

Supporting Information

**Mechanism and Origins of Cobalt-Catalyzed Ligand-Controlled Regiodivergent C–H
Functionalization of Aldehydes with Enynes**

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1. Supplementary results for the cyclization in the presence of dppen

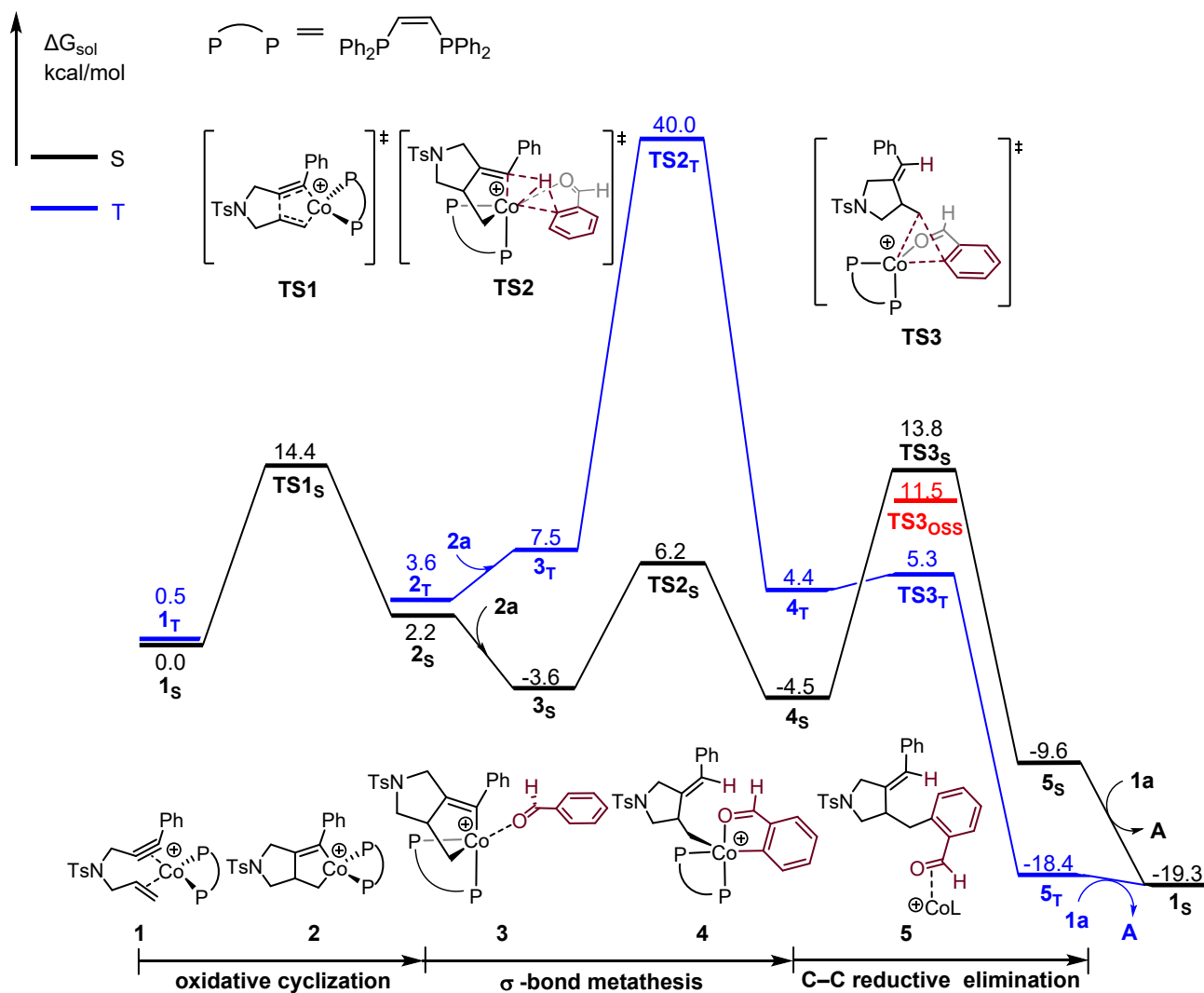


Figure S1. Free energy profiles of the cobalt-catalyzed cyclization of enynes with benzaldehydes forming the hydroarylate product **A** in the presence of dppen ligand.

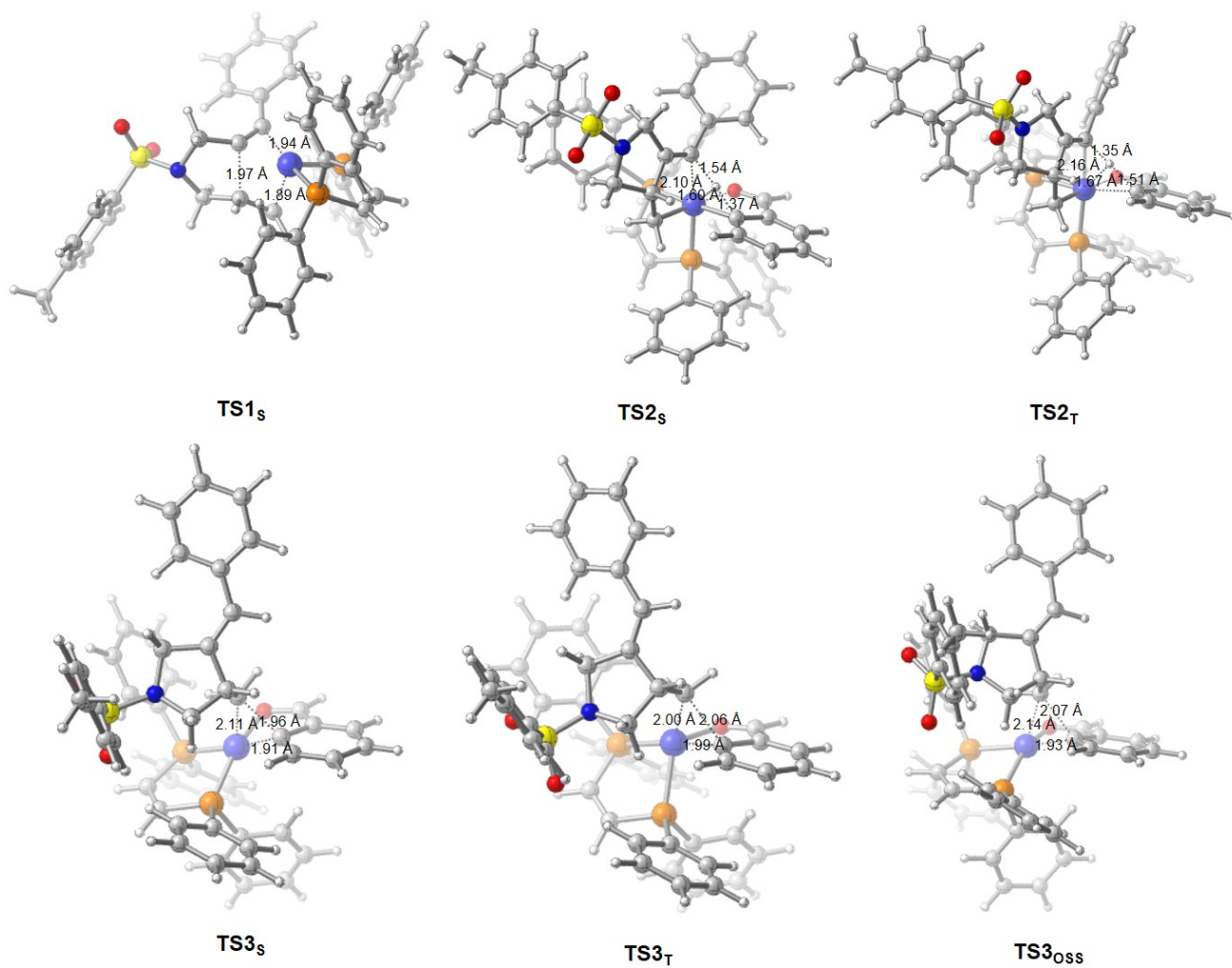


Figure S2. Optimized structures of the key transition states in Figure S1 with selected bond distances.

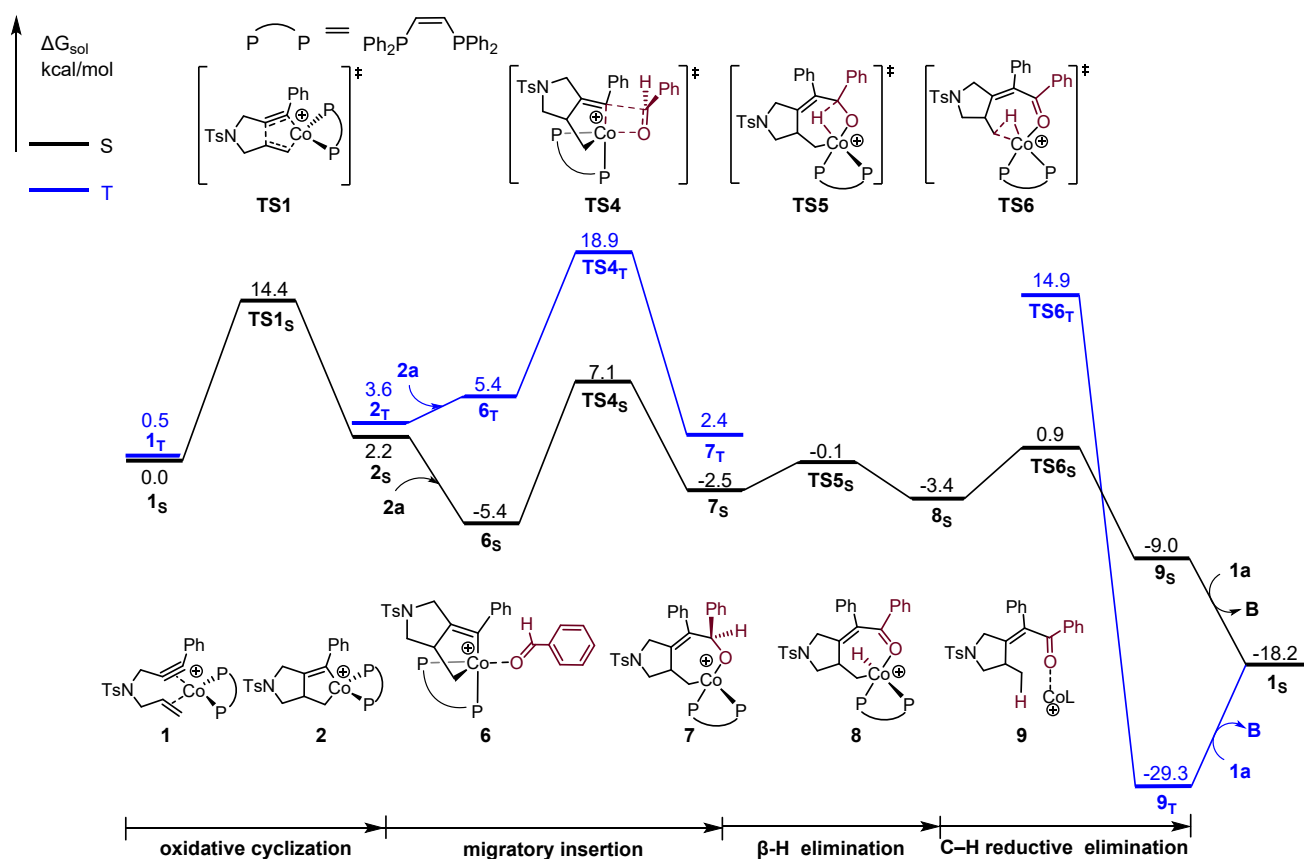


Figure S3. Free energy profiles of the cobalt-catalyzed cyclization of enynes with benzaldehydes forming the hydroacylative product **B** in the presence of dppen ligand.

