	-0.30129300
C	-1.22892900	2.06426600	-0.49745300	C	0.70252000	-2.15413200	0.80048300
C	-2.92401900	1.85400400	1.21606800	H	0.80512600	-1.55432000	1.69578600
C	-2.09958400	2.88785300	-1.23076900	C	-0.48267000	-2.91276500	0.44389100
C	-3.80360500	2.62230700	0.45566100	H	-1.38113900	-2.96269800	1.04236900
C	-3.38837900	3.14551100	-0.77184600	C	-0.28660500	-3.44804000	-0.84988500
H	-1.77781400	3.29734600	-2.18414900	H	-1.00142700	-4.02226000	-1.42441900
H	-4.80328500	2.82641900	0.82726000	O	-1.40187900	-1.26388100	2.71808500
H	-4.06151300	3.75664900	-1.36501900	C	-1.01059000	0.72125900	1.58499800
O	-0.45109500	1.33938600	2.77939000	C	-1.59364000	1.76056000	0.65503200
C	2.77178700	2.19382400	-0.02607100	C	-0.84728600	2.31260100	-0.40451500
C	3.80930200	1.87868100	-0.91050900	C	-2.88655900	2.24012500	0.88991800
C	2.61007400	1.48899100	1.16789100	C	-1.40061600	3.34269900	-1.18094100
C	4.68140000	0.83316700	-0.59607200	C	-3.44151900	3.24688800	0.09732900
H	3.92824000	2.44524600	-1.82932200	C	-2.69630000	3.80140200	-0.94278900
C	3.49331900	0.45192300	1.47688200	H	-0.83015500	3.76442100	-2.00411500
H	1.78479800	1.73436800	1.82698400	H	-4.44695700	3.60326600	0.30156900
C	4.52390100	0.11517300	0.59478000	H	-3.11317400	4.58821300	-1.56395200
H	5.48851900	0.58614800	-1.27989200	O	0.13268500	0.85900400	2.06274100
H	3.35234300	-0.10588800	2.39763000	C	3.31733100	1.59423200	0.24617700
H	5.20302600	-0.69829200	0.83295100	C	4.24988600	1.35407700	-0.77070000

C	3.22299600	0.73832500	1.34683400	O	-0.09811500	2.32795400	-0.73203300
C	5.09203300	0.24275600	-0.67795700	C	-1.07983600	3.04602700	-0.08623000
H	4.32856700	2.03352700	-1.61395100	C	-1.02116200	3.43098100	1.25678300
C	4.08648600	-0.35579200	1.43866900	C	-2.19123000	3.38148400	-0.87089700
H	2.45607100	0.92742000	2.08743200	C	-2.09199900	4.14515200	1.80826400
C	5.01749300	-0.61233800	0.42653900	H	-0.16724900	3.18562900	1.87696800
H	5.81760000	0.05642200	-1.46454200	C	-3.24836800	4.08993900	-0.30750500
H	4.01667900	-1.02015500	2.29559500	H	-2.20702500	3.08043300	-1.91436500
H	5.68038700	-1.46958200	0.49766100	C	-3.20613700	4.47571200	1.03795800
C	-1.61377300	-0.85091600	4.06556600	H	-2.04385000	4.44069700	2.85271200
H	-1.27958100	-1.68437900	4.69094300	H	-4.10760800	4.34357100	-0.92216900
H	-1.02299800	0.04305700	4.29794100	H	-4.03157000	5.02881500	1.47595500
H	-2.67674800	-0.65047100	4.25379100	C	2.65563400	-1.52126900	-0.73137800
C	-3.05024300	-1.08074800	-1.19435900	O	2.85922800	-2.10189900	-1.80113700
O	-3.73824200	-1.44710000	-2.14377900	O	1.29682800	-0.89760300	1.09619600
O	-1.87829600	-0.42992600	-1.41456900	C	1.48654700	-1.61340100	2.32226900
H	1.72238200	0.48933000	-1.43136300	H	0.82490400	-2.48469400	2.36431000
C	0.49254200	1.83918600	-0.82086700	H	2.53128700	-1.92922700	2.42929800
N	0.75420800	0.61625400	-1.13613700	H	1.22926700	-0.90537200	3.11406200
C	1.63187100	2.86062600	-0.90808200	H	4.01712700	2.86870400	0.13918100
H	1.24827300	3.87828300	-0.84994800	O	-0.91263800	-1.68538100	-1.02977900
H	2.17964600	2.74144400	-1.85043900	C	-1.70916500	-1.68329800	0.07171600
O	2.49012700	2.70604400	0.22582500	H	-1.28018700	-1.17300300	0.95898700
O	-3.38854600	-1.24454900	0.06047000	C	-3.02838700	-0.94063700	-0.20306000
H	-2.69415200	-0.76348800	0.84201000	F	-3.82472100	-0.82931100	0.87995500
H	-3.45346100	1.81634500	1.71143300	F	-3.75249400	-1.50584800	-1.18949200
15				F	-2.74510600	0.33518500	-0.60988800
N	1.67062300	0.89428400	-2.08267500	Na	-0.65663200	0.20540600	-2.17720700
C	3.33436200	0.86652300	-0.28272600	C	-1.99061400	-3.11914100	0.55032900
C	3.63311300	-0.50861000	-0.18373300	F	-2.57651000	-3.87760100	-0.39830900
C	4.24109200	1.80856900	0.21519100	F	-0.81973400	-3.71982100	0.87817900
C	4.84152500	-0.91785000	0.37986500	F	-2.78036600	-3.16727000	1.65067300
C	5.44736800	1.39120000	0.78306400	TS10			
C	5.74709100	0.03029500	0.86526800	N	-1.66740200	0.96791300	2.10140300
H	5.06789400	-1.97782600	0.44891700	C	-3.29926400	0.90759700	0.27194500
H	6.15086400	2.12920600	1.15656400	C	-3.57586600	-0.47094300	0.16757300
H	6.68372000	-0.29580000	1.30771100	C	-4.20056900	1.84388900	-0.24779100
H	2.39254000	0.32315900	-2.52972400	C	-4.76742600	-0.88661900	-0.42815500
N	1.53277100	-1.76023500	0.00042000	C	-5.38951400	1.41715000	-0.84397900
H	0.60698400	-1.93235000	-0.49240700	C	-5.67139100	0.05238300	-0.93415500
C	2.04680000	1.27338600	-0.91807700	H	-4.98316300	-1.94874600	-0.50400600
C	1.11900900	2.08334000	-0.04369400	H	-6.09153600	2.14840100	-1.23366000
H	0.94546700	1.49863500	0.86846500	H	-6.59391100	-0.28308100	-1.39960800
H	1.60073800	3.02863500	0.24412000	H	-2.39463300	0.39478600	2.53792300

N	-1.47718600	-1.75495400	0.07731600	C	5.61266300	1.26122200	0.07015100
H	-0.21994000	-1.82149900	0.63800200	C	5.92330500	-0.03787900	0.47630700
C	-2.02338700	1.32177900	0.92249500	H	5.19740700	-2.05948100	0.71011300
C	-1.07656200	2.09663400	0.03779500	H	6.35822500	2.04778800	0.13802100
H	-0.90180600	1.48220200	-0.85562000	H	6.91121500	-0.26530800	0.86601500
H	-1.54267000	3.03931200	-0.28174400	H	2.22538300	-0.49401600	-2.48716100
O	0.13925800	2.34435700	0.73034800	N	1.61087400	-1.81459400	0.65974000
C	1.11987400	3.06767400	0.08884100	H	0.62581200	-1.99003100	0.28148400
C	1.06486700	3.44942400	-1.25515300	C	2.02638400	0.80764500	-1.11503100
C	2.22684600	3.40886500	0.87729900	C	1.17683600	1.80237300	-0.36132200
C	2.13333900	4.16967300	-1.80302900	H	1.03121300	1.39445600	0.64688700
H	0.21608400	3.19525400	-1.87881900	H	1.70683100	2.76091000	-0.27107800
C	3.28211000	4.12300400	0.31717000	O	-0.06936600	1.97617400	-1.02167900
H	2.24070400	3.10966100	1.92149400	C	-0.98829800	2.83248200	-0.45813300
C	3.24241400	4.50784100	-1.02859900	C	-0.83071700	3.45038700	0.78613600
H	2.08781800	4.46340600	-2.84810400	C	-2.14256800	3.05940100	-1.21949900
H	4.13753700	4.38232700	0.93477600	C	-1.84444500	4.28973900	1.26372500
H	4.06602500	5.06578600	-1.46386100	H	0.05497300	3.28728500	1.38861700
C	-2.60185300	-1.47430400	0.75305300	C	-3.14226000	3.89485400	-0.73003200
O	-2.85239200	-1.97992000	1.86751000	H	-2.23890800	2.57225500	-2.18584600
O	-1.32036900	-0.95723300	-1.11833100	C	-2.99977700	4.51612900	0.51688700
C	-1.56779200	-1.77171200	-2.25957600	H	-1.71895200	4.76618300	2.23218000
H	-0.92370800	-2.66015900	-2.25174300	H	-4.03527800	4.06304700	-1.32563100
H	-2.61971000	-2.08646100	-2.29879000	H	-3.78012200	5.16860100	0.89697900
H	-1.33807700	-1.15240600	-3.13223700	C	2.63891900	-1.84007800	-0.23594200
H	-3.98542900	2.90596500	-0.16771600	O	2.68460300	-2.67920400	-1.13939100
O	0.84721300	-1.68952100	0.97809800	O	1.60953700	-0.70878200	1.54018400
C	1.65713400	-1.76276900	-0.14685000	C	1.49226000	-1.16953300	2.88500700
H	1.17960700	-1.34352700	-1.04345600	H	0.54717300	-1.70429500	3.03654500
C	2.91995500	-0.93659400	0.10527900	H	2.33465500	-1.81798300	3.15403000
F	3.77977400	-0.96859600	-0.92607800	H	1.50189100	-0.26666700	3.50099600
F	3.57365500	-1.33290600	1.21308200	H	4.10742700	2.56005100	-0.76323000
F	2.56975400	0.36551100	0.29924300	O	-0.80162200	-1.94591100	-0.42883200
Na	0.63765900	0.27083300	2.19545900	C	-1.86885300	-2.04969700	0.40056500
C	1.98847800	-3.22540700	-0.47412700	H	-1.73123400	-2.72845900	1.26773700
F	2.63360700	-3.83980700	0.53573300	C	-2.22924500	-0.68413700	1.02481800
F	0.84317100	-3.90259400	-0.70261600	F	-3.23189300	-0.74160600	1.92613600
F	2.75411000	-3.33582400	-1.58104700	F	-2.60250300	0.21801400	0.07028000
16				F	-1.15336800	-0.16059900	1.64667600
N	1.54616900	0.17856600	-2.12209700	Na	-0.82130500	-0.33919700	-1.96867500
C	3.37874100	0.54265300	-0.53663900	C	-3.07653000	-2.61988300	-0.36741500
C	3.69039800	-0.76448900	-0.10691600	F	-3.34280100	-1.89253600	-1.48584400
C	4.34141000	1.55233300	-0.43140000	F	-2.81639400	-3.87976900	-0.76997200
C	4.96294500	-1.04983500	0.38566000	F	-4.21691700	-2.65587300	0.35955300