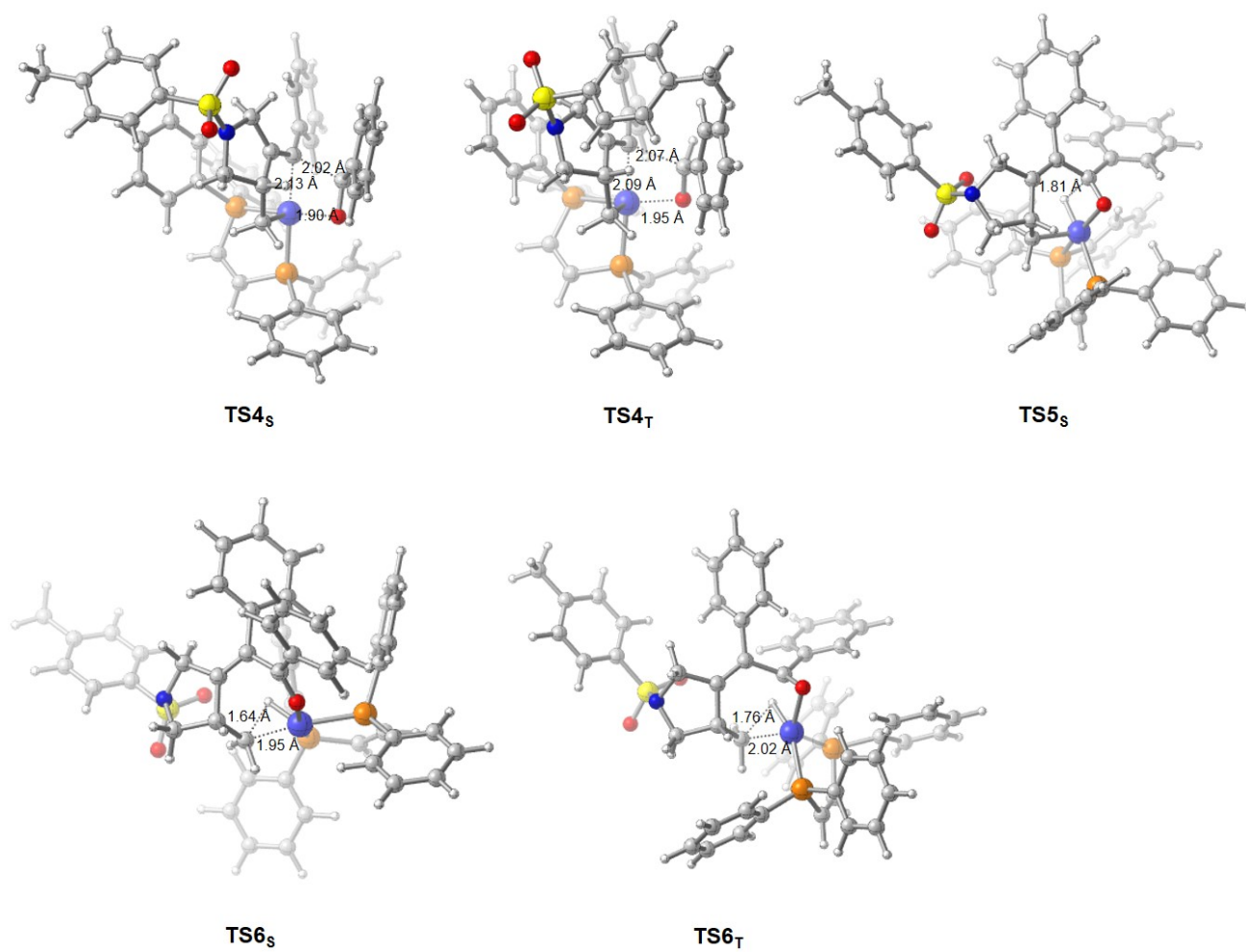


Figure S4. Optimized structures of the key transition states in Figure S3 with selected bond distances.

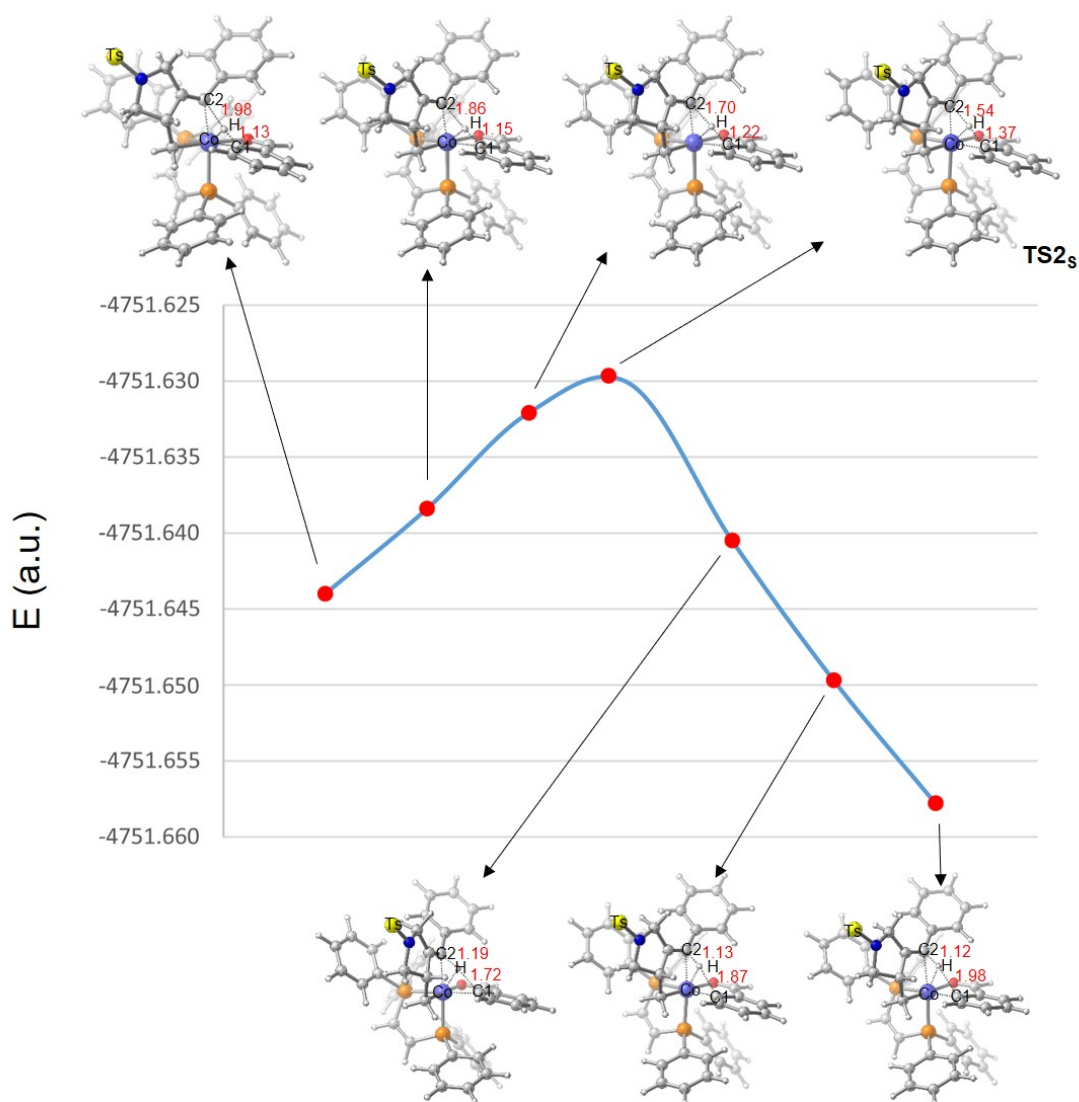


Figure S5. The geometry changes along the intrinsic reaction coordinate (IRC) of $TS2_s$, with selected bond distances in Å.

We carefully examined the geometry changes along the intrinsic reaction coordinate (IRC) of $TS2_s$. The results in Figure S5 reveal that the transition state $TS2_s$ indeed connects the corresponding reactant 3_s instead of 6_s .

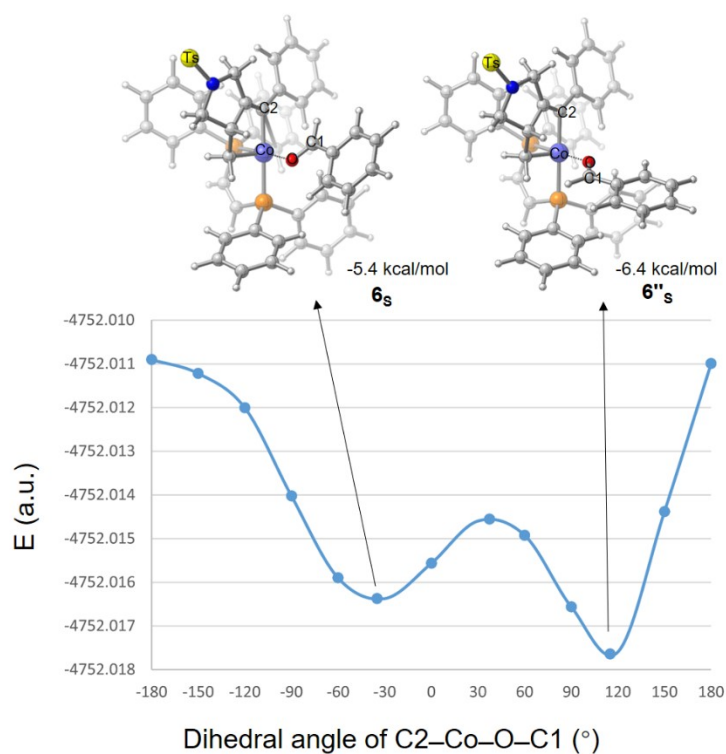


Figure S6. The relaxed potential energy surface scan along the C2-Co-O-C1 dihedral angle.

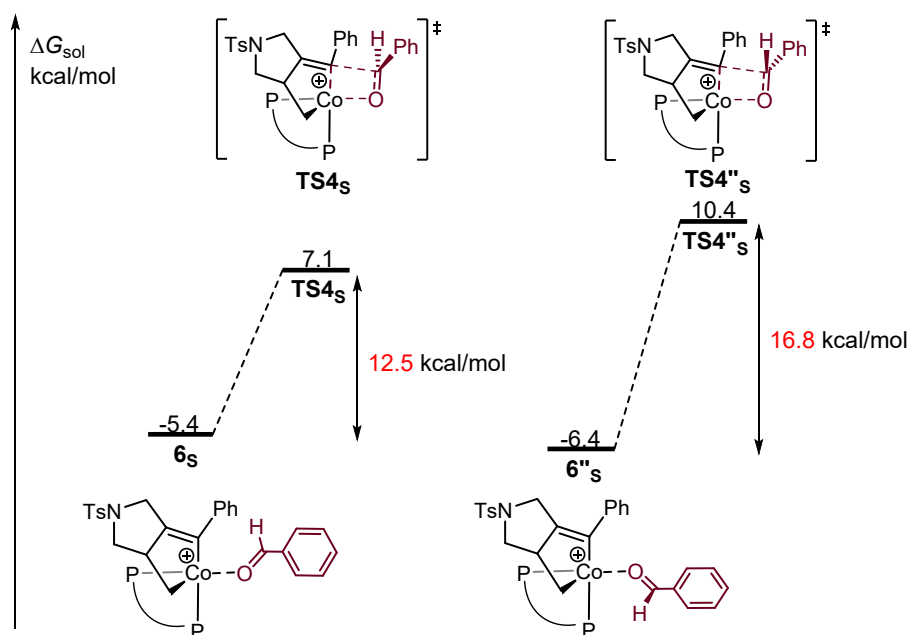


Figure S7. A comparison of the migratory insertion step from **6_s** or **6''_s** intermediate.

The relaxed potential energy surface in Figure S6 reveals that, in addition to **6_s**, there exists the other isomer **6''_s** with lower energy. We further calculated the migratory insertion of the C=O into the Co–C(sp²) from **6''_s**. However, as shown in Figure S7, the migratory insertion from **6''_s** is kinetically less favorable, with the corresponding activation barrier being 4.3 kcal/mol higher than that from **6_s**.