TS11				F	-3.77259500	-0.02788400	-1.64817800
N	0.11862400	0.02821800	1.33933000	Na	-1.77228700	-1.95680100	-1.50799100
C	2.46865600	0.56699400	0.94225500	C	-4.29338200	-0.82094800	1.13840200
C	3.20691600	1.67618100	0.48770900	F	-3.97512200	-1.41659900	2.30222200
C	3.08797200	-0.40635700	1.73982700	F	-5.41076000	-0.09380300	1.33611900
C	4.56938100	1.76601800	0.78387400	F	-4.59127000	-1.79698000	0.24918900
C	4.44506300	-0.29750600	2.04476700	3			
C	5.18799000	0.78603700	1.56012600	C	1.68930700	0.40651800	0.11786200
H	5.12293800	2.61862300	0.40204800	C	2.88041200	0.29512500	-0.60297000
H	4.92680700	-1.06603800	2.64271200	C	1.32182700	1.61789400	0.69612700
H	6.24732100	0.86307900	1.79041300	C	3.74229200	1.37409500	-0.77388800
H	0.38083100	0.06146100	2.32249100	C	2.18451500	2.70898800	0.53090500
N	1.20243000	2.70277600	0.00551400	C	3.38018800	2.59287900	-0.19427200
H	-1.08983000	-0.41155800	0.87775500	H	4.66108600	1.26172500	-1.34167100
C	1.05450400	0.39651200	0.51735400	H	1.92159500	3.66611600	0.97281800
C	0.74706400	0.23485800	-0.96833900	H	4.02613700	3.45893800	-0.30583200
H	-0.16620900	0.76322800	-1.23104900	N	0.89671700	-1.59499900	1.46711500
H	1.56996800	0.59822500	-1.58358600	C	0.98349200	-0.94333700	0.13704800
O	0.48473400	-1.16389600	-1.27623700	C	-0.38869000	-0.92159400	-0.55362600
C	1.54777300	-2.03157300	-1.04573900	H	-0.24366900	-0.62246200	-1.59934200
C	2.73450200	-1.92154100	-1.77453200	H	-0.81462700	-1.93336100	-0.52460700
C	1.38955800	-3.02897400	-0.08140600	O	-1.23554000	-0.00116500	0.11714900
C	3.77609400	-2.81602700	-1.52175800	C	-2.52976700	0.12829900	-0.30838700
H	2.83907200	-1.14443800	-2.52511800	C	-3.07445800	-0.54317500	-1.40970200
C	2.43347700	-3.92668400	0.15564800	C	-3.32443900	1.00534400	0.44510000
H	0.46556100	-3.07496200	0.48680500	C	-4.41615200	-0.32803100	-1.74667600
C	3.63026200	-3.81848900	-0.55769100	H	-2.47581200	-1.22326000	-2.00436500
H	4.70213500	-2.73010700	-2.08307500	C	-4.65625300	1.20907100	0.09610700
H	2.31368800	-4.70149300	0.90772400	H	-2.87691800	1.51151500	1.29513700
H	4.44432700	-4.51105200	-0.36502400	C	-5.21234400	0.54266500	-1.00327500
C	2.50989200	2.75068100	-0.29998300	H	-4.83366100	-0.85200900	-2.60231900
O	3.13805200	3.50679200	-1.07666600	H	-5.26378100	1.89005100	0.68606700
O	0.43397700	3.50668500	-0.88590100	H	-6.25208100	0.70202300	-1.27323800
C	-0.66386100	4.04302100	-0.16744300	C	3.02022000	-1.09816800	-1.10443200
H	-1.26702800	3.25372700	0.29672800	O	3.92181700	-1.58538300	-1.77562200
H	-0.33260900	4.74327800	0.61355900	O	0.30608000	-0.68840000	2.41203400
H	-1.27683000	4.57940700	-0.89941200	C	-0.88952600	-1.26438800	2.92889300
H	2.52162200	-1.27338300	2.06641000	H	-1.63634600	-1.41256600	2.14167700
O	-2.04227400	-0.80250700	0.40716600	H	-0.68758500	-2.21765200	3.43350800
C	-3.11534600	0.03142900	0.65197300	H	-1.26852600	-0.53806200	3.65423900
H	-2.91725500	0.78082500	1.43227400	H	0.39941600	1.70488000	1.25513000
C	-3.46689200	0.81375900	-0.62285300	N	1.89612800	-1.75710000	-0.65411100
F	-2.39947400	1.53733100	-1.02352200	H	1.73369600	-2.73827800	-0.83599400
F	-4.50082400	1.65327800	-0.46224200	H	1.85858100	-1.68642300	1.80040100

17				TS12			
N	-0.62820100	0.54239000	-2.52002800	N	-0.60114500	0.65296800	-2.38870200
C	-1.74872000	-1.13822300	-1.08651900	C	-1.67545400	-1.14817700	-1.06718300
C	-2.87253200	-0.43599700	-0.60034200	C	-2.84275700	-0.50780800	-0.59452000
C	-1.73037200	-2.53892300	-0.97239700	C	-1.58888000	-2.54954800	-0.97559300
C	-3.93277900	-1.13257600	-0.01254600	C	-3.87418300	-1.27466700	-0.04188200
C	-2.80022000	-3.22958200	-0.40017600	C	-2.63156600	-3.30598600	-0.43789900
C	-3.90163800	-2.52470400	0.09136600	C	-3.77744700	-2.66523200	0.04021800
H	-4.78685100	-0.57757200	0.36523300	H	-4.76170100	-0.76956900	0.32951900
H	-2.77209200	-4.31375800	-0.34123600	H	-2.54889600	-4.38845400	-0.39818500
H	-4.73530800	-3.05432800	0.54322100	H	-4.59315600	-3.24385100	0.46491500
H	-1.60066400	0.75361900	-2.76056700	H	-1.58244000	0.87621900	-2.58566300
N	-2.56362800	1.73862800	0.32417500	N	-2.70320000	1.62533000	0.40960600
H	-2.03879100	1.30842900	1.13469200	H	-1.87962400	1.05203400	1.40334500
C	-0.57374100	-0.41360600	-1.67473800	C	-0.52256400	-0.36204700	-1.61812600
C	0.76822700	-0.89229900	-1.15195100	C	0.84190600	-0.86222300	-1.16763100
H	0.73830200	-0.91656000	-0.05352100	H	0.83656400	-0.99203200	-0.07711700
H	0.95190900	-1.91852100	-1.50474000	H	1.04051300	-1.84614100	-1.61770300
O	1.80232200	-0.02912700	-1.60187100	O	1.85258400	0.05771200	-1.54921600
C	3.05912600	-0.22735200	-1.11229500	C	3.11730800	-0.15612100	-1.08545800
C	3.45124400	-1.32984300	-0.33569800	C	3.54052900	-1.31785000	-0.42023100
C	3.99470800	0.77527400	-1.42128100	C	4.02462600	0.89696000	-1.29608000
C	4.77339000	-1.41456700	0.12311900	C	4.86263300	-1.40751900	0.03478100
H	2.74808500	-2.11540100	-0.08611100	H	2.86059100	-2.14468000	-0.25267700
C	5.30257900	0.67760100	-0.95382500	C	5.33510100	0.79138000	-0.83701800
H	3.67009500	1.61847600	-2.02315500	H	3.67587100	1.78508700	-1.81411300
C	5.70198300	-0.41737200	-0.17548200	C	5.76340300	-0.36105800	-0.16424100
H	5.06767200	-2.27373500	0.72000000	H	5.18165200	-2.31155600	0.54667700
H	6.01500000	1.46040100	-1.19931100	H	6.02592300	1.61300500	-1.00552200
H	6.72354700	-0.49179500	0.18482800	H	6.78625000	-0.44119600	0.19131800
C	-2.98941200	1.06488900	-0.75650600	C	-3.03874000	0.99509600	-0.71225800
O	-3.44602500	1.56862300	-1.79086500	O	-3.46333700	1.46729500	-1.79334200
O	-2.55422100	3.13243000	0.27669200	O	-2.86064800	3.04436800	0.34332400
C	-1.29589500	3.58392800	-0.26462200	C	-1.70967300	3.62353800	-0.27497300
H	-0.47004100	3.21216500	0.35172700	H	-0.79754500	3.32878000	0.25739100
H	-1.17969400	3.24289400	-1.30005600	H	-1.63368900	3.32128700	-1.32722800
H	-1.34501400	4.67580200	-0.23407200	H	-1.85056400	4.70849100	-0.21541100
H	-0.88370800	-3.10159100	-1.35289300	H	-0.70864900	-3.06486700	-1.34740700
C	0.06278000	0.60560500	2.12348600	C	0.04571900	0.61100300	1.98904200
O	0.63845200	1.71806600	1.86034200	O	0.50721800	1.71302700	1.59001900
Na	2.66593700	0.72209400	1.89616000	Na	2.64506100	0.92493500	1.94662300
O	0.76615900	-0.50226100	2.20357300	O	0.77293100	-0.40150400	2.31533200
O	-1.22690200	0.52858200	2.31110100	O	-1.28296700	0.42226000	2.10072100
Na	-1.13959900	-1.71115600	2.49816700	Na	-1.04021700	-1.82078500	2.50984300

18				TS13			
N	-0.63432800	0.52642300	-2.53174000	N	-0.85818200	-0.09425000	-2.02853500
C	-1.75473500	-1.14261700	-1.08415100	C	-2.56030000	-0.86073600	-0.48322800
C	-2.87426300	-0.43574500	-0.59520500	C	-3.53301400	-0.22670900	0.31649200
C	-1.73916700	-2.54291400	-0.96534300	C	-2.77834000	-2.16091000	-0.96211900
C	-3.93345600	-1.12739000	0.00009300	C	-4.69032300	-0.93478200	0.65317200
C	-2.80823000	-3.22878300	-0.38585200	C	-3.94222400	-2.85214800	-0.61938900
C	-3.90537000	-2.51927700	0.10853000	C	-4.89570400	-2.23769000	0.19695100
H	-4.78430500	-0.56895100	0.38008400	H	-5.42415700	-0.42934500	1.27299600
H	-2.78277200	-4.31282800	-0.32340700	H	-4.09665100	-3.86459200	-0.98131500
H	-4.73827600	-3.04512100	0.56617900	H	-5.80147900	-2.77216800	0.47116600
H	-1.60691500	0.73559600	-2.77363100	H	-1.53836600	-0.33338100	-2.74770400
N	-2.55658700	1.74225100	0.31872700	N	-2.38834700	1.78225900	0.11353400
H	-2.03183000	1.31458500	1.13059500	H	0.30123100	0.18757300	-2.34992400
C	-0.58006300	-0.42262200	-1.67868700	C	-1.26900100	-0.20464100	-0.80848400
C	0.76064800	-0.89617300	-1.14898500	C	-0.24870500	0.04163200	0.28625100
H	0.73031200	-0.90166500	-0.05028400	H	0.30668600	0.95508500	0.06916600
H	0.94130800	-1.92885300	-1.48387300	H	-0.73998900	0.10479900	1.25784200
O	1.79789300	-0.04430000	-1.61303700	O	0.64916100	-1.08840100	0.25271100
C	3.05304000	-0.23960900	-1.11817300	C	1.69620600	-1.07048300	1.12985400
C	3.43548400	-1.32446900	-0.31228900	C	1.94227300	-0.04152700	2.05188400
C	3.99700800	0.74706800	-1.45192900	C	2.56062900	-2.17590800	1.07588700
C	4.75622600	-1.40765400	0.15052400	C	3.06656200	-0.11705200	2.88471900
H	2.72587100	-2.09740400	-0.04264800	H	1.27952200	0.81222000	2.13011700
C	5.30378100	0.65066100	-0.98104500	C	3.67757300	-2.23287000	1.90531900
H	3.67998400	1.57677500	-2.07620000	H	2.33479900	-2.98034700	0.38134400
C	5.69329100	-0.42632900	-0.17317300	C	3.94347400	-1.20012300	2.81308400
H	5.04280300	-2.25307300	0.77035500	H	3.24574700	0.68363100	3.59761800
H	6.02284700	1.42083300	-1.24632500	H	4.33930500	-3.09288400	1.84800100
H	6.71385300	-0.49948000	0.19024600	H	4.81114300	-1.24963400	3.46396400
C	-2.98639200	1.06466100	-0.75798900	C	-3.39214500	1.20807500	0.77414700
O	-3.44223800	1.56485000	-1.79436400	O	-4.19048100	1.68508100	1.62055400
O	-2.54016200	3.13582900	0.26315700	O	-2.20893200	3.14318600	0.52489300
C	-1.28124400	3.57715900	-0.28491100	C	-0.87167300	3.52011200	0.26311500
H	-0.45528000	3.20547700	0.33147100	H	-0.16812400	3.05942600	0.97556500
H	-1.16994500	3.22885400	-1.31843400	H	-0.55036500	3.24189700	-0.74887000
H	-1.32438900	4.66947000	-0.26128000	H	-0.82940800	4.60873800	0.38022600
H	-0.89568500	-3.10894600	-1.34788300	H	-2.02009600	-2.63899800	-1.57671500
C	0.06954700	0.62056900	2.12868300	C	2.28558000	0.94108400	-1.86340300
O	0.64579500	1.73403200	1.87127700	O	1.82771200	1.95539500	-1.24953300
Na	2.67359300	0.73647800	1.89581400	Na	3.73150300	1.94026300	0.05902900
O	0.77220900	-0.48760600	2.20619600	O	3.49610800	0.51561900	-1.70789100
O	-1.22099700	0.54272400	2.31249100	O	1.50867500	0.23545100	-2.68473200
Na	-1.13430200	-1.69642700	2.50234700	Na	2.87511000	-1.58123300	-2.40193800

19				O	1.20989300	-2.35191200	0.69631100
N	-1.32361200	-0.56417600	1.63330500	H	-0.31300700	-0.60144300	1.55411000
C	-3.44930100	0.06931900	0.60210600	C	2.67893600	-0.73321600	1.62183300
C	-4.07779300	-0.71548200	-0.36670500	F	3.22648400	-1.66839000	2.41268700
C	-4.19418600	0.76702800	1.54466100	F	3.62084100	0.19091600	1.34523400
C	-5.46316800	-0.82675700	-0.43180700	F	1.70005500	-0.12082600	2.32299500
C	-5.59029800	0.66483300	1.48507700	TS14			
C	-6.21910600	-0.12058700	0.50812900	N	0.33111500	0.35930600	-1.79233600
H	-5.93093900	-1.44718100	-1.18999000	C	0.73201700	2.50287200	-0.77087900
H	-6.19543800	1.19822200	2.21233200	C	0.66567200	2.95106200	0.56178100
H	-7.30300700	-0.18328200	0.48717400	C	1.58039500	3.13730300	-1.69374500
H	-1.66562000	-1.50644700	1.80633100	C	1.40985700	4.07441000	0.93231000
N	-1.85749500	-0.83013500	-0.78499200	C	2.32844900	4.24559400	-1.29998800
H	0.44885300	-2.28351700	0.08249900	C	2.23192200	4.72207300	0.01069800
C	-1.93433500	0.00085200	0.45750400	H	1.34472000	4.41476200	1.96054600
C	-1.36595600	1.40036400	0.19547900	H	2.97536900	4.73972500	-2.01812800
H	-1.87807200	1.84572800	-0.66472200	H	2.80791000	5.59048100	0.31637600
H	-1.54250300	2.01569200	1.08474700	H	1.24113100	0.01853900	-1.43764000
O	0.03446100	1.29422400	-0.06340100	N	-0.03672000	0.86532800	1.40955500
C	0.72566600	2.45761000	-0.32144600	H	0.96666400	0.19453200	0.83923800
C	0.15746100	3.73512500	-0.24640400	C	-0.15589200	1.44717900	-1.29597700
C	2.07313200	2.31171700	-0.68285700	C	-1.62815800	1.72892600	-1.47191900
C	0.94636500	4.85685900	-0.52459500	H	-2.03885700	2.02703700	-0.50132700
H	-0.88243500	3.87334900	0.02311800	H	-1.72800100	2.58147400	-2.15448200
C	2.84478600	3.43881500	-0.95403200	O	-2.28571000	0.60799400	-2.03643800
H	2.51471600	1.32532500	-0.75316300	C	-3.13179600	-0.13284500	-1.21721300
C	2.28839100	4.72011200	-0.87666100	C	-4.20156300	0.46875900	-0.55070300
H	0.49579400	5.84362600	-0.46264700	C	-2.90939400	-1.50733800	-1.13010000
H	3.88763000	3.31135800	-1.23090100	C	-5.04203900	-0.32099100	0.23670700
H	2.89329700	5.59605600	-1.09069500	H	-4.37426900	1.53608400	-0.64941900
C	-3.05213800	-1.38232300	-1.20842000	C	-3.76375300	-2.28807500	-0.34952200
O	-3.19006300	-2.21172600	-2.09743800	H	-2.06370900	-1.95047400	-1.64493800
O	-0.66456200	-1.43784900	-1.14322100	C	-4.82644700	-1.69815600	0.34028600
C	-0.18152200	-0.91732000	-2.40434000	H	-5.87079300	0.14334900	0.76311900
H	-0.91768500	-1.11716800	-3.18572300	H	-3.58552800	-3.35640900	-0.26966500
H	0.02067500	0.15249000	-2.31228700	H	-5.48290800	-2.30750300	0.95411200
H	0.73914400	-1.46736900	-2.59842500	C	-0.08025400	2.19948900	1.63518700
H	-3.71148600	1.36215800	2.31344300	O	-0.61270700	2.79596000	2.58328400
C	2.09810500	-1.33024800	0.33811900	O	-0.59432200	0.10160600	2.46887800
H	1.59075400	-0.51479300	-0.18329000	C	-2.00894300	-0.01003700	2.32351200
C	3.19023600	-1.86377500	-0.59798200	H	-2.49074600	0.97298900	2.38202300
F	4.02413600	-2.71974100	0.01474100	H	-2.26928600	-0.49647400	1.37983900
F	2.61833200	-2.51650700	-1.63232200	H	-2.34344900	-0.63016000	3.16102400
F	3.92655100	-0.85234800	-1.10711900	H	1.62170300	2.78378100	-2.71937300