2. Supplementary results for the cyclization in the presence of dppp

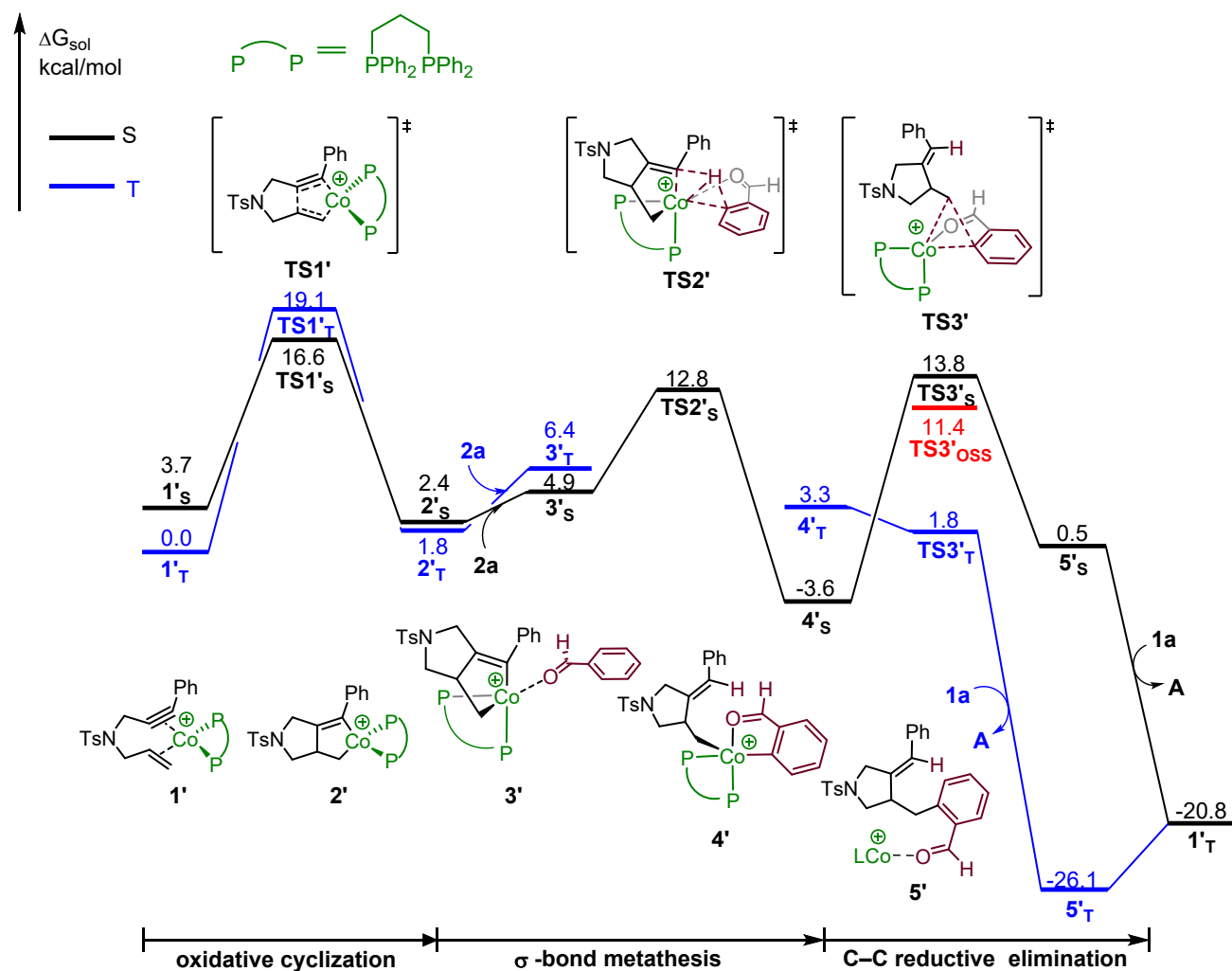


Figure S8. Free energy profiles of the cobalt-catalyzed cyclization of enynes with benzaldehydes forming the hydroarylate product **A** in the presence of dppp ligand.

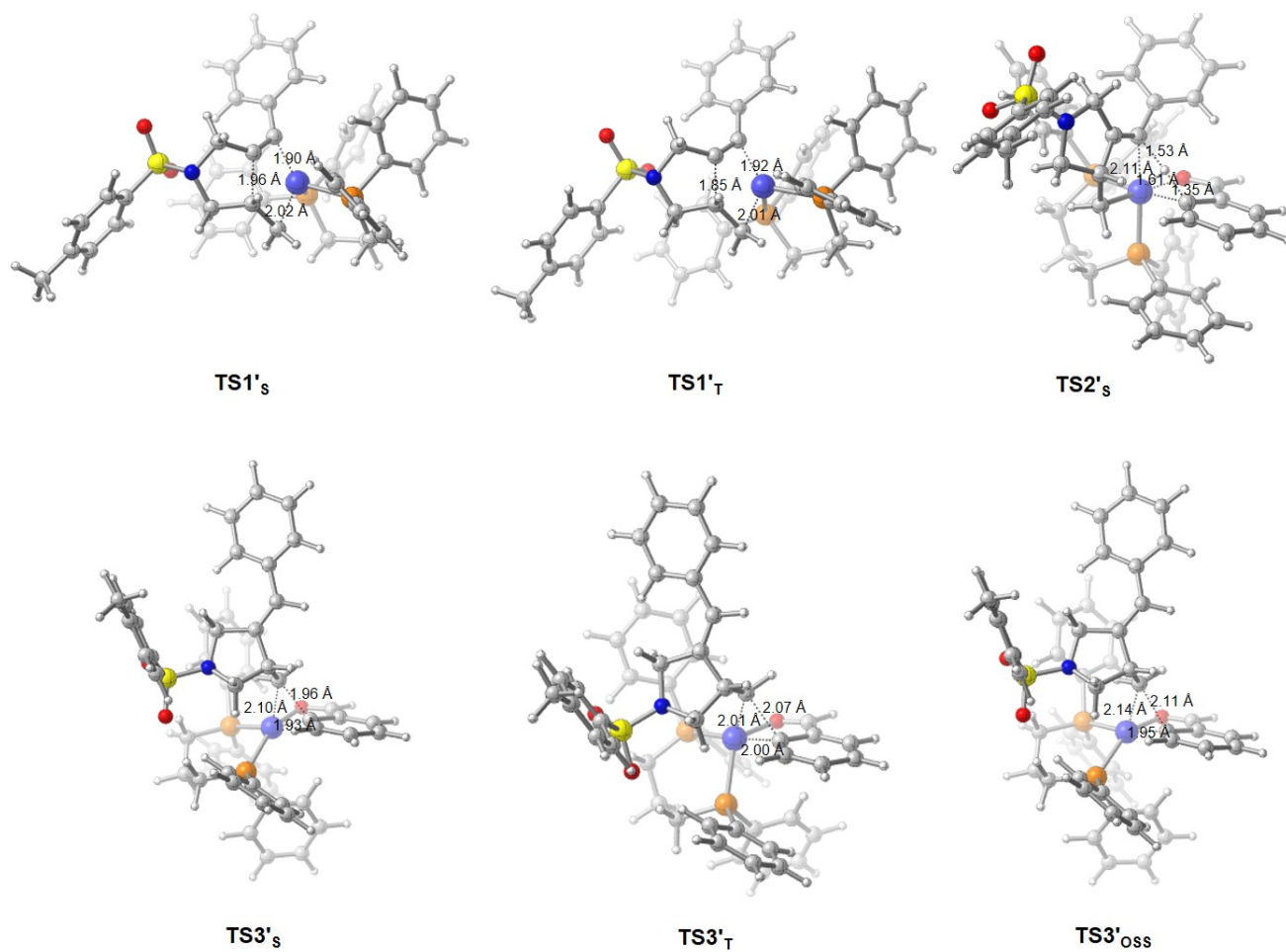


Figure S9. Optimized structures of the key transition states in Figure S8 with selected bond distances.

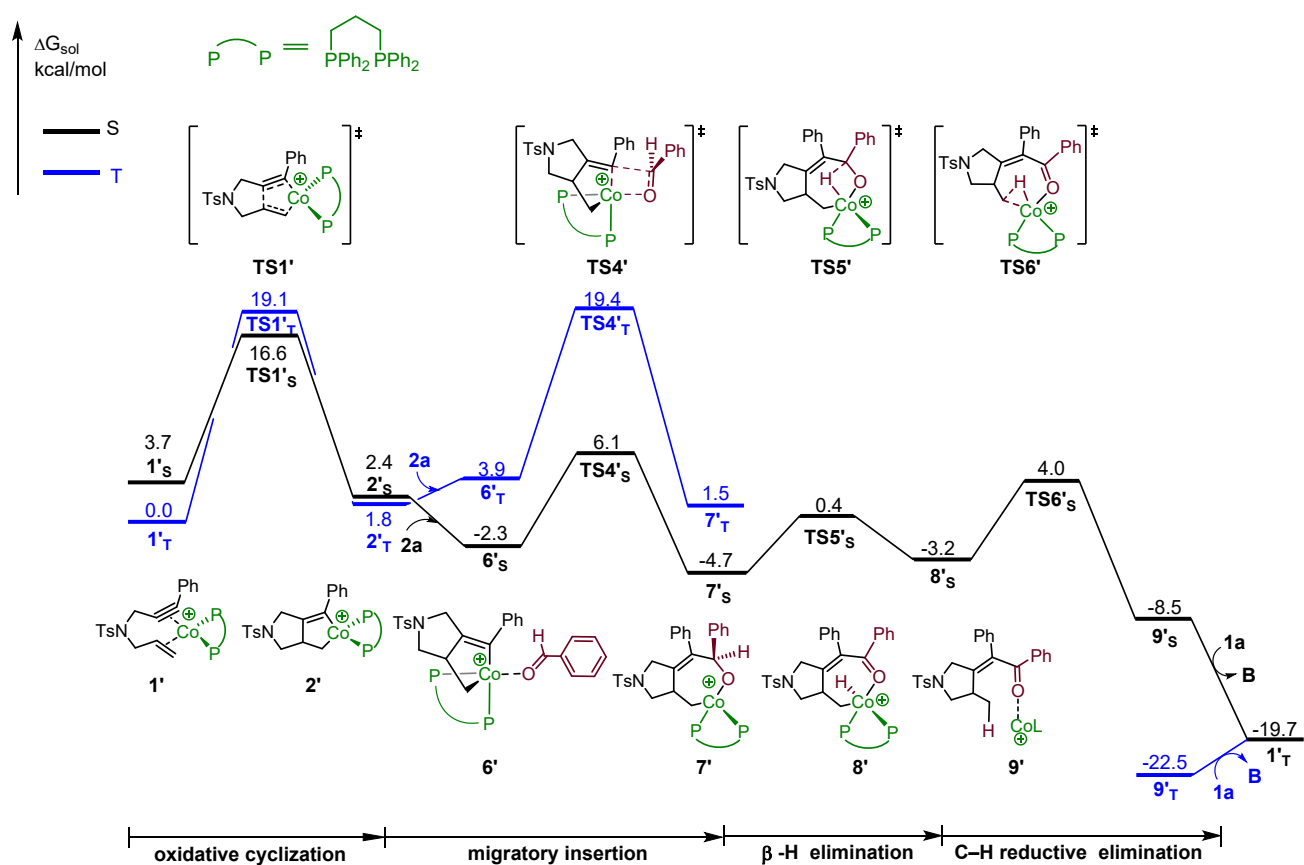


Figure S10. Free energy profiles of the cobalt-catalyzed cyclization of enynes with benzaldehydes forming the hydroacylative product **B** in the presence of dppp ligand.

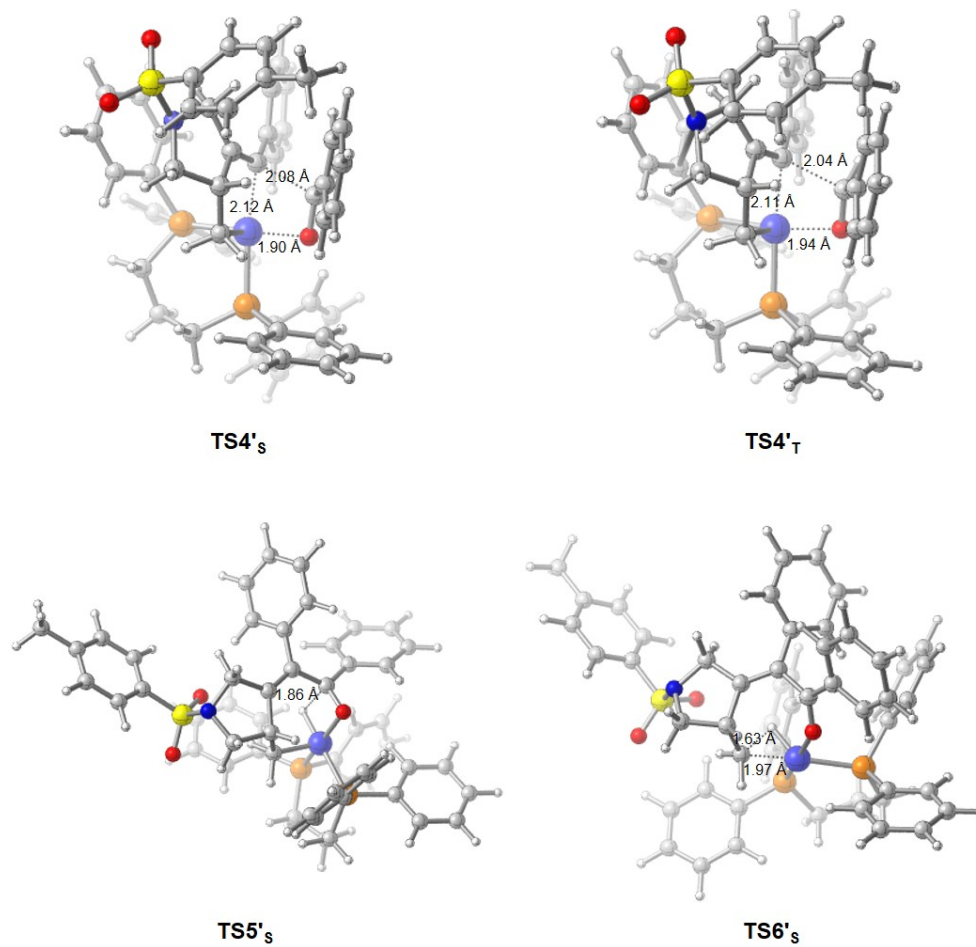


Figure S11. Optimized structures of the key transition states in Figure S10 with selected bond distances.

3. Detailed free energy profiles of the other potential reaction pathways

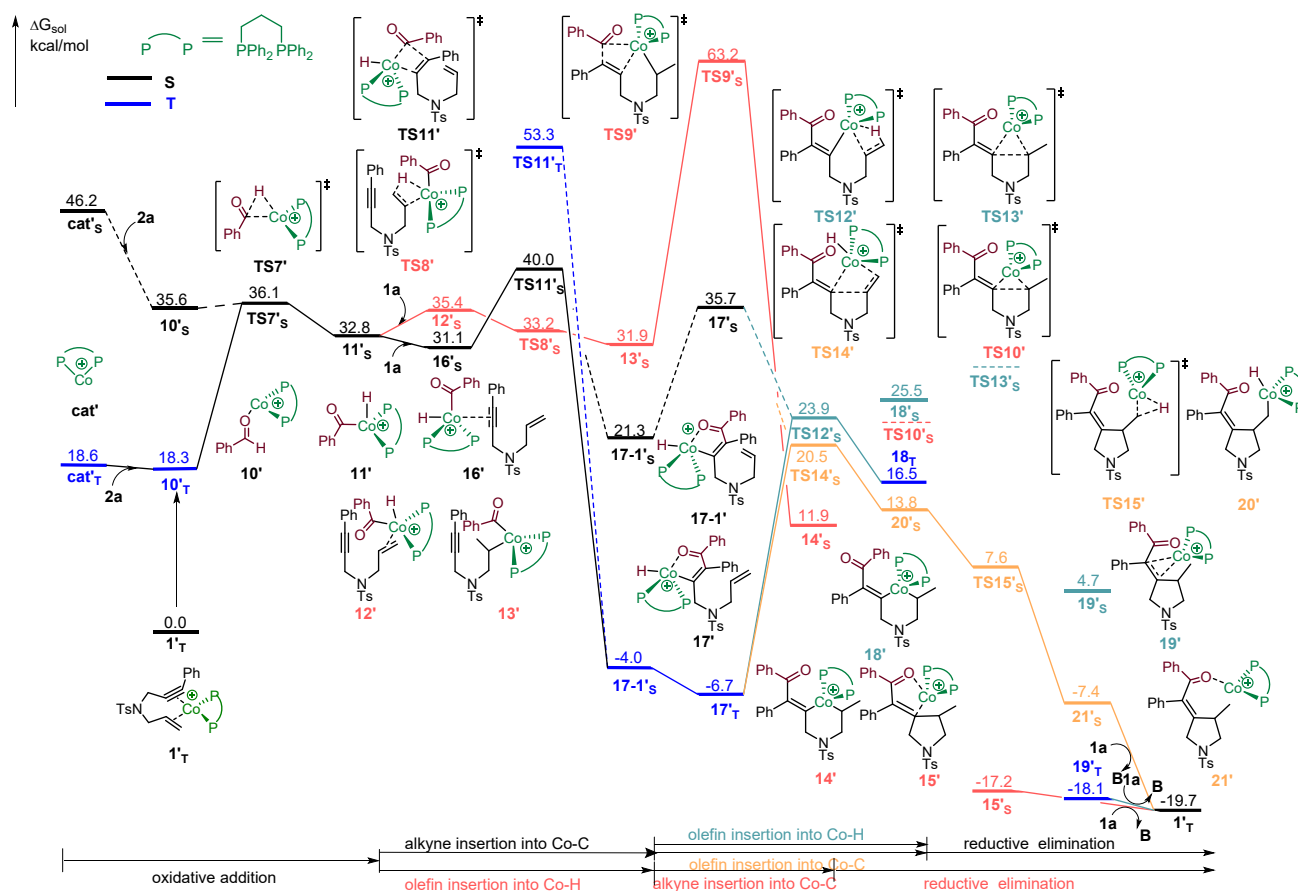
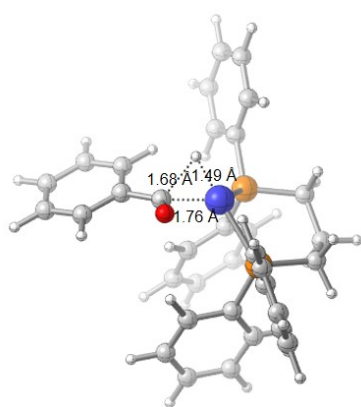
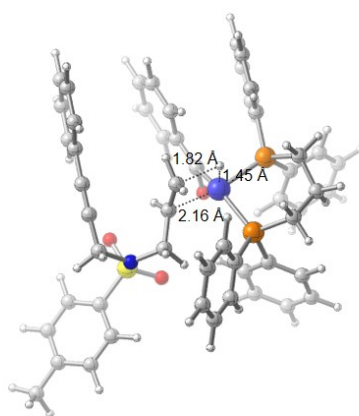


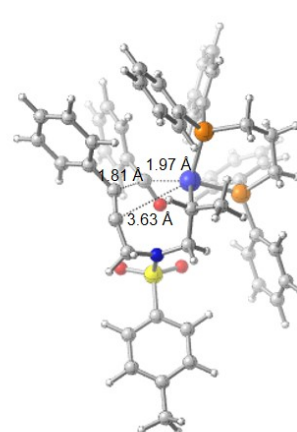
Figure S12. Free energy profiles of the other possible catalytic cycles for the formation of product **B** in the presence of dppp ligand.



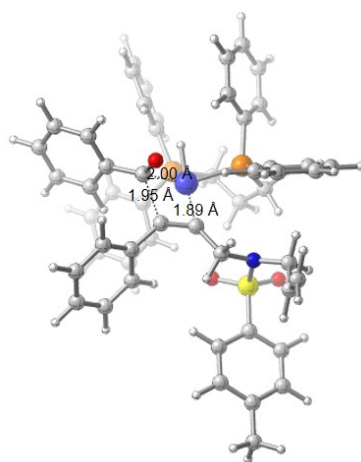
TS7'_s



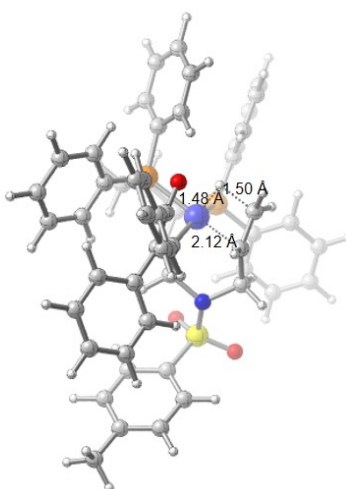
TS8'_s



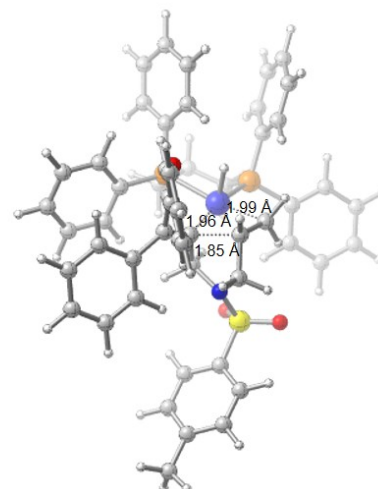
TS9'_s



TS11'_s



TS12'_s



TS14'_s

Figure S13. Optimized structures of the key transition states in Figure S12 with selected bond distances.

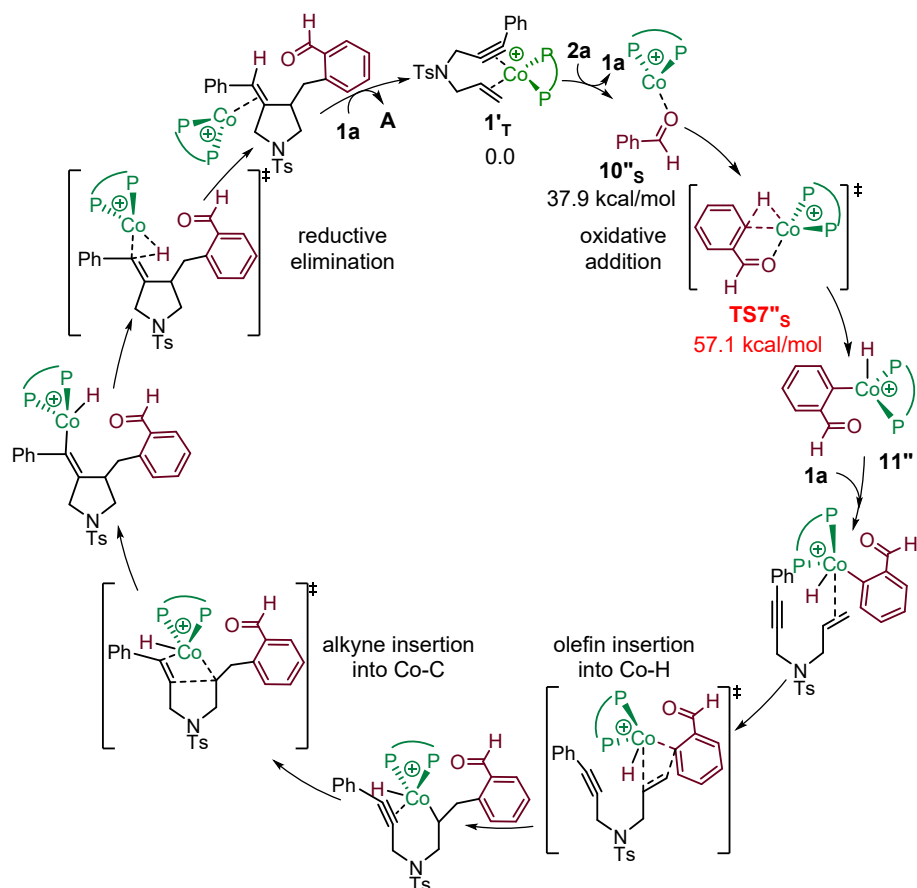


Figure S14. The other possible reaction pathway for formation of product **A** in the presence of dppp.

4. Results of the minimum energy crossing points (MECPs)

The minimum energy crossing points (MECPs) were searched at SMD(dichloromethane)/B3LYP-D3(BJ)/def2-SVP theoretical level via sobMECP, which is a modified version of Harvey's MECP program by Tian Lu.^[S1]

Table S1. Calculated energies of the MECPs

Low-spin state (energies in a.u.)	High-spin state (energies in a.u.)	MECPs (energies in a.u.)
4_S (-4752.0114547)	4_T (-4752.0025042)	MECP1 (-4751.99482122)
9_S (-4752.0341098)	9_T (-4752.0798349)	MECP2 (-4752.03406844)
1'_S (-4447.1393007)	1'_T (-4447.1528311)	MECP3 (-4447.13730083)
4'_S (-4792.5456003)	4'_T (-4792.5394016)	MECP4 (-4792.53056831)

[S1] (a) J. N. Harvey, M. Aschi, H. Schwarz, W. Koch, *Theor. Chem. Acc.* **1998**, 99, 95-99; (b) T. Lu, The sobMECP Program. Website: <http://sobereva.com/286>.