C	1.91942000	-1.69145800	0.61696700	O	-1.15434400	-0.06991900	2.59657700
H	1.92384500	-1.86997000	1.70351400	C	-2.16958800	-1.01468400	2.22386500
C	3.25103100	-2.22332700	0.07447900	H	-3.09909200	-0.50048800	1.96223500
F	3.33008900	-2.07343600	-1.26569900	H	-1.83691300	-1.63756000	1.39103700
F	4.27608600	-1.54503000	0.62236000	H	-2.32311300	-1.62786400	3.11540100
F	3.43311200	-3.53214200	0.35062400	H	0.57070000	3.32358400	-2.53399100
O	1.82814100	-0.35796600	0.27436700	C	2.68560600	-0.62359300	0.77192900
H	-0.31199800	-0.30652200	-2.21428600	H	2.93999500	-0.68979900	1.83296500
C	0.72691000	-2.50029900	0.06956500	C	4.00390700	-0.61349600	-0.01584100
F	0.62060300	-2.39873700	-1.28409500	F	3.77943200	-0.39954200	-1.32871300
F	0.80189200	-3.81038000	0.36826400	F	4.79535800	0.37623000	0.43186900
F	-0.42293400	-2.02574900	0.58404900	F	4.67407800	-1.77521900	0.10982500
20				O	1.99093300	0.56893500	0.55706500
N	0.49200700	0.56393100	-1.64211900	H	0.24275300	-0.32171700	-2.09220400
C	-0.43523500	2.60207200	-0.77735600	C	1.83461300	-1.86513200	0.44989300
C	-0.96146900	2.94717900	0.48436200	F	1.63307100	-2.01201900	-0.88236300
C	0.16857600	3.59494800	-1.56287900	F	2.41610700	-2.98917200	0.90007000
C	-0.91026600	4.28063800	0.91073500	F	0.62621800	-1.75586600	1.03194700
C	0.23164900	4.91541400	-1.11910100	TS16			
C	-0.31893800	5.26147000	0.11736100	N	0.75435400	0.14400000	2.00472900
H	-1.32861500	4.52999500	1.88044100	C	2.16676500	-0.98207300	0.45190400
H	0.70134600	5.67143100	-1.74115100	C	2.66744600	0.19764600	-0.17706400
H	-0.28155100	6.28939600	0.46526200	C	2.84316200	-2.20095900	0.38721900
H	1.66006400	0.61104000	-0.39506100	C	3.88980700	0.07197200	-0.84535800
N	-0.85761500	0.77094800	1.52214300	C	4.07231600	-2.27850100	-0.27034200
H	0.13170400	0.71005600	1.27136600	C	4.59036300	-1.13769400	-0.88218600
C	-0.55805500	1.23958800	-1.37498400	H	4.27454600	0.94757100	-1.35471000
C	-1.96406400	0.77904700	-1.72933600	H	4.61236800	-3.21954600	-0.30484500
H	-2.61110900	0.87499000	-0.85095300	H	5.54120000	-1.18706800	-1.40508200
H	-2.36283400	1.44080500	-2.50759200	H	1.65777300	0.46477300	2.35335800
O	-1.93897100	-0.55082600	-2.23271800	N	0.69626500	1.71690000	0.12618100
C	-2.46073800	-1.55617600	-1.43633600	H	0.25616500	1.00470300	1.49444400
C	-3.76873600	-1.49404200	-0.94607600	C	0.86138900	-0.78403500	1.09003000
C	-1.65936900	-2.67364500	-1.19018400	C	-0.36743300	-1.31941300	0.42474900
C	-4.26558300	-2.55436400	-0.18496200	H	-0.29951400	-1.07773400	-0.64458700
H	-4.39026300	-0.63092200	-1.16370500	H	-0.35763200	-2.41970900	0.50942400
C	-2.17189000	-3.73403800	-0.44034300	O	-1.51050500	-0.74538800	1.01557700
H	-0.64317700	-2.69412200	-1.56674300	C	-2.68673800	-0.75153100	0.30373300
C	-3.47200400	-3.67618900	0.07051400	C	-2.94421000	-1.59861500	-0.77885600
H	-5.27981700	-2.50388500	0.20080000	C	-3.66018700	0.15444500	0.74413400
H	-1.54557600	-4.59947700	-0.24308200	C	-4.18504500	-1.52423200	-1.42221400
H	-3.86383900	-4.49873700	0.66135200	H	-2.20463400	-2.31548900	-1.11787700
C	-1.53692400	1.96169600	1.46440700	C	-4.89165400	0.21289400	0.09655300
O	-2.53120800	2.20796400	2.14104300	H	-3.42842200	0.80147000	1.58427500

C	-5.16063200	-0.62456400	-0.99275100	C	-5.30256400	-1.85676300	-0.81673500
H	-4.38237500	-2.18259600	-2.26366700	H	-4.45377600	-3.53707500	0.23778200
H	-5.64149400	0.92013100	0.44001500	H	-5.97372700	0.01591200	-1.65675100
H	-6.12000000	-0.57382500	-1.49890900	H	-5.92473700	-2.46883700	-1.46264500
C	1.97102400	1.58594300	-0.32145200	C	1.37599000	-0.25418300	3.79202300
O	2.61383000	2.46447400	-0.92599800	H	1.96146100	-0.88463700	4.46504800
O	0.19946400	3.00677200	-0.19604100	H	1.53324700	0.79801000	4.04534600
C	-1.19995300	2.98984700	0.02757200	H	0.31599200	-0.51438200	3.88039000
H	-1.70201300	2.22726600	-0.58349700	C	0.94294500	0.97293900	-2.62735800
H	-1.44023100	2.79908300	1.08536500	O	1.29719100	1.75457400	-3.50248500
H	-1.56178000	3.98432500	-0.24910900	O	1.62433400	0.75305900	-1.53254900
H	2.42088500	-3.07329300	0.87669600	H	-1.09052200	-1.50664700	0.18156200
TS17				C	-0.72197600	0.33933500	0.74989800
N	1.27332800	0.22521100	1.46878700	N	-0.66015500	-0.64587600	-0.15162600
C	3.04724000	-2.30858100	0.35115400	C	-1.61123700	0.20577500	1.98149000
H	3.60743200	-2.06521700	1.24354300	H	-1.29987300	0.92144500	2.74189400
Rh	1.43636000	-0.95846600	-0.36278500	H	-1.54843100	-0.80557600	2.39528100
C	1.79549000	-3.01338100	0.32476100	O	-2.95000900	0.57038700	1.63840000
H	1.29842300	-3.46510500	1.17192100	O	-0.23110900	0.29374200	-2.78831700
C	1.35860900	-3.05170800	-1.04541600	H	-0.47967900	-0.13935300	-1.93608500
H	0.43667700	-3.49053700	-1.40606000	H	1.87804600	4.18190100	0.69783100
C	2.30025700	-2.33979300	-1.83930800	23			
H	2.22964100	-2.16154100	-2.90395900	TS18			
C	3.35792000	-1.87925600	-0.96613000	N	0.94580700	-0.00633700	1.31776100
H	4.21635100	-1.29109500	-1.26096300	C	0.26154100	-3.38153300	0.76745200
O	1.87346800	-0.55905000	2.48234100	H	-0.14903700	-3.39864300	1.76742000
C	1.66218000	1.57408400	1.50794300	Rh	0.77320000	-1.49470200	-0.29196400
C	0.70849700	2.38452800	0.71901800	C	-0.47300600	-3.30626300	-0.44283900
C	-0.45818100	1.73892600	0.29231900	H	-1.55023800	-3.24020700	-0.52958800
C	0.96411900	3.70709900	0.35530100	C	0.46155700	-3.24232700	-1.53842600
C	-1.35866100	2.40140600	-0.54356300	H	0.21158700	-3.18268100	-2.58897600
C	0.05158800	4.37986500	-0.45558900	C	1.78670700	-3.35990100	-0.98098600
C	-1.10079600	3.72536700	-0.90828500	H	2.71147400	-3.31764800	-1.54116100
H	-2.24722500	1.89167300	-0.89914400	C	1.67041500	-3.41484500	0.42619200
H	0.23954800	5.40859900	-0.74782300	H	2.48986600	-3.44883600	1.13212900
H	-1.80450600	4.24953700	-1.54813000	O	0.68974200	-0.69707300	2.52909600
O	2.60454200	2.02259200	2.15354800	C	2.19191800	0.77821900	1.27918700
C	-3.68673800	-0.28448100	0.83863000	C	1.86334900	2.02828800	0.60113200
C	-3.66683200	-1.67786900	0.97029100	C	0.50286800	2.07583400	0.28962700
C	-4.52159100	0.32382300	-0.10369900	C	2.73618300	3.06499300	0.26223200
C	-4.47282200	-2.45579400	0.13409300	C	-0.02549400	3.16544600	-0.39351600
H	-3.04761200	-2.15929400	1.72023300	C	2.20525300	4.16675200	-0.40334000
C	-5.32915900	-0.46323500	-0.92534800	C	0.83799900	4.21355300	-0.72529700
H	-4.52812600	1.40682800	-0.17449900	H	-1.07680700	3.20181700	-0.65213700