5. Influences of different DFT methods on the calculated results

Table S2. The Gibbs free energies of **TS2_s** and **TS4_s** calculated at different theoretical levels.

DFT methods	$G(\text{TS2}_s)$ (in a.u.)	$G(\text{TS4}_s)$ (in a.u.)	$\Delta G(\text{TS4}_s - \text{TS2}_s)$ (kcal/mol)
TPSSH-D3(BJ)	-4754.389934	-4754.388553	0.9
B3LYP-D3(BJ)	-4754.313119	-4754.317198	2.6
M06	-4752.069315	-4752.070829	-1.0
ω B97XD	-4753.166523	-4753.168531	-1.3
TPSS-D3(BJ)	-4754.721699	-4754.717997	2.3

6. Calculated energies and imaginary frequencies

Table S3. Calculated energies and imaginary frequencies in Sections 1 and 2.

Stationary point	Corrected thermal correction to Gibbs free energy at B3LYP-D3(BJ)/ def2-SVP (in a.u.)	Single-point energy including solvation energy at TPSSh- D3(BJ)/def2-TZVP (in a.u.)	Imaginary frequencies (in cm ⁻¹)
1a	0.281788	-1339.276017	
2a	0.07776	-345.7496885	
A	0.395068	-1685.120787	
B	0.392999	-1685.116922	
L=dppen			
cat_S	0.345911	-3070.004594	
cat_T	0.344167	-3070.055461	
1_S	0.666212	-4409.400527	
1_T	0.661416	-4409.394903	
TS1_S	0.663641	-4409.375006	280.76 <i>i</i>
2_S	0.669853	-4409.400686	
2_T	0.665535	-4409.394176	
3_S	0.773824	-4755.182543	
3_T	0.768712	-4755.159747	
TS2_S	0.770509	-4755.163662	1147.47 <i>i</i>
TS2_T	0.763492	-4755.102795	1433.27 <i>i</i>
4_S	0.772364	-4755.182534	
4_T	0.770508	-4755.166576	
TS3_S	0.772793	-4755.153846	454.85 <i>i</i>
TS3_T	0.771136	-4755.165722	257.56 <i>i</i>
TS3_{Oss}	0.770837	-4755.1555	418.63 <i>i</i>

5_S	0.77411	-4755.192504	
5_T	0.771918	-4755.204336	
6_S	0.77452	-4755.186147	
6''_S	0.774268	-4755.1874195	
6_T	0.771792	-4755.166232	
TS4_S	0.773856	-4755.165628	278.63 <i>i</i>
TS4''_S	0.776566	-4755.1630182	244.03 <i>i</i>
TS4_T	0.771758	-4755.144598	264.84 <i>i</i>
7_S	0.775828	-4755.182899	
7_T	0.773078	-4755.172324	
TS5_S	0.770884	-4755.174126	278.66 <i>i</i>
8_S	0.770691	-4755.179152	
TS6_S	0.769083	-4755.17064	803.27 <i>i</i>
TS6_T	0.765855	-4755.145159	752.08 <i>i</i>
9_S	0.774549	-4755.191979	
9_T	0.772629	-4755.222306	
L=dppp			
cat'_S	0.397968	-3110.588716	
cat'_T	0.394979	-3110.629664	
1'_S	0.71876	-4449.968229	
1'_T	0.711999	-4449.967327	
TS1'_S	0.718741	-4449.947693	235.87 <i>i</i>
TS1'_T	0.714669	-4449.939539	245.63 <i>i</i>
2'_S	0.722213	-4449.973777	
2'_T	0.716195	-4449.968592	
3'_S	0.82953	-4795.745693	
3'_T	0.82436	-4795.738185	

TS2'_S	0.824254	-4795.727886	979.37 <i>i</i>
4'_S	0.825862	-4795.755631	
4'_T	0.823478	-4795.742229	
TS3'_S	0.824814	-4795.726813	436.74 <i>i</i>
TS3'_T	0.821279	-4795.742439	263.01 <i>i</i>
TS3'_{OSS}	0.823932	-4795.729785	355.14 <i>i</i>
5'_S	0.830241	-4795.753455	
5'_T	0.82441	-4795.790101	
6'_S	0.827279	-4795.755058	
6'_T	0.821539	-4795.739363	
TS4'_S	0.827437	-4795.741703	271.15 <i>i</i>
TS4'_T	0.824222	-4795.717281	289.00 <i>i</i>
7'_S	0.829574	-4795.761088	
7'_T	0.821936	-4795.743532	
TS5'_S	0.824698	-4795.748126	194.82 <i>i</i>
8'_S	0.823855	-4795.753029	
TS6'_S	0.82156	-4795.739161	801.06 <i>i</i>
9'_S	0.823079	-4795.760684	
9'_T	0.821835	-4795.781664	

Table S4. Calculated energies and imaginary frequencies in Section 3.

Stationary point	Corrected thermal correction to Gibbs free energy at B3LYP-D3(BJ)/ def2-SVP (in a.u.)	Single-point energy including solvation energy at TPSSh- D3(BJ)/def2-TZVP (in a.u.)	Imaginary frequencies (in cm ⁻¹)
1a	0.281788	-1339.276017	
2a	0.07776	-345.7496885	
cat'_s	0.397968	-3110.588716	
cat'_T	0.394979	-3110.629664	
1'_T	0.711999	-4449.967327	
10'_s	0.503027	-3456.379382	
10'_T	0.500063	-3456.403951	
TS7'_s	0.49945	-3456.374877	182.05 <i>i</i>
11'_s	0.502191	-3456.382981	
12'_s	0.816551	-4795.684159	
TS8'_s	0.815865	-4795.687003	205.77 <i>i</i>
13'_s	0.818013	-4795.691178	
TS9'_s	0.822929	-4795.646206	348.92 <i>i</i>
14'_s	0.825617	-4795.730713	
15'_s	0.8284	-4795.779876	
16'_s	0.817334	-4795.691731	
TS11'_s	0.816165	-4795.676399	345.71 <i>i</i>
TS11'_T	0.812247	-4795.651399	396.06 <i>i</i>
17-1'_s	0.821562	-4795.711723	
17-1'_T	0.80308	-4795.733421	
17'_s	0.82389	-4795.690964	
17'_T	0.821433	-4795.756144	
TS12'_s	0.821297	-4795.707312	629.98 <i>i</i>

18'_s	0.827476	-4795.710925	
18'_T	0.824246	-4795.721946	
19'_s	0.831965	-4795.748478	
19'_T	0.826263	-4795.779209	
TS14'_s	0.821886	-4795.713194	248.81 <i>i</i>
20'_s	0.821253	-4795.723246	
TS15'_s	0.822118	-4795.734083	799.99 <i>i</i>
21'_s	0.825687	-4795.761473	
B	0.392999	-1685.116922	
10''_s	0.50103	-3456.3736791	
TS7''_s	0.497527	-3456.3395572	558.92 <i>i</i>

7. Cartesian coordinates of all optimized structures

1a

N	-0.27039900	0.37777300	0.44282300
S	-1.62744800	0.55821900	1.41033200
O	-1.84416200	1.99907200	1.56082900
O	-1.42312900	-0.29822500	2.58463300
C	-2.99608300	-0.10341800	0.47261000
C	-3.78239900	0.75879200	-0.29968300
C	-4.81621300	0.22646500	-1.06791100
C	-5.07993400	-1.15473400	-1.07770000
C	-4.28025900	-1.99371000	-0.28429400
C	-3.24109300	-1.47952400	0.49234300
H	-3.59187100	1.83252400	-0.28066100
H	-5.43704800	0.89653200	-1.66852800
H	-4.47975800	-3.06803800	-0.26816200
H	-2.63770700	-2.13789900	1.11914900
C	-6.19524700	-1.70900000	-1.92196700
H	-6.33813400	-2.78529900	-1.74949500
H	-7.14617600	-1.19414300	-1.70876100
H	-5.98458400	-1.56007800	-2.99462400
C	0.32110900	-0.96378100	0.35847700
H	-0.12426000	-1.54548900	-0.47207100
H	0.09029800	-1.49435200	1.29256200
C	1.77139500	-0.89166200	0.18593000
C	2.97197800	-0.80774500	0.01320200
C	4.38565900	-0.69995800	-0.18861700
C	5.28724200	-1.35959700	0.67234300
C	4.89566900	0.07250200	-1.25314800
C	6.66258800	-1.24808800	0.46865700
H	4.89775300	-1.95714000	1.49903800
C	6.27256400	0.18069600	-1.44691600
H	4.20157700	0.58611300	-1.92160600
C	7.15957800	-0.47875900	-0.58900400
H	7.35192900	-1.76393400	1.14155500
H	6.65620700	0.78342800	-2.27373900
H	8.23775800	-0.39263400	-0.74445000
C	-0.16474800	1.24874300	-0.73916300
H	0.46572000	0.70378600	-1.45960100
H	-1.14395600	1.38507200	-1.22956000
C	0.47490400	2.57328500	-0.43762300

C	0.02205900	3.74748800	-0.88049900
H	1.38937300	2.52020800	0.16503100
H	0.54928400	4.68198600	-0.66664200
H	-0.89874200	3.81869200	-1.47041200

2a

C	1.99349400	0.46705400	0.00004000
H	2.27356200	1.55034800	0.00006900
O	2.84697400	-0.39648400	-0.00000700
C	0.53648200	0.21257200	0.00002000
C	-0.35748900	1.29452000	0.00000500
C	0.04421600	-1.10429500	0.00001200
C	-1.73443500	1.06400000	-0.00003000
H	0.03370700	2.31594400	0.00001200
C	-1.32951200	-1.33258500	-0.00000700
H	0.75646700	-1.93236400	0.00002500
C	-2.21876300	-0.24834300	-0.00003100
H	-2.43152500	1.90523200	-0.00004800
H	-1.71544700	-2.35479200	-0.00000700
H	-3.29651800	-0.43003300	-0.00004900

cats

H	-1.33407300	0.62414300	-2.82222400
C	0.54316800	0.63909700	-1.77606400
H	1.17509100	0.85688200	-2.64392400
P	1.28860500	0.39450400	-0.10798100
C	-0.78644300	0.49097900	-1.88356900
P	-1.65461300	0.09295100	-0.33947700
C	-3.28539200	0.87535700	-0.38393400
C	-4.45472900	0.14580700	-0.11820900
C	-3.36237200	2.25056000	-0.66558100
C	-5.69365700	0.79067900	-0.14017000
H	-4.39848000	-0.92319300	0.09706300
C	-4.60500000	2.88557200	-0.69120400
H	-2.45237800	2.82119800	-0.87026600
C	-5.77044200	2.15722300	-0.42731900
H	-6.60354700	0.22059800	0.06185300
H	-4.66430100	3.95285700	-0.91714300
H	-6.74186500	2.65685900	-0.44744900
C	-1.66316900	-1.67621300	-0.01687400
C	-1.27851800	-2.70491600	-0.92147700
C	-1.88782600	-1.98829600	1.36567200
C	-1.04995800	-3.98218800	-0.44597400
H	-1.13719000	-2.46976100	-1.97831700

C	-1.63560800	-3.30848900	1.81412100	C	5.28187900	-3.10476800	-0.36511300
H	-2.41689900	-1.29332600	2.02736500	H	5.79192700	-1.90000700	-2.09023600
C	-1.20413600	-4.28412100	0.93026000	H	4.52841500	-4.12485000	1.38866400
H	-0.74318100	-4.77004200	-1.13841000	H	6.16039000	-3.74792000	-0.45867300
H	-1.80929300	-3.55584900	2.86453000	C	2.10997900	1.29224200	-0.13292400
H	-1.01286500	-5.29927500	1.28533700	C	1.35706300	2.22883900	-0.85834200
C	2.06820200	2.00112700	0.27901900	C	3.26580100	1.71533400	0.54547700
C	2.21545200	2.33000700	1.63639300	C	1.75811500	3.56702500	-0.90828900
C	2.50465000	2.90537200	-0.70265600	H	0.45367600	1.91829100	-1.38531300
C	2.80712000	3.53878300	2.00880100	C	3.66411700	3.05262700	0.49036800
H	1.85804300	1.63498700	2.40154100	H	3.86124800	0.99653500	1.11431300
C	3.08952700	4.11766100	-0.32635100	C	2.91070200	3.98239700	-0.23555800
H	2.39140200	2.67095000	-1.76267400	H	1.16352000	4.28597200	-1.47709900
C	3.24392800	4.43430100	1.02700100	H	4.56785000	3.37030800	1.01648200
H	2.91999300	3.78625500	3.06707000	H	3.22383400	5.02842600	-0.27712400
H	3.42619400	4.81779800	-1.09475800	C	-3.22339500	-1.31790200	-0.10312700
H	3.70094900	5.38350200	1.31709900	C	-4.42046400	-0.76499300	0.38013600
C	2.66123600	-0.77498400	-0.41527800	C	-3.24648700	-2.58950900	-0.70084000
C	3.95076000	-0.38995900	-0.80975900	C	-5.62123200	-1.46873800	0.25654700
C	2.36633200	-2.13524800	-0.22044200	H	-4.41786900	0.22237500	0.84766100
C	4.93246200	-1.36276100	-1.01643600	C	-4.44967200	-3.28854000	-0.82560500
C	3.35037300	-3.10353400	-0.42823900	H	-2.32145100	-3.03792100	-1.07351700
H	1.35804400	-2.42367700	0.09095900	C	-5.63958000	-2.73014200	-0.34744800
C	4.63437600	-2.71703500	-0.82722700	H	-6.54805100	-1.02643600	0.63031000
H	5.93715800	-1.06181200	-1.32331900	H	-4.45731400	-4.27353600	-1.29890100
H	3.11570200	-4.15970600	-0.27509300	H	-6.58032000	-3.27714500	-0.44605000
H	5.40739100	-3.47271300	-0.98694200	C	-2.00771700	1.32107100	0.06622100
H	4.19126600	0.66582700	-0.95065300	C	-2.66204900	1.91293700	-1.02563400
Co	-0.25255800	-0.54751900	1.09789600	C	-1.52848700	2.12720800	1.10862400
cat_T				C	-2.82839000	3.29856000	-1.07015000
H	1.14091100	-0.87123600	-2.41649000	C	-1.69949700	3.51333200	1.06511500
C	-0.75140000	-0.76167700	-1.44856400	H	-1.01851800	1.66139000	1.95852200
H	-1.33687700	-0.92325900	-2.36098600	C	-2.34544300	4.09919600	-0.02719200
P	-1.62317100	-0.46858200	0.14353200	H	-3.33459200	3.75826400	-1.92252700
C	0.59001100	-0.73592600	-1.47831300	H	-1.32280000	4.13603700	1.87993700
P	1.52411900	-0.43607700	0.07121400	H	-2.47539100	5.18340500	-0.06762900
C	3.03286200	-1.45090000	-0.12748600	H	-3.03797000	1.29018000	-1.84081100
C	3.95660300	-1.24004600	-1.16496400	Co	-0.00140300	-0.76756900	1.69338400
C	3.24576100	-2.49120400	0.78816400	1_s			
C	5.07541600	-2.06625600	-1.28205300	N	-2.32092200	1.00701100	-1.81297700
H	3.80296300	-0.42530700	-1.87707700	S	-3.24074000	1.52187300	-0.50485700
C	4.36771600	-3.31719100	0.67039200	C	-2.02252800	-0.42651300	-1.85927000
H	2.52680300	-2.64717700	1.59731300	C	-1.26090400	1.88173400	-2.31300900

O	-3.21203500	2.98995900	-0.53725300	C	-0.59889800	1.82044300	3.08012700
O	-2.84538800	0.83525600	0.74214500	C	0.84166300	-5.70906400	0.21258300
C	-4.86585200	0.93461400	-0.93136900	H	2.84836700	-5.06930300	0.71092500
H	-1.96149000	-0.72642200	-2.91990900	H	-1.22161800	-6.05293800	-0.34640800
H	-2.86684000	-0.98711800	-1.42746300	H	4.73021100	-0.30920600	1.05924300
C	-0.77107100	-0.76294900	-1.16017400	P	2.81837400	0.29922600	-0.54778100
H	-1.68351100	2.89101700	-2.43129600	C	-1.91930800	-2.62699700	2.90721000
C	0.02408300	2.00366600	-1.51067200	H	-1.73246600	-0.82293400	1.74482400
H	-1.02258900	1.51458600	-3.32215300	C	0.11842100	-3.48955600	3.88348800
C	-5.46910100	1.39704000	-2.10748900	H	1.90743200	-2.34986200	3.52825700
C	-5.53002900	0.06507900	-0.06706600	C	1.49592000	3.28139700	4.22291200
C	0.07092600	-1.61680700	-0.65092400	H	2.81325800	1.83611700	3.32315000
C	0.11929000	2.30124100	-0.17800300	C	-0.87035900	2.95821100	3.84134800
H	0.91211400	2.14961500	-2.13610000	H	-1.42632500	1.28014000	2.61842800
C	-6.75561900	0.96783400	-2.41493800	H	1.03564900	-6.76006200	0.44067200
H	-4.93639500	2.07844300	-2.77326900	C	3.51885700	-0.78555800	-1.84158700
C	-6.82186100	-0.35501200	-0.39398300	C	3.52760700	1.94773300	-0.89942900
H	-5.04134300	-0.27610500	0.84609100	C	-1.25641800	-3.59971700	3.66349800
Co	0.64216000	0.12057100	-0.32051000	H	-2.99327900	-2.71127700	2.72389100
C	0.34139000	-3.00848500	-0.36842700	H	0.64482000	-4.25055200	4.46445000
H	-0.76755300	2.36689000	0.45281300	C	0.17437400	3.69150300	4.41464500
H	1.03386000	2.73338300	0.22968000	H	2.31786500	3.84759600	4.66757500
C	-7.45349200	0.08606000	-1.56571000	H	-1.90612400	3.27723500	3.98003100
H	-7.23507800	1.32164100	-3.33131700	C	2.68190200	-1.34524800	-2.81697100
H	-7.34824300	-1.03792800	0.27715900	C	4.89818400	-1.05449600	-1.87062600
P	1.07167100	-0.04633600	1.81617100	C	3.66444300	2.87540400	0.14699800
C	1.60935900	-3.41877500	0.08318100	C	3.83389900	2.33382900	-2.21382400
C	-0.67488300	-3.97361800	-0.52550300	H	-1.81042700	-4.44695200	4.07472600
C	-8.84353200	-0.36461700	-1.92081600	H	-0.04274900	4.58313400	5.00773000
C	2.85060100	-0.36264500	2.07408900	C	3.21697100	-2.17173800	-3.80878100
C	0.17036300	-1.43680100	2.59288400	H	1.61157400	-1.13788200	-2.79716700
C	0.72913800	1.40218500	2.88784000	C	5.42629700	-1.88691300	-2.85872300
C	1.85920300	-4.76076700	0.36450700	H	5.56544000	-0.61127500	-1.12825200
H	2.39267800	-2.67290000	0.21124000	C	4.11125000	4.17115400	-0.11956700
C	-0.42611600	-5.31287700	-0.23092400	H	3.41785900	2.58761200	1.17075300
H	-1.66182000	-3.65705400	-0.86979100	C	4.27778800	3.63282100	-2.47472100
H	-9.51978100	0.49916100	-2.03137000	H	3.73010600	1.62010500	-3.03365000
H	-8.84860200	-0.89924500	-2.88534000	C	4.58657500	-2.44764200	-3.82777700
H	-9.26064100	-1.03331800	-1.15450500	H	2.55836700	-2.60555000	-4.56481700
H	3.24391100	-0.62317800	3.06157100	H	6.49829500	-2.09748500	-2.87322200
C	3.64266200	-0.19483800	1.00892000	C	4.41748500	4.55206100	-1.43023200
C	-1.21148300	-1.55372800	2.36555800	H	4.21835400	4.88582100	0.69985300
C	0.83269100	-2.41045100	3.35388900	H	4.51744700	3.92648200	-3.49950200
C	1.77504600	2.14231200	3.46130600	H	5.00281600	-3.09981100	-4.59941400

H	4.76554400	5.56676600	-1.63758300	H	-9.23969400	-1.66814900	-3.37435600
I _T				H	-8.67736400	-3.25888800	-2.78824800
N	-2.57160300	-0.37876400	-0.98978700	H	2.76512500	1.76764400	2.94470100
S	-3.84690600	0.32993900	-0.18966900	C	3.37446800	1.12869000	1.01955200
C	-2.03563200	-1.66074900	-0.54974000	C	-1.00847300	-0.80347500	2.92923800
C	-2.09221600	0.14684500	-2.26287900	C	1.17222500	-0.61013900	3.96683100
O	-3.83271800	1.75084600	-0.55665000	C	0.56375300	3.77110200	2.20707500
O	-3.73563900	-0.07855400	1.22032400	C	-1.54359100	2.57499200	2.26448400
C	-5.33632100	-0.39421400	-0.84276900	C	3.77662600	-4.66242700	0.78988300
H	-2.29118300	-2.45561300	-1.27365000	H	4.50935800	-3.12022800	2.11951900
H	-2.49249200	-1.92540600	0.41377700	H	2.80192000	-6.00771500	-0.59801300
C	-0.56745300	-1.61436800	-0.38269000	H	4.43296100	1.35049400	1.19233500
H	-2.86811600	0.79077000	-2.70466900	P	2.83701900	0.53241300	-0.62240700
C	-0.81029100	0.95046300	-2.14212600	C	-1.36919200	-1.77073100	3.86908000
H	-1.95003800	-0.69822000	-2.95364500	H	-1.72674100	-0.51905000	2.15995300
C	-6.01068400	0.24863100	-1.88294900	C	0.81131700	-1.58878600	4.89771600
C	-5.79067700	-1.61346100	-0.32577600	H	2.17126000	-0.17479800	4.01644200
C	0.59162000	-1.99305100	-0.09151900	C	-0.11462100	4.97134600	2.44224200
C	-0.61701600	1.91266000	-1.19377600	H	1.64873700	3.78672100	2.08581600
H	-0.12183800	0.88628700	-2.99327500	C	-2.21488800	3.77567400	2.50124400
C	-7.15214500	-0.35021200	-2.41893200	H	-2.12538300	1.65685300	2.17138100
H	-5.65573500	1.20996000	-2.25672600	H	4.60356800	-5.34600700	0.99610400
C	-6.93079900	-2.19397100	-0.87505100	C	4.10013200	-0.66227800	-1.17966400
H	-5.26709500	-2.09140200	0.50351800	C	3.12655800	2.01777600	-1.66719100
Co	0.51480400	0.06442800	-0.50733100	C	-0.45930100	-2.16926000	4.85368000
C	1.66632400	-2.89379600	0.24108600	H	-2.36461500	-2.21953900	3.82348400
H	-1.38053000	2.12204800	-0.44197700	H	1.52980800	-1.89775100	5.66086400
H	0.21440400	2.61591900	-1.27344200	C	-1.50371500	4.97709400	2.59201800
C	-7.62936200	-1.57603300	-1.92905300	H	0.44927000	5.90515500	2.50805100
H	-7.68726700	0.14998200	-3.22980300	H	-3.30277900	3.77014800	2.60235600
H	-7.29419600	-3.14340400	-0.47328500	C	3.68476900	-1.70608800	-2.02003500
P	0.69927400	0.99827000	1.66383600	C	5.45005700	-0.57088000	-0.80523000
C	2.67983600	-2.53322800	1.14602600	C	2.70244600	3.27487100	-1.20302300
C	1.71613900	-4.15853900	-0.37913000	C	3.67203700	1.90570300	-2.95516600
C	-8.86859200	-2.21385400	-2.49512500	H	-0.73818700	-2.93409500	5.58251900
C	2.46320100	1.35736200	1.97461600	H	-2.03246300	5.91592000	2.77349300
C	0.26226900	-0.20633200	2.97737200	C	4.60491100	-2.65197600	-2.47669100
C	-0.14448800	2.56125100	2.12382600	H	2.63437700	-1.78364100	-2.30755800
C	3.72444400	-3.41446000	1.41911500	C	6.36637600	-1.52260200	-1.25799800
H	2.64487800	-1.55908500	1.62976600	H	5.79604000	0.24093900	-0.16301500
C	2.76706400	-5.03298600	-0.10551500	C	2.82801400	4.40344200	-2.01593100
H	0.93269900	-4.43986500	-1.08570400	H	2.27254800	3.37344300	-0.20412700
H	-9.67425700	-2.23539700	-1.74177500	C	3.79226800	3.03842500	-3.76573500
				H	4.00806800	0.93572700	-3.32715700