H	2.85019900	4.99402600	-0.68231200	O	-1.35234600	-0.46354300	2.17598300
H	0.44447100	5.08091800	-1.24687200	C	0.21344700	2.67817100	-0.88907100
O	3.22719200	0.37394500	1.75652600	C	-0.64217000	3.19086100	0.09158700
C	-3.41612900	0.98129900	0.51170100	C	1.58264200	2.96934000	-0.85327700
C	-3.96687200	-0.16929000	1.08867800	C	-0.11201900	3.99043900	1.11277000
C	-3.89598700	1.45783600	-0.71285200	H	-1.70348000	2.96934600	0.09292300
C	-4.98760400	-0.84931800	0.41726700	C	2.09433600	3.77055200	0.16167800
H	-3.62019700	-0.52963800	2.05128900	H	2.22691000	2.52052500	-1.60130400
C	-4.92348300	0.77704000	-1.36571700	C	1.25091000	4.28452600	1.15630500
H	-3.45326600	2.35227000	-1.13920200	H	-0.78124900	4.38374600	1.87337800
C	-5.46906100	-0.38374400	-0.80829300	H	3.15904700	3.98668200	0.18470800
H	-5.41243800	-1.74226100	0.86705700	H	1.65273200	4.90886400	1.94901700
H	-5.28973300	1.15064000	-2.31766400	C	-0.85793800	-3.26296400	-1.29763900
H	-6.26286800	-0.91727800	-1.32219400	H	-1.40090200	-3.71795100	-2.13256100
C	1.02730500	0.02541000	3.73799800	H	-0.31026800	-2.38422700	-1.65746900
H	0.52959300	-0.54385900	4.52446000	H	-0.14212500	-3.98999600	-0.88999900
H	2.10652300	0.03442900	3.89662700	C	-1.90061000	0.46681900	-0.90324000
H	0.63933900	1.04757500	3.72186900	N	-1.03929100	-0.12700900	-0.15864500
C	1.53143700	0.50218100	-2.46342500	C	-1.52733600	1.43842600	-1.99069700
O	2.38745400	0.96857500	-3.22707500	H	-2.22287500	2.28862400	-1.98056000
O	1.95207900	-0.24466100	-1.42311500	H	-1.63990000	0.94198400	-2.96041200
H	-1.61613000	-0.32606300	-0.31714800	O	-0.17913800	1.85953300	-1.92464400
C	-0.21338300	0.81574100	0.73207000	H	0.10273200	0.00625300	-0.07756400
N	-0.65934900	0.00642100	-0.41023500	H	-1.58340400	-2.83884700	1.60108700
C	-1.33950600	1.06312000	1.75383300	O	1.40116400	0.09090900	0.33855600
H	-0.99356100	1.73145300	2.54239700	C	2.06350000	-1.05905300	0.02065700
H	-1.63659400	0.11324100	2.20321400	C	2.58767400	-0.98190000	-1.42152700
O	-2.42174300	1.73176200	1.11600700	F	3.39928800	0.07737000	-1.62517200
O	0.24435900	0.70937000	-2.59874800	F	3.26783900	-2.09085100	-1.79637600
H	-0.34033100	0.41633500	-1.51243200	F	1.53938400	-0.84980500	-2.26996100
H	3.79023700	2.99914000	0.51131400	Na	0.60589800	0.58023600	2.37873000
TS19				H	1.43862200	-1.97110800	0.06233900
N	-1.21090100	-2.31319400	0.80733300	H	-4.27572100	-1.81685300	2.10351700
O	-1.84986500	-2.91406300	-0.34035300	C	3.20175500	-1.30433500	1.01841000
C	-1.70744000	-0.92163700	0.99783700	F	4.12497400	-0.32146700	1.01128300
C	-3.18324200	-0.71573400	0.60613000	F	2.68895100	-1.35501200	2.27998600
C	-3.27426500	0.12071600	-0.51417700	F	3.84622400	-2.47149800	0.80854500
C	-4.33260600	-1.17491800	1.22860200	24			
C	-4.50278400	0.51792400	-1.04258700	N	0.79579300	-2.27726300	-0.24536800
C	-5.57543100	-0.79016900	0.70311100	O	1.30993400	-2.69181100	1.03133600
C	-5.66214900	0.04496300	-0.41939900	C	1.59001800	-1.10769000	-0.83205000
H	-4.56489400	1.16993400	-1.90914800	C	3.09815800	-1.28728600	-0.60030900
H	-6.48843700	-1.14167800	1.17602900	C	3.52107800	-0.32561100	0.32327400
H	-6.63643800	0.33004300	-0.80473500	C	4.00353700	-2.17357600	-1.16134800

C	4.85416300	-0.22553200	0.71648800	N	0.76171100	-2.20193800	-0.12639100
C	5.35023100	-2.08540200	-0.77329600	O	1.22516900	-2.52558200	1.18178400
C	5.77079400	-1.12530700	0.15574100	C	1.59908400	-1.06131100	-0.84359800
H	5.18193100	0.52148500	1.43462600	C	3.09023100	-1.31850900	-0.60630900
H	6.07869000	-2.76963800	-1.20047800	C	3.56082000	-0.34625300	0.28271000
H	6.81779900	-1.07556500	0.44125800	C	3.94609800	-2.26640400	-1.14225700
O	1.17585300	-0.91065000	-2.06878600	C	4.89826200	-0.29945300	0.66957900
C	0.59753700	2.99244900	0.62766900	C	5.29660200	-2.23124400	-0.75906200
C	1.31523900	3.29367600	-0.53832900	C	5.76609200	-1.26248800	0.13675300
C	-0.74189800	3.38938900	0.74506800	H	5.26556500	0.45446700	1.36049000
C	0.68173100	3.98431800	-1.57777400	H	5.98940100	-2.96321600	-1.16528500
H	2.34673300	2.98330000	-0.65760600	H	6.81535100	-1.25481000	0.41764900
C	-1.36150600	4.07224200	-0.29924200	O	1.15023000	-0.95084800	-2.06040900
H	-1.28251300	3.12806400	1.64837200	C	0.67140800	3.01986600	0.57794000
C	-0.65548100	4.37380200	-1.47033300	C	1.35870900	3.36753600	-0.59219300
H	1.24578100	4.21150500	-2.47850500	C	-0.69064000	3.32216300	0.70664800
H	-2.40323900	4.36456200	-0.19928800	C	0.66914600	4.00198000	-1.63053800
H	-1.13944300	4.90756500	-2.28287600	H	2.40911700	3.13022500	-0.71596700
C	0.33063400	-2.46405900	2.03787800	C	-1.36577300	3.95390000	-0.33605500
H	0.81932700	-2.70224000	2.98709100	H	-1.20635300	3.01998800	1.61144900
H	0.00324700	-1.41946500	2.04542400	C	-0.69185200	4.29608500	-1.51429800
H	-0.53870100	-3.12568200	1.90781000	H	1.20780700	4.26392300	-2.53737300
C	2.31357000	0.46014700	0.67092700	H	-2.42525900	4.16978000	-0.22959100
N	1.24584900	0.05737200	0.08751000	H	-1.21870800	4.78815500	-2.32655400
C	2.35376400	1.65646900	1.58829700	C	0.27258000	-2.12828700	2.17462000
H	3.15360600	2.34297500	1.27440300	H	0.78359100	-2.27322300	3.12891100
H	2.60476800	1.32498000	2.60152300	H	-0.00880000	-1.07933600	2.05626700
O	1.10868200	2.32670600	1.71079100	H	-0.62090700	-2.76556300	2.14066900
H	-0.76241700	-1.76107800	-0.41438600	C	2.39244700	0.50594800	0.60823100
H	0.98540300	-3.06827300	-0.86529400	N	1.30632700	0.13780700	0.03452800
O	-1.62315800	-1.28678400	-0.71763500	C	2.47707900	1.71825500	1.49980900
C	-2.63067300	-1.30776300	0.24244800	H	3.26842800	2.39209400	1.14065600
H	-2.45124700	-2.02938900	1.04740000	H	2.76817700	1.40344800	2.50755700
C	-2.73721000	0.07873600	0.89692400	O	1.23911100	2.39269400	1.65956200
F	-1.60179800	0.35314200	1.56850300	H	-0.39820800	-1.84105800	-0.18869300
F	-3.76502500	0.17088500	1.75696400	H	0.89659900	-3.04832700	-0.68548000
F	-2.88772700	1.04887100	-0.03837100	O	-1.51797400	-1.27051200	-0.48974400
Na	-0.47832500	0.58016100	-1.56459700	C	-2.62148500	-1.30590100	0.31295900
H	3.68356300	-2.91910100	-1.88525800	H	-2.55638300	-2.00455000	1.16498100
C	-3.93383100	-1.72299800	-0.44976300	C	-2.86954400	0.08268800	0.93357100
F	-3.78572600	-2.93965700	-1.00365300	F	-1.84186800	0.41560200	1.74679400
F	-4.96238500	-1.78523700	0.41874900	F	-4.00106300	0.15504900	1.66146400
F	-4.27098700	-0.86047800	-1.42973700	F	-2.93887700	1.04664600	-0.02181900
TS20				Na	-0.58667000	0.49941900	-1.51506300

H	3.58723700	-3.01583900	-1.84300700	F	-3.46633000	-1.12665800	2.24115900
C	-3.83528200	-1.76410100	-0.51151100	F	-3.16375400	0.82789200	1.33959200
F	-3.59794500	-2.98450800	-1.03274500	H	-4.43908600	-0.83398000	-0.18171200
F	-4.96602400	-1.85235700	0.22469600	TS2 3			
F	-4.08707900	-0.92417600	-1.54055400	N	2.32756000	1.99165500	1.28888600
25				O	2.71664500	2.39051800	-0.03830300
C	2.67523500	-1.88377900	-0.57213400	C	2.26913400	0.52131600	1.39451700
C	3.99961300	-1.40211200	-0.07662300	C	3.22293500	-0.24994900	0.47045400
C	3.85767500	-0.02585700	0.14279400	C	2.62126300	-0.84531100	-0.64378400
C	5.19186700	-2.06082800	0.16279500	C	4.57638300	-0.44506800	0.71297500
C	4.91294200	0.74195100	0.61302300	C	3.35482000	-1.62645300	-1.53846600
C	6.26911100	-1.29173000	0.63920600	C	5.32533800	-1.21997900	-0.18323300
C	6.13069500	0.08206300	0.85921800	C	4.72146500	-1.80602700	-1.30202900
H	4.81656700	1.80878700	0.78860400	H	2.88363500	-2.08688900	-2.40244000
H	7.22219600	-1.77121000	0.83970200	H	6.38677400	-1.37160500	-0.00611000
H	6.97825500	0.65146700	1.22779200	H	5.31411900	-2.40632900	-1.98601700
O	2.33711000	-3.00274600	-0.89044100	O	2.09431900	0.09767800	2.56343600
C	-0.21720800	2.80452800	-0.38572500	C	-1.85121600	-1.55021900	-0.71121300
C	0.35723700	4.04756200	-0.10144800	C	-1.32034900	-2.39927100	0.26748500
C	-1.59792900	2.67938300	-0.58759400	C	-3.23976900	-1.44282100	-0.86917100
C	-0.46753700	5.17653300	-0.02227600	C	-2.18842800	-3.12889100	1.08768500
H	1.42362500	4.15780000	0.05720500	H	-0.25057300	-2.48390800	0.41660600
C	-2.39900300	3.81610000	-0.50378200	C	-4.09317100	-2.17471200	-0.04590600
H	-2.03043700	1.69807200	-0.78172600	H	-3.62694800	-0.78558400	-1.64005100
C	-1.84294500	5.07018400	-0.22266100	C	-3.57318400	-3.02277300	0.94124700
H	-0.01914000	6.14124900	0.19902800	H	-1.76870700	-3.78350900	1.84650800
H	-3.47117100	3.71744100	-0.65286500	H	-5.16803600	-2.08655200	-0.17931200
H	-2.47606300	5.95032800	-0.15725900	H	-4.23890300	-3.59728900	1.57847100
C	2.45287500	0.28807400	-0.22262100	C	1.72613900	3.27532400	-0.55886200
N	1.78234100	-0.74654800	-0.62574400	H	2.04025000	3.48973700	-1.58679900
C	1.87425200	1.66062100	-0.13809500	H	0.72735000	2.82328800	-0.56305000
H	2.45186800	2.31909100	-0.80611500	H	1.69540800	4.21698200	0.00877200
H	2.01442000	2.03910200	0.88603500	C	1.17935600	-0.52250400	-0.66451800
O	0.50677200	1.62957100	-0.49154100	N	0.84051600	0.23128800	0.30375100
H	5.29086600	-3.12783700	-0.00986700	C	0.27030100	-1.07545300	-1.73553700
O	-2.66453500	-0.35816400	-1.17827900	H	0.43052200	-2.15956500	-1.82092400
Na	-0.50868300	-0.74885200	-1.29026500	H	0.55735700	-0.62835500	-2.69347800
C	-3.33390300	-0.98163400	-0.19243600	O	-1.10263900	-0.77678300	-1.56299900
C	-3.16433500	-2.51670800	-0.27808700	H	-0.12569000	0.62733200	0.49848000
F	-1.85057600	-2.88425900	-0.16789900	H	3.10960300	2.27763900	1.88283400
F	-3.83930300	-3.20925800	0.66700100	H	5.04773100	0.00012800	1.58538700
F	-3.58884300	-2.96371500	-1.47802700	C	-2.21089300	1.85045800	0.15072600
C	-2.88078500	-0.48483700	1.20181100	O	-1.69652400	2.43030500	-0.86964500
F	-1.53393700	-0.61660900	1.37086200	Na	-3.70829700	2.36969200	-1.89264200