C	5.94566400	-2.56462800	-2.09111900
H	4.27041200	-3.46561900	-3.12420900
H	7.41465700	-1.44965400	-0.95852800
C	3.37214000	4.28781300	-3.29953100
H	2.49885300	5.37662000	-1.64371200
H	4.22022100	2.94240100	-4.76668000
H	6.66452200	-3.31015800	-2.43946200
H	3.46956800	5.17112300	-3.93518100

TS1_s

N	-2.93579900	-0.31286200	-1.01570400
S	-4.09353500	-1.48684300	-1.38061100
C	-1.79698900	-0.22564600	-1.96065800
C	-2.47438900	-0.30108600	0.38337600
O	-3.75346300	-2.77781600	-0.75157000
O	-4.27326700	-1.43417200	-2.83688100
C	-5.53206900	-0.83688800	-0.56522600
H	-1.81555200	0.74812000	-2.47483000
H	-1.84430900	-1.01553400	-2.72224400
C	-0.57040400	-0.38714000	-1.13249600
H	-2.26392700	-1.31741200	0.75434100
C	-1.22764500	0.55936000	0.46774200
H	-3.24803200	0.15149400	1.02345800
C	-6.08962000	-1.52882300	0.50900800
C	-6.09480700	0.35291200	-1.04274300
C	0.35217800	-1.30371700	-0.89504700
C	-0.32901600	0.36219600	1.58985400
H	-1.42844500	1.59700200	0.18154300
C	-7.23361200	-1.01100900	1.12130400
H	-5.63333500	-2.45655500	0.85638200
C	-7.23231900	0.85293700	-0.41824600
H	-5.64545000	0.87560600	-1.88900300
Co	0.84236100	0.25931100	0.04616100
C	0.64021500	-2.65102600	-1.34432700
H	-0.38918600	-0.59886400	2.11222000
H	-0.15527900	1.20965000	2.25957100
C	-7.82098700	0.18071000	0.67127000
H	-7.67832500	-1.54517000	1.96432600
H	-7.68049200	1.78152100	-0.78124200
P	2.61072300	-0.31490300	1.19155300
C	1.96277400	-3.08273300	-1.56878200
C	-0.41897300	-3.56405300	-1.54348400
C	-9.05952300	0.73389600	1.32051600
C	3.29686700	1.20627100	1.94771700

C	4.06284700	-0.95838300	0.28145900
C	2.29441400	-1.47035900	2.56225900
C	2.22111000	-4.38720100	-1.98733400
H	2.78325200	-2.38385100	-1.41479600
C	-0.15161500	-4.87315100	-1.94610900
H	-1.44897600	-3.25099800	-1.36069600
H	-9.91075900	0.70774100	0.61920000
H	-9.33832600	0.16105300	2.21637100
H	-8.91712100	1.78765500	1.61029100
H	4.13644200	1.13149600	2.64752300
C	2.82512500	2.39020400	1.53368000
C	4.76093100	-2.11261700	0.66134000
C	4.44950200	-0.25653000	-0.87339500
C	2.40533400	-1.07386100	3.90284200
C	1.83926800	-2.76501500	2.25550200
C	1.16574300	-5.28831300	-2.17172400
H	3.25193700	-4.70438300	-2.16298500
H	-0.97848500	-5.57375000	-2.08674200
H	3.24139300	3.33710300	1.89359500
P	1.48918900	2.38634300	0.28752800
C	5.82663400	-2.56939700	-0.12087900
H	4.47178600	-2.66448200	1.55687300
C	5.51706900	-0.71340800	-1.64588100
H	3.91176100	0.64541300	-1.17316600
C	2.07643400	-1.96864600	4.92627000
H	2.73956700	-0.06635800	4.15739200
C	1.51940000	-3.65518300	3.28087600
H	1.73461100	-3.07581300	1.21464600
H	1.36991400	-6.31363400	-2.48993700
C	2.25234500	3.00739900	-1.24897800
C	0.31972900	3.67614700	0.81882300
C	6.20325900	-1.87589000	-1.27445200
H	6.36370500	-3.47376700	0.17495200
H	5.80965200	-0.16416200	-2.54391200
C	1.63696500	-3.25852000	4.61830000
H	2.16419700	-1.65259400	5.96847400
H	1.17186600	-4.66113900	3.03415000
C	2.09242300	2.25487700	-2.42291400
C	3.00778300	4.19094400	-1.27196700
C	0.14913400	3.97597500	2.18002900
C	-0.50637900	4.29162700	-0.13718500
H	7.03370200	-2.23930700	-1.88444700
H	1.38126600	-3.95534800	5.42007000
C	2.68542000	2.68448300	-3.61375700

H	1.50318500	1.33385400	-2.40240400	H	-5.28033100	0.47581000	-0.23233400
C	3.59967100	4.61340600	-2.46316700	H	-2.56494900	-0.47530800	-3.44476300
H	3.13091000	4.78321300	-0.36209100	P	2.21287900	0.90306200	0.98259900
C	-0.82989600	4.89090100	2.57743900	C	2.09278500	-1.16150900	-2.52642400
H	0.78087800	3.49853300	2.93290900	C	2.74507700	-3.01402900	-1.11618700
C	-1.48311400	5.20382800	0.26621000	C	-4.09830200	1.55936400	-2.45451300
H	-0.38302800	4.06065200	-1.19812600	C	1.97233300	2.58985800	1.65288900
C	3.43998400	3.86086100	-3.63323100	C	3.35606000	1.16686900	-0.41443900
H	2.55725500	2.09824400	-4.52668200	C	3.14672500	-0.04387800	2.22754000
H	4.18834500	5.53368500	-2.47999100	C	3.08182200	-1.50961400	-3.44557200
C	-1.64631200	5.50482000	1.62307100	H	1.45400800	-0.29640700	-2.72059000
H	-0.95331400	5.12471300	3.63756300	C	3.74441300	-3.35465000	-2.03062600
H	-2.11876200	5.68297800	-0.48220400	H	2.61903700	-3.60149000	-0.20410600
H	3.90570000	4.19531000	-4.56338700	H	-4.10667100	1.54663700	-3.55481800
H	-2.41095800	6.21954800	1.93633300	H	-5.03001100	2.02417200	-2.10142000
				H	-3.26364500	2.21194800	-2.15041600
2s				H	2.82349600	3.11471300	2.09822300
N	-1.76826200	-3.87487300	0.71803600	C	0.78605400	3.19354700	1.49946200
S	-3.25329200	-3.99094000	-0.07887000	C	4.48963300	0.36223500	-0.59910400
C	-0.57398700	-3.70279700	-0.13332200	C	3.02153800	2.13974700	-1.37215400
C	-1.67186800	-2.89411800	1.81763300	C	3.99368500	0.60450600	3.14214900
O	-4.25762100	-4.20536300	0.96733800	C	3.06499100	-1.44521600	2.23176000
O	-3.05238500	-4.97148900	-1.15013000	C	3.91522700	-2.60640900	-3.19991000
C	-3.57825900	-2.40018300	-0.83421600	H	3.21107300	-0.91608400	-4.35359700
H	-0.78087600	-3.97542500	-1.17626300	H	4.39241400	-4.21168700	-1.82957600
H	0.21279400	-4.38769500	0.22363700	H	0.61802400	4.22247100	1.83661600
C	-0.15426900	-2.25970200	0.08254200	P	-0.55881700	2.27621100	0.67405300
H	-0.97690100	-3.29228200	2.57413400	C	5.28673200	0.53855900	-1.73180600
C	-1.07433000	-1.63918900	1.13399600	H	4.74835000	-0.40489200	0.13200400
H	-2.64971800	-2.73842300	2.28756300	C	3.82148900	2.30719700	-2.50329200
C	-4.43113500	-1.50009700	-0.19050400	H	2.13799600	2.76615900	-1.23265600
C	-2.91161800	-2.04233900	-2.01216100	C	4.74334300	-0.14616000	4.05074200
C	0.86197000	-1.51820100	-0.39196500	H	4.08402300	1.69134800	3.15142800
C	-0.28469500	-0.60338500	1.89996700	C	3.82165100	-2.18979300	3.13846000
H	-1.92159400	-1.13596300	0.63775600	H	2.40914700	-1.95049100	1.52372800
C	-4.60280100	-0.22328400	-0.72654800	H	4.69703900	-2.87435700	-3.91466900
H	-4.95553800	-1.80215100	0.71682700	C	-0.85635900	3.13273600	-0.90793800
C	-3.08279700	-0.75724600	-2.52434000	C	-2.02270600	2.55529200	1.71683000
H	-2.27381800	-2.76057800	-2.52820700	C	4.95491000	1.50706500	-2.68396700
Co	0.33048800	0.20808600	0.25110100	H	6.16687300	-0.09211000	-1.87464300
C	1.89974800	-1.91065300	-1.34831200	H	3.55835000	3.06526900	-3.24471900
H	0.52058500	-1.04179200	2.50093200	C	4.65910800	-1.54184000	4.05116900
H	-0.89416600	0.07700900	2.50965200	H	5.39811500	0.36445300	4.76067800
C	-3.92716700	0.17444000	-1.89270400	H	3.75239200	-3.27999700	3.13259400

C	-0.47146200	2.44757100	-2.07231000	C	-4.88506500	-1.27703900	-1.93146300
C	-1.42350000	4.41240200	-1.00645900	H	-4.65679700	-2.83513000	-0.44713300
C	-1.87417500	2.68256700	3.10819400	Co	0.52363700	0.24768200	-0.06039100
C	-3.30968800	2.53486800	1.15523300	C	0.35680300	-2.82257600	0.22091000
H	5.57956800	1.63724100	-3.57082000	H	-0.10625200	1.02399800	2.17833700
H	5.24686300	-2.12452000	4.76447300	H	-1.01875900	2.13667600	1.10652900
C	-0.64803300	3.03391900	-3.32702600	C	-5.15993200	0.07949600	-2.18313600
H	-0.03395500	1.44750100	-1.98994200	H	-5.63262600	1.97976400	-1.26518900
C	-1.60354500	4.99413600	-2.26315700	H	-4.70805400	-1.95399500	-2.77143100
H	-1.73055200	4.94835500	-0.10536000	P	2.76776200	-0.21602800	-0.67474800
C	-3.00206100	2.79850600	3.92440700	C	0.21422700	-3.47104600	-1.02183900
H	-0.87793300	2.69281000	3.55640600	C	1.09039000	-3.47418300	1.23188900
C	-4.43282600	2.64922200	1.97680000	C	-5.21214300	0.59283100	-3.59657500
H	-3.43612400	2.43764400	0.07708800	C	3.43176700	1.23995900	-1.56129000
C	-1.21640400	4.30793100	-3.42089100	C	3.16896800	-1.63273400	-1.73808900
H	-0.34850700	2.49510600	-4.22879500	C	3.75643400	-0.34764500	0.84550700
H	-2.04715000	5.98943700	-2.34151200	C	0.76278300	-4.73613200	-1.23713700
C	-4.28189100	2.78124200	3.36109700	H	-0.34009600	-2.97187600	-1.82092800
H	-2.87912600	2.90366600	5.00488700	C	1.64193700	-4.73923700	1.01399500
H	-5.43089800	2.63813300	1.53242600	H	1.22166600	-2.97982000	2.19716700
H	-1.36117200	4.76926500	-4.40069000	H	-6.00896700	0.08614100	-4.16624800
H	-5.16256200	2.87211300	4.00121100	H	-5.40773600	1.67389600	-3.62868500
2_T				H	-4.26684400	0.39347000	-4.12728200
N	-3.28950000	-1.36907800	2.52083100	H	4.38906100	1.15554700	-2.08746100
S	-4.91024900	-1.51000300	2.11543700	C	2.74127700	2.38769800	-1.52534700
C	-2.32775300	-2.24564600	1.81130400	C	3.79866200	-2.77974600	-1.23600700
C	-2.71832200	-0.00743200	2.60501200	C	2.77159500	-1.58223200	-3.08574500
O	-5.63593400	-0.59297200	3.00071900	C	5.16067000	-0.32076800	0.82878600
O	-5.20189000	-2.94746300	2.11002300	C	3.06821000	-0.41633200	2.06643000
C	-5.08340900	-0.90752700	0.43977300	C	1.47662400	-5.37733900	-0.21922600
H	-2.84460700	-2.93698500	1.13110300	H	0.63847100	-5.22236200	-2.20785600
H	-1.78373000	-2.86927400	2.53926500	H	2.20278900	-5.23012900	1.81369000
C	-1.39873900	-1.28243300	1.10053100	H	3.11143800	3.30358000	-1.99986100
H	-2.06069000	0.04193100	3.48895000	P	1.17323500	2.43046300	-0.59052000
C	-1.89551600	0.12386600	1.30784600	C	4.04120600	-3.86361800	-2.08306000
H	-3.51101600	0.73974400	2.72834100	H	4.09090900	-2.83329600	-0.18656700
C	-5.37038500	0.44194200	0.21973600	C	3.02034900	-2.66805000	-3.92596900
C	-4.84952500	-1.77761100	-0.63194700	H	2.27233700	-0.69256700	-3.47974800
C	-0.23928800	-1.49510400	0.44981100	C	5.86603100	-0.36395300	2.03246700
C	-0.72531900	1.09170300	1.26766100	H	5.70031500	-0.26741200	-0.11962600
H	-2.60031200	0.37054900	0.49392100	C	3.77982800	-0.46092900	3.26766900
C	-5.40420300	0.92570800	-1.08949200	H	1.97483200	-0.43407100	2.06606900
H	-5.57351300	1.10215400	1.06376600	H	1.91012600	-6.36569700	-0.39001000
				C	-0.06897300	3.18309600	-1.67933500