O	-3.51327900	1.74116600	0.26857100	Na	-0.97704800	-1.88787800	-0.55093900
O	-1.46419000	1.33648000	1.08900200	O	0.15424700	-3.08857900	1.08995700
Na	-3.21950500	0.34057700	2.04518100	O	2.35387800	-3.11992300	0.52205300
28				TS24			
N	2.60329700	-0.43766000	0.95762900	N	2.49203400	-0.58705000	0.97330600
O	2.11667000	0.32019000	2.08078800	O	2.06343100	0.08711700	2.15712300
C	2.12257400	0.16230300	-0.36480200	C	2.13642200	0.08649800	-0.41924300
C	2.27843700	1.69303300	-0.32911500	C	2.38257000	1.59286200	-0.28521900
C	1.01307100	2.27643400	-0.25536100	C	1.14740500	2.24296100	-0.27706200
C	3.41747500	2.48141300	-0.37545600	C	3.56554300	2.30982900	-0.21147000
C	0.84312200	3.65937900	-0.21697000	C	1.05236600	3.63016600	-0.18218400
C	3.26420800	3.87619500	-0.33793500	C	3.48581800	3.70792300	-0.11486700
C	1.99269900	4.45926200	-0.25687300	C	2.24547900	4.35957400	-0.09786500
H	-0.14306400	4.11238600	-0.15751900	H	0.09198600	4.13812000	-0.17327900
H	4.14274300	4.51515800	-0.37439600	H	4.39794700	4.29540500	-0.05521900
H	1.89775400	5.54112000	-0.22888700	H	2.20923600	5.44253800	-0.02295400
O	2.72253800	-0.45846700	-1.35607800	O	2.78655200	-0.56582000	-1.33627300
C	-3.51520900	0.24929800	-0.16192300	C	-3.44347000	0.37142900	-0.29534400
C	-4.33053800	0.14649000	-1.28856900	C	-4.36746800	0.46146500	-1.33543500
C	-4.05873900	0.40267200	1.11502300	C	-3.85381900	0.32414100	1.03861000
C	-5.71846100	0.19410000	-1.13133700	C	-5.73121000	0.50240800	-1.03134600
H	-3.87257000	0.02935300	-2.26624100	H	-4.01223100	0.49450200	-2.36092700
C	-5.44651000	0.45583600	1.26075300	C	-5.21819100	0.37183900	1.33205600
H	-3.39735000	0.47018300	1.97387200	H	-3.10818600	0.24435300	1.82464100
C	-6.27722900	0.35160200	0.14020700	C	-6.15745600	0.46086500	0.29931900
H	-6.36070000	0.11079900	-2.00343900	H	-6.45847400	0.56916700	-1.83544700
H	-5.87800300	0.57173600	2.25087100	H	-5.54657200	0.33271600	2.36674800
H	-7.35614800	0.38948000	0.25882900	H	-7.21793700	0.49412300	0.53135700
C	1.43124300	-0.55645200	2.97108800	C	0.78757800	-0.37971800	2.63271000
H	0.96386300	0.08997500	3.72090100	H	0.79709900	-0.17792000	3.70730500
H	0.67365700	-1.14502900	2.44443400	H	-0.03370700	0.17286400	2.16412100
H	2.12977800	-1.24310800	3.47223800	H	0.64869700	-1.44656500	2.43749100
C	0.05308100	1.14982000	-0.26593600	C	0.13079900	1.17417300	-0.40127200
N	0.59781800	-0.01127300	-0.32859700	N	0.61766300	-0.01350100	-0.47606100
C	-1.42898300	1.38578500	-0.22816500	C	-1.33850100	1.47241600	-0.40197900
H	-1.72409200	2.04614400	-1.05679400	H	-1.57733700	2.20333400	-1.18762900
H	-1.68648500	1.90171800	0.70775300	H	-1.60239700	1.93139600	0.56184400
O	-2.13609900	0.14552300	-0.32140200	O	-2.08850500	0.27226400	-0.60224000
H	2.41979800	-2.19452900	0.92247800	H	2.25048400	-1.79134900	0.92858200
H	3.61205900	-0.26320500	0.95518400	H	3.51140100	-0.51154500	1.01996500
Na	2.77829500	-2.60796400	-1.77596100	Na	2.77121400	-2.78084700	-1.57961800
H	4.40628800	2.03354700	-0.44056600	H	4.52939400	1.80732900	-0.22909000
C	1.01332000	-3.31308000	0.20406000	C	0.87464300	-3.26483400	0.27855200
O	0.79246200	-3.65043000	-0.99758900	O	0.67916300	-3.56367200	-0.95977600

Na	-1.02777100	-1.88066900	-0.65683300	C	-3.45207100	0.52321000	-0.47365600
O	-0.08014900	-3.08740300	1.10029800	C	-4.59632600	-1.54764400	0.03867000
O	2.13748000	-3.05022400	0.67524000	C	-4.58366900	1.28535800	-0.17942500
29				C	-5.73943800	-0.79191400	0.33783300
C	-2.32426900	-0.19427800	-0.59664600	C	-5.73357100	0.60609100	0.23276400
C	-2.65182900	-1.58165700	-0.15532000	H	-4.58124400	2.36713100	-0.27099700
C	-1.42484100	-2.20714500	0.09838900	H	-6.64677300	-1.29737400	0.65538300
C	-3.85701100	-2.23553500	0.02503100	H	-6.63302600	1.16620200	0.46815000
C	-1.36244600	-3.51822900	0.54439600	O	-2.01269300	-2.42292400	-1.56608900
C	-3.80599200	-3.56747600	0.47627400	C	0.48284900	2.49652500	-0.06327600
C	-2.58299300	-4.19431200	0.73052900	C	0.02524000	2.06134100	1.18441900
H	-0.41886600	-4.01467400	0.74806900	C	1.80002500	2.94335800	-0.21869700
H	-4.72978000	-4.11625700	0.63059700	C	0.90376400	2.07773700	2.27461300
H	-2.57252100	-5.22216600	1.07952600	H	-0.97892500	1.67895100	1.32230200
O	-3.09732900	0.69763900	-0.89050000	C	2.66534700	2.94002700	0.87137300
C	3.17922600	-0.36973100	-0.21228800	H	2.13060000	3.25694200	-1.20247700
C	3.98547200	-1.09283000	-1.09176400	C	2.22143600	2.51031400	2.12738800
C	3.71875500	0.30382800	0.88325500	H	0.54643300	1.73852300	3.24232200
C	5.36313700	-1.13844200	-0.86556400	H	3.69100800	3.27083000	0.73755300
H	3.53506800	-1.60000200	-1.93986300	H	2.89682400	2.50905700	2.97742500
C	5.09901700	0.25705700	1.09620800	C	-0.61593200	-1.09500900	2.73058200
H	3.05960200	0.85310800	1.54891800	H	-0.96795400	-0.41585300	3.50932800
C	5.92086000	-0.46445900	0.22562600	H	-0.66750600	-2.12924500	3.09369100
H	6.00021900	-1.69620000	-1.54588100	H	0.41106900	-0.84779300	2.45232400
H	5.52895600	0.78303300	1.94373100	C	-2.12414500	0.94005000	-0.93068500
H	6.99305100	-0.49962500	0.39494000	N	-1.37968300	-0.08320600	-1.16240400
C	-0.39512400	-1.17995900	-0.20656600	C	-1.67729800	2.36549100	-1.09911800
N	-0.88952900	-0.04781600	-0.60818400	H	-2.07883100	2.97356300	-0.27868100
C	1.06650800	-1.41857500	-0.03704600	H	-2.10792900	2.74733700	-2.03185900
H	1.35801700	-2.30709600	-0.61646600	O	-0.27696900	2.50113000	-1.21712500
H	1.25982500	-1.64767700	1.02276600	H	-0.35518300	-0.12254900	-1.32166000
O	1.80610900	-0.27465200	-0.44627700	H	-0.12383600	-1.63406700	0.17945700
Na	-3.18536000	3.10964000	-0.67325400	H	-1.45731900	-2.72815500	0.82950800
H	-4.80318100	-1.74157000	-0.17260300	O	0.92212800	-1.28131500	-0.66046600
C	-1.02350400	3.28979900	0.70721800	C	2.07125000	-0.71282700	-0.19462400
O	-0.95984400	3.48121800	-0.60196600	H	1.93885000	0.13856600	0.49741700
Na	0.68975900	1.92275000	-0.61366900	C	2.91280900	-1.73178000	0.58861200
O	0.03459500	2.89150500	1.32955800	F	2.20904600	-2.16044100	1.66806600
O	-2.15376600	3.46169300	1.30785100	F	4.06892400	-1.20259900	1.05359700
TS27				F	3.22690500	-2.82461600	-0.13272900
N	-1.21473000	-1.76724400	0.56059100	C	2.86994500	-0.15124100	-1.38304100
O	-1.51965500	-0.89231300	1.63518100	F	2.08468300	0.67110200	-2.11607200
C	-2.11194900	-1.46594200	-0.77323700	F	3.94830800	0.56679300	-0.99026700
C	-3.45333200	-0.87286600	-0.35346800	F	3.31283200	-1.11762400	-2.21537100

H	-4.60373900	-2.63076200	0.11432000	C	0.24934400	1.96082500	1.69744500
32				C	0.38662200	2.74795600	0.44518700
C	-1.76029400	-0.72198500	1.29960200	C	0.65020800	1.84787800	-0.60452700
C	-3.06621900	-0.70822100	0.57190300	C	0.30100900	4.11026900	0.22735200
C	-2.85653800	0.03512300	-0.59637900	C	0.83364800	2.29183600	-1.91011800
C	-4.29707700	-1.26116700	0.87435100	C	0.47593100	4.56438000	-1.09260300
C	-3.88027500	0.25104100	-1.50748800	C	0.73532900	3.67224400	-2.13956100
C	-5.34203500	-1.05083700	-0.04395100	H	1.03983900	1.60442100	-2.72385200
C	-5.13602800	-0.30958500	-1.21138100	H	0.40825100	5.62679000	-1.30337500
H	-3.73240200	0.82673900	-2.41577300	H	0.86480700	4.05474800	-3.14661600
H	-6.32358700	-1.46932500	0.15631900	O	-0.00985800	2.29220500	2.82763500
H	-5.96017200	-0.16224900	-1.90252600	C	2.91549500	-1.62343500	-0.01230800
O	-1.48283600	-1.24100700	2.35674800	C	3.60966400	-0.58826800	-0.64697900
C	0.72391800	2.68047600	-0.39008700	C	3.61618900	-2.64486700	0.64377100
C	-0.30650200	3.43482500	0.17907200	C	5.00955400	-0.58190400	-0.61310700
C	2.05953600	2.93969100	-0.05679800	H	3.08903600	0.20943700	-1.16344000
C	0.01392200	4.46280000	1.07363700	C	5.00776400	-2.62420400	0.66918300
H	-1.34737200	3.23470800	-0.04917300	H	3.05116200	-3.43594100	1.12675200
C	2.36176500	3.96548200	0.83403500	C	5.71453500	-1.59163600	0.04003000
H	2.82881100	2.31097500	-0.49035700	H	5.54317700	0.22579300	-1.10639300
C	1.34092800	4.73709800	1.40330200	H	5.54286800	-3.41786700	1.18326600
H	-0.79011900	5.04611300	1.51424000	H	6.80009400	-1.57778400	0.06103500
H	3.39982900	4.15991000	1.09015600	C	0.70130500	0.51451200	-0.02790900
H	1.57939400	5.53534200	2.10002000	N	0.50379500	0.60376500	1.28754500
C	-1.43229900	0.45172100	-0.54931800	C	0.75778900	-0.78984600	-0.66699600
N	-0.81071400	0.03242200	0.50758100	H	0.98267200	-0.75086600	-1.73555000
C	-0.76181900	1.25013100	-1.62709700	H	-0.31248300	-1.19102400	-0.41787300
H	-1.40381000	2.09116000	-1.92421700	O	1.54307700	-1.73716200	0.03994800
H	-0.65940500	0.60334800	-2.50610000	C	-2.55192400	-1.44954700	0.61322800
O	0.54423000	1.66176100	-1.29795000	H	-3.22174000	-1.85529300	1.40207300
C	2.41335400	-1.31849000	0.34833600	C	-2.81167900	0.07101300	0.63618000
H	3.46422600	-1.43262100	0.63222300	F	-2.37456200	0.59268000	1.80710200
C	1.71195500	-2.61886100	0.77825500	F	-4.11123500	0.41293000	0.50856600
F	1.74963800	-2.73582700	2.11665100	F	-2.13102300	0.71412700	-0.35238100
F	2.31215100	-3.70560400	0.24947500	C	-3.08095500	-2.05966700	-0.70100400
F	0.41486100	-2.64750800	0.40065000	F	-2.92504400	-3.39890000	-0.68207200
C	2.40360700	-1.14559500	-1.18008200	F	-4.39534300	-1.81245400	-0.91815000
F	3.03298900	-0.00708100	-1.52152600	F	-2.40493600	-1.59289900	-1.77951900
F	3.03935100	-2.16465100	-1.79616800	H	0.10294800	4.79951800	1.04138200
F	1.14878700	-1.09350200	-1.67963300	O	-1.24561600	-1.74327400	0.79998200
H	-4.44961900	-1.83394000	1.78376000	H	0.24231500	-0.21702900	1.83376600
O	1.90242100	-0.20964100	1.00971800	33			
H	0.93931500	-0.08035500	0.78571600	C	-1.80987500	2.17494500	-1.59450800
TS28				C	-3.13861200	2.50097600	-2.16655100

C	-4.07878500	1.58149800	-1.66574700	C	6.05077300	-1.89235800	-2.50334600
C	-3.50099600	3.51213200	-3.05159700	C	6.23488600	-0.52586400	-2.29212500
C	-5.41848200	1.66501000	-2.04939700	H	5.29490700	1.33223900	-1.81160700
C	-4.84082900	3.59496300	-3.43577400	H	6.89594400	-2.53446300	-2.73295000
C	-5.78449100	2.67984500	-2.93746800	H	7.22374800	-0.08244100	-2.36000500
H	-6.16024000	0.96753900	-1.67183100	O	2.36601200	-3.59496100	-1.61922000
H	-5.16064000	4.37159300	-4.12411900	C	1.82818500	3.04996400	1.16915300
H	-6.82177300	2.76374700	-3.24897500	C	2.93364800	3.37938700	1.95232600
O	-0.72456600	2.73496800	-1.77900200	C	0.59578900	3.68632400	1.34197300
C	-3.26110800	-2.41824100	1.00068900	C	2.79024100	4.36918700	2.93190000
C	-3.84251500	-3.25906300	0.04853300	H	3.88546700	2.87710200	1.82135300
C	-2.86197100	-2.90399300	2.24864000	C	0.46956700	4.66339300	2.32600000
C	-4.02763500	-4.60822400	0.36197100	H	-0.22759900	3.40875600	0.69197200
H	-4.12382100	-2.87131800	-0.92508300	C	1.56591000	5.00932000	3.12549800
C	-3.04353500	-4.25585400	2.54132900	H	3.64650400	4.63093400	3.54699000
H	-2.42577600	-2.22237300	2.97139200	H	-0.48620000	5.16073600	2.46491600
C	-3.62904700	-5.11142300	1.60267500	H	1.46468300	5.77343500	3.89041500
H	-4.47630900	-5.26709200	-0.37580900	C	-0.60934800	-2.58504300	-1.44029600
H	-2.73283100	-4.63742200	3.50957000	H	-1.46683200	-3.24786500	-1.57371200
H	-3.77093600	-6.16227300	1.83593300	H	0.03047200	-2.96127700	-0.63747500
C	-3.35920700	0.66227800	-0.77984300	H	-0.95353500	-1.57355600	-1.20555600
N	-2.02310200	1.08558900	-0.78045500	C	2.75748100	0.71319800	-1.53015100
C	-3.83015600	-0.39034000	-0.08945400	N	1.67002000	0.81115100	-2.18865300
H	-1.27777900	0.63830400	-0.24685800	C	3.08000100	1.56456400	-0.30071000
H	-4.86981000	-0.69864000	-0.12274900	H	3.73823500	2.40053600	-0.56745100
O	-2.99714100	-1.08111500	0.75031300	H	3.58430500	0.95227100	0.45330000
C	0.16436300	-0.78262000	1.66217000	O	1.84250300	2.06270300	0.19746300
H	-0.55324000	-1.59292000	1.52788600	H	1.02710800	1.51883600	-1.80915400
C	1.51595100	-1.41640900	2.00988900	H	1.18643000	-0.86571300	-2.77428600
F	1.85962900	-2.30500700	1.06230000	H	4.62076200	-3.49852300	-2.54544100
F	1.48097100	-2.04751000	3.19505800	O	0.26052300	-0.09459200	0.44994100
F	2.49071900	-0.47829800	2.06243800	H	0.86651500	0.68361200	0.51873700
H	-2.75729300	4.20963500	-3.42522600	TS25			
C	-0.37238100	0.12151500	2.78210000	C	-3.15125500	0.21325900	1.69199900
F	0.54594700	1.02756200	3.17603600	C	-3.73496400	-0.47444100	0.48854500
F	-1.45160800	0.79508400	2.35081000	C	-2.73959400	-0.46121600	-0.49394700
F	-0.73186300	-0.60550800	3.85951000	C	-4.97393600	-1.05073200	0.26267100
N	1.27128900	-1.88598100	-2.65587300	C	-2.95220300	-1.03077700	-1.74342000
O	0.08726600	-2.61324800	-2.69899600	C	-5.19889800	-1.63227900	-0.99602600
C	2.35988300	-2.44745700	-2.06858300	C	-4.20322100	-1.62310000	-1.98071900
C	3.64554100	-1.63965100	-2.13713500	H	-2.18572000	-1.02775400	-2.51251500
C	3.83276300	-0.25300800	-1.91218300	H	-6.15730100	-2.09602700	-1.21096600
C	4.77220000	-2.43332400	-2.41067000	H	-4.40215000	-2.08135000	-2.94509400
C	5.13698300	0.27176300	-1.98241700	O	-3.69979100	0.37713100	2.77417000

C	0.61979000	2.57952900	-0.30952200	C	1.80692500	2.91130500	-1.18720800
C	-0.34361300	3.14160500	-1.15174200	C	1.62898300	2.68444700	1.58932100
C	1.71290600	3.33715000	0.13043700	H	-0.47713400	2.30480400	1.27015100
C	-0.20470600	4.47682200	-1.54636200	C	2.94709300	3.05793900	-0.39787500
H	-1.19018100	2.55471400	-1.49018500	H	1.85283200	2.98449300	-2.26926400
C	1.83415500	4.66653300	-0.26731400	C	2.86649200	2.94279800	0.99534600
H	2.45374400	2.85759600	0.76347800	H	1.55376700	2.58101000	2.66816100
C	0.87598900	5.24451400	-1.10932500	H	3.90324600	3.25463300	-0.87480200
H	-0.95471300	4.91460200	-2.19968000	H	3.75765800	3.04732900	1.60666100
H	2.68385100	5.25115300	0.07492500	C	-2.18664400	0.96790300	-0.68059700
H	0.97419400	6.28006400	-1.42139200	N	-1.43891400	-0.19913000	-0.84017200
C	-1.59364000	0.25781600	0.11944600	C	-1.75027200	2.22086600	-0.91179900
N	-1.84749100	0.63097800	1.37605400	H	0.00058800	-0.47790100	-0.95619600
C	-0.29971600	0.34983600	-0.46235300	H	-2.36818100	3.09929700	-0.75085500
H	-0.21511100	0.31358800	-1.54856200	O	-0.49157300	2.47245700	-1.43490400
H	0.24760500	-0.73817000	0.08811800	O	0.97372500	-0.94757800	-1.05523700
O	0.57862600	1.28541600	0.15086900	C	1.89644000	-0.55261800	-0.09568900
O	0.80935400	-1.45519800	1.00314600	H	2.05422800	0.52889100	-0.05563900
C	2.05199200	-1.92437200	0.65173900	C	1.46125200	-0.98117000	1.31501100
H	2.50127000	-2.52292100	1.45926000	F	0.24349600	-0.48557400	1.59639600
C	1.94897900	-2.86496400	-0.56082500	F	2.31283100	-0.55658100	2.26519200
F	1.23051700	-3.95693100	-0.23303500	F	1.37193400	-2.33679800	1.42069700
F	3.15807000	-3.28573800	-0.99410700	Na	0.26259900	-3.15713500	-1.04736400
F	1.32751900	-2.26962700	-1.60251100	H	-4.66581500	-2.55740900	0.43997400
Na	0.37313300	0.35197800	2.47157800	C	3.24014800	-1.16950500	-0.48914100
H	-5.74023300	-1.05268900	1.03223600	F	3.65840000	-0.65474600	-1.65846000
C	3.06546500	-0.79252400	0.38088500	F	3.14187800	-2.51429900	-0.65115100
F	3.02172800	0.11597600	1.38980200	F	4.19607500	-0.94097500	0.43052700
F	4.33120400	-1.25719900	0.32387400	TS26			
F	2.82274500	-0.13271800	-0.76845000	C	2.86307800	-1.03400900	0.93632700
30				C	3.87820500	-0.19192300	0.23070000
C	-2.19740100	-1.26562600	-0.48657300	C	3.25245700	1.00510800	-0.14249000
C	-3.54971900	-0.78489600	-0.07981000	C	5.21355100	-0.44259800	-0.06769400
C	-3.54073600	0.61219900	-0.20093700	C	3.96263500	1.99277000	-0.82739100
C	-4.67728500	-1.47447600	0.35288600	C	5.92790100	0.54167900	-0.75746100
C	-4.67656500	1.35768000	0.11270000	C	5.30528000	1.74452900	-1.13160200
C	-5.81833000	-0.72977800	0.67027800	H	3.49591900	2.92891200	-1.12154700
C	-5.81437200	0.66932300	0.55030800	H	6.97260800	0.37996900	-1.00839100
H	-4.68844600	2.44049600	0.02452200	H	5.87817900	2.49676100	-1.66719400
H	-6.71746800	-1.23461600	1.01256800	O	3.04706000	-2.17125700	1.39020100
H	-6.71167000	1.22823500	0.80181900	C	-1.42485200	2.22598700	0.22334400
O	-1.82617900	-2.46655500	-0.49339100	C	-1.53894500	2.24177300	-1.16876300
C	0.57349400	2.64244900	-0.57989500	C	-2.47098300	2.66388700	1.03784600
C	0.47731700	2.53404400	0.81110300	C	-2.72695700	2.69857300	-1.74633200

H	-0.71851900	1.88839100	-1.78530700	H	1.90093600	2.86637600	-2.39298300
C	-3.65174200	3.11224300	0.44771100	C	3.02091100	3.13598900	0.82538500
H	-2.34945700	2.64550600	2.11666900	H	1.78268000	2.86090200	2.57032600
C	-3.78511200	3.13203800	-0.94510700	H	3.98278400	3.33684000	-1.09889200
H	-2.82201600	2.70616600	-2.82835700	H	3.92611300	3.32881000	1.39328000
H	-4.46847700	3.45052500	1.07897100	C	-2.18390100	0.97612700	-0.66633100
H	-4.70660000	3.48278600	-1.39989600	N	-1.53638700	-0.24120600	-0.91211600
C	1.86175200	0.90506100	0.34022900	C	-1.63005700	2.18581400	-0.84951700
N	1.68281900	-0.32687400	0.98237300	H	-0.49124600	-0.35888800	-1.02894600
C	0.92680800	1.86756300	0.22738700	H	-2.13626300	3.11325800	-0.59694600
H	0.48862500	-1.12692500	0.93819100	O	-0.38507500	2.29762800	-1.42784600
H	1.08662700	2.81408300	-0.27710600	O	1.03415600	-0.96008600	-1.10318200
O	-0.30111900	1.72215400	0.86276800	C	1.91678400	-0.62523200	-0.12704800
O	-0.47039100	-1.64136500	1.01342700	H	2.20031200	0.44209400	-0.09180900
C	-1.22131000	-1.34035800	-0.11446000	C	1.35105500	-0.92705100	1.27739600
H	-0.96289800	-0.37004400	-0.55922200	F	0.15666100	-0.31984200	1.44454000
C	-0.97658500	-2.38446100	-1.21005400	F	2.15060700	-0.52500700	2.28735900
F	0.32484900	-2.35319000	-1.56346100	F	1.12744900	-2.26509200	1.45389300
F	-1.71089100	-2.12986100	-2.31517000	Na	0.25973600	-3.05962000	-1.06675900
F	-1.26236100	-3.63429400	-0.80413300	H	-4.81525700	-2.48053400	0.36847700
Na	-0.40954300	-0.03292900	2.74608700	C	3.24821500	-1.37047100	-0.33154800
H	5.67814300	-1.37868800	0.22979700	F	3.82080300	-0.98286600	-1.48924700
C	-2.69668300	-1.24895300	0.28240900	F	3.07110500	-2.71933900	-0.41135600
F	-2.83163000	-0.37660700	1.31650700	F	4.14894700	-1.15249800	0.65415500
F	-3.19669200	-2.42872900	0.69140700	H ₂ CO ₃			
F	-3.46130700	-0.79696600	-0.72725500	O	0.69879100	-1.14910000	-0.00005500
31				O	0.55828200	1.12327700	-0.00011800
C	-2.31353100	-1.30837000	-0.54889700	C	0.05273100	-0.12753800	0.00012800
C	-3.61591500	-0.75136000	-0.10960400	H	1.52968600	1.05027900	0.00057300
C	-3.53139900	0.64997000	-0.17721200	O	-1.28675700	-0.11087600	-0.00000200
C	-4.77070000	-1.39650300	0.32217300	H	-1.60859200	0.80854000	0.00006000
C	-4.62087600	1.44146300	0.18574700	CpRhCO ₃			
C	-5.86084000	-0.60414000	0.69098400	C	1.78249700	0.02709300	1.25504500
C	-5.78260900	0.79694500	0.62203800	H	1.66990200	0.05006200	2.33160500
H	-4.57633400	2.52519200	0.13457900	Rh	0.07302800	-0.00028000	-0.04573500
H	-6.77907500	-1.07200100	1.03346400	C	1.87999200	-1.16262800	0.44543700
H	-6.64329100	1.39245300	0.91283600	H	1.83518700	-2.18103700	0.80675500
O	-1.96207400	-2.50025600	-0.58039700	C	1.94531500	-0.74877200	-0.90356800
C	0.70025000	2.61415300	-0.63232900	H	1.96440900	-1.39403100	-1.77216700
C	0.64916900	2.61691200	0.76289100	C	1.94478400	0.70660000	-0.93451200
C	1.89473100	2.88278500	-1.30775500	H	1.96329300	1.31439600	-1.82980800
C	1.81762700	2.87650700	1.48463500	C	1.88323100	1.17935000	0.39616300
H	-0.27661900	2.37636200	1.27229000	H	1.84059000	2.21265200	0.71257600
C	3.05219900	3.13927600	-0.57420900	C	-2.39606200	0.00012500	0.00966300

O	-1.61933400	-1.09767200	-0.00248100
O	-3.61100200	-0.00006500	0.02962000
O	-1.61943500	1.09773100	-0.00216900
Na ₂ CO ₃			
C	-0.00000100	0.57256400	0.00157800
O	-1.12882800	1.19432400	-0.00033100
O	0.00000400	-0.75582200	0.00511600
O	1.12882200	1.19432700	-0.00065700
Na	-2.23878000	-0.74991100	-0.00206300
Na	2.23878200	-0.74990800	-0.00180000
(CF ₃) ₂ CHONa			
O	0.00299800	1.18527600	1.18944200
C	-0.00103300	-0.11152100	0.84548000
H	-0.00371200	-0.84315100	1.68859200
C	-1.26694500	-0.47860200	0.03509500
F	-2.37309100	-0.23204300	0.76887000
F	-1.32850400	-1.77416700	-0.35371100
F	-1.37650900	0.27483100	-1.09938900
Na	0.01323000	2.66493000	-0.40005300
C	1.26270600	-0.48752800	0.03573500
F	2.37068900	-0.24041400	0.76634100
F	1.31907400	-1.78555000	-0.34529100
F	1.37343300	0.25874500	-1.10364300
NH ₂ OMe			
N	1.23462800	0.11553700	-0.00012100
O	0.01000700	-0.62104500	-0.00012200
C	-1.13143600	0.22933900	0.00005800
H	-2.00518900	-0.42928600	0.00119500
H	-1.15825900	0.86983300	0.89517800
H	-1.15939000	0.86832800	-0.89610200
H	1.19430800	0.73827600	-0.81493200
H	1.19469200	0.73641900	0.81614200