C	1.51487300	3.55771500	0.79646700	C	-5.79822700	0.50409400	1.51391600
C	3.65649800	-3.80975600	-3.42528600	C	-5.91096800	-0.94780500	-0.43655400
H	4.52824000	-4.75744000	-1.68735400	C	-0.82354900	0.16476300	1.03635400
H	2.71558700	-2.62394700	-4.97421400	C	-0.65369900	-1.89555700	-0.66311100
C	5.17732800	-0.43283900	3.25000700	H	-0.86761700	-2.95051900	1.23233300
H	6.95832600	-0.34301100	2.02208400	C	-6.14792500	1.59048000	0.71450200
H	3.24170400	-0.51543100	4.21667500	H	-5.63932000	0.62728500	2.58571100
C	-1.20458300	2.41896800	-1.99450100	C	-6.26383700	0.15175600	-1.22032500
C	0.09288100	4.46384100	-2.23196700	H	-5.83920300	-1.94473100	-0.87299600
C	2.67982100	3.33313600	1.55125700	C	-1.07094300	1.52327000	1.54037700
C	0.60825300	4.55436100	1.18752400	H	-1.35821300	-1.47654200	-1.39016600
H	3.84804300	-4.66064300	-4.08329700	H	-0.19355300	-2.78425100	-1.11963200
H	5.73530800	-0.46496300	4.18887500	C	-6.38300700	1.43501400	-0.66306500
C	-2.17726000	2.93660000	-2.85291900	H	-6.25090000	2.57893300	1.16990000
H	-1.32433500	1.42047400	-1.56159900	H	-6.45858600	0.00852000	-2.28538400
C	-0.88328700	4.97571000	-3.08850800	C	-0.18149900	2.18777100	2.40837400
H	0.97433000	5.06116200	-1.98713900	C	-2.23107200	2.20914900	1.12335700
C	2.93764900	4.11016000	2.68118600	C	-6.75204600	2.62241900	-1.50958800
H	3.38150300	2.54821100	1.26008800	C	-0.43304500	3.49689900	2.82451000
C	0.87500800	5.32869000	2.32039400	H	0.71312800	1.66980800	2.75402000
H	-0.30158200	4.73017700	0.61061700	C	-2.47716100	3.52045300	1.53437200
C	-2.01687500	4.21424800	-3.39744400	H	-2.93564100	1.70151000	0.46300200
H	-3.06002200	2.34323800	-3.09520800	H	-7.04471800	2.32079600	-2.52520800
H	-0.76061100	5.97353300	-3.51607200	H	-7.58729200	3.18358300	-1.06071700
C	2.03642200	5.10898500	3.06680700	H	-5.90288800	3.32112200	-1.59162200
H	3.84495400	3.93243800	3.26322700	C	-1.57501600	4.17384300	2.38112900
H	0.16961100	6.10719500	2.62013800	H	0.26948100	3.99351200	3.49892300
H	-2.77888900	4.62014300	-4.06709100	H	-3.37906100	4.03447800	1.19155100
H	2.24030100	5.71632300	3.95185000	H	-1.76473200	5.20146200	2.70076900
3_s				P	0.39728800	0.57299600	-1.79499800
N	-3.46639500	-2.17898200	1.77688200	P	2.32178100	-1.71630600	-1.06964600
S	-5.12301300	-2.14132700	1.92252800	C	-1.26338500	0.97353200	-2.44531000
C	-2.69968800	-1.04581600	2.35262800	C	1.31335400	2.15679000	-1.78555700
C	-2.87616700	-2.65859900	0.50805600	C	4.04299400	-1.14056600	-0.83346700
O	-5.41141500	-1.82618700	3.32649700	C	2.42470100	-3.51769600	-0.82261800
O	-5.62159400	-3.37682400	1.30669700	C	-1.88998800	2.19111000	-2.13877100
C	-5.67338200	-0.76146200	0.92856000	C	2.30013600	2.43573000	-2.74503900
H	-2.37275800	-1.29686800	3.37555500	C	4.60362000	-0.15510400	-1.66044700
H	-3.29221000	-0.12038400	2.41074800	C	1.85166300	-4.06042000	0.33722300
C	-1.55192500	-0.90803600	1.38690500	C	-1.93212100	0.03958600	-3.25682200
H	-3.34254500	-2.16861100	-0.36608100	C	1.06391100	3.08661600	-0.76139600
C	-1.40890200	-2.20419800	0.62343700	C	4.76771000	-1.60499300	0.27772100
H	-3.00203300	-3.74498800	0.41612200	C	3.09560900	-4.35394300	-1.72893200
				C	-3.17034300	2.46298800	-2.62539200

C	3.02668000	3.62774400	-2.67605200	H	4.96542500	0.56727200	5.10040100
C	5.87607000	0.35276200	-1.38314000	H	6.78114000	2.16953200	4.52627800
C	1.94660100	-5.43161200	0.58942300	C	1.16448500	-0.39927800	-3.14432400
C	-3.21133600	0.31802100	-3.74147600	C	1.99021900	-1.40854300	-2.83825200
C	1.78807000	4.27774400	-0.70116400	H	0.94292100	-0.12708200	-4.18176300
C	6.03583700	-1.09183100	0.55199200	H	2.48519800	-2.00033200	-3.61527800
C	3.18090900	-5.72435400	-1.47659800				
C	-3.83492000	1.52819800	-3.42280000	3_T			
C	2.77350500	4.54963600	-1.65583200	N	-4.07779100	-0.17732000	-1.15682800
C	6.59238800	-0.11149800	-0.27669400	S	-4.92086100	-1.52666800	-0.57284100
C	2.60736800	-6.26348000	-0.31902900	C	-3.44795100	0.65013700	-0.09220000
H	-1.38713000	2.93578300	-1.52462300	C	-3.01726900	-0.50862000	-2.14284200
H	2.51025600	1.72748800	-3.54764900	O	-4.21560200	-2.17246700	0.55199900
H	4.04750000	0.22361700	-2.51835900	O	-5.25462500	-2.34345000	-1.74855500
H	1.33003500	-3.40862600	1.04176400	C	-6.39958700	-0.76589400	0.06352800
H	-1.45513600	-0.90648000	-3.51931800	H	-3.86630900	0.41104100	0.89596000
H	0.32469000	2.87112600	0.00751600	H	-3.65880100	1.71378400	-0.28836200
H	4.33735900	-2.36560100	0.93327100	C	-1.96837300	0.34451600	-0.20497300
H	3.55892400	-3.93692000	-2.62611500	H	-2.90803800	0.35546500	-2.81870000
H	-3.64966700	3.41208000	-2.37614100	C	-1.75572100	-0.68826900	-1.27764600
H	3.79412900	3.83467100	-3.42551900	H	-3.30730700	-1.38343700	-2.73549600
H	6.30459600	1.11875800	-2.03385400	C	-6.71566900	-0.90040100	1.41691700
H	1.49990300	-5.84983500	1.49440200	C	-7.24180100	-0.08133300	-0.81686900
H	-3.72111700	-0.41485100	-4.37108400	C	-0.88733100	0.93247900	0.33118300
H	1.58637900	4.98866400	0.10311300	C	-0.38337800	-0.42558300	-1.87291300
H	6.58860400	-1.45226700	1.42244700	H	-1.79743000	-1.70207200	-0.83653700
H	3.70027700	-6.37476900	-2.18438500	C	-7.89471100	-0.32820000	1.89335700
H	-4.83657200	1.74441000	-3.79901000	H	-6.04217800	-1.44442400	2.08039200
H	3.34539800	5.47911300	-1.60438900	C	-8.41513500	0.48470500	-0.32174100
H	7.58262200	0.29318200	-0.05584700	H	-6.97982600	0.01174500	-1.87223400
H	2.67774300	-7.33646500	-0.12487400	C	-0.84873300	2.06612100	1.26253700
Co	0.65858000	-0.56411500	0.00706100	H	-0.37649000	0.53771800	-2.40769300
C	2.97006600	1.14135200	0.94198300	H	-0.00408300	-1.20974200	-2.53767300
H	3.09511300	1.64920200	-0.02778300	C	-8.76126200	0.37147700	1.03626800
O	2.01438400	0.38080700	1.12658300	H	-8.14834800	-0.42620900	2.95214100
C	3.97678600	1.42779600	1.94869400	H	-9.07876200	1.02481700	-1.00143100
C	5.00442000	2.33338100	1.62732800	C	-0.68746800	1.87767700	2.65009300
C	3.96096100	0.79022600	3.20502800	C	-0.89868200	3.38559100	0.76782300
C	6.00974300	2.60126300	2.55512800	C	-10.03145600	0.97788500	1.56761900
H	5.00776200	2.81600000	0.64760200	C	-0.57896000	2.97152900	3.51118400
C	4.96775300	1.05943900	4.12543400	H	-0.64557400	0.86141000	3.04796500
H	3.16177200	0.08329500	3.43578000	C	-0.78760700	4.47777800	1.63017800
C	5.99097000	1.96352700	3.80011800	H	-1.01224100	3.54521100	-0.30596600
H	6.81053200	3.30204200	2.30998400	H	-10.57099600	1.53408700	0.78788800

H	-10.70433700	0.19659000	1.95918900	H	-0.30421700	3.84637000	-4.78746900
H	-9.82127500	1.66650700	2.40237400	H	6.56965300	3.53476700	0.88600700
C	-0.62250200	4.27606500	3.00486700	H	4.76143600	-4.59520100	1.74370100
H	-0.45692600	2.80587600	4.58482700	H	3.43548800	-4.95192300	-4.42627000
H	-0.82369100	5.49233200	1.22511900	H	-0.31091100	6.16521600	-3.86385600
H	-0.52995900	5.13073100	3.67945700	H	5.54648900	4.11664300	3.08480700
P	2.25893800	1.90443300	-1.04088600	H	6.20206300	-2.90510400	2.88197200
P	2.53475700	-1.25227500	-1.20326900	H	1.34117900	-6.17967600	-3.85565500
C	1.51394400	3.30597700	-1.94479800	Co	0.77568300	0.11220500	-0.32561300
C	3.33849400	2.64478300	0.23222400	C	1.94678400	-0.64896400	2.45710300
C	3.78098300	-1.81228300	0.02674200	H	2.56624700	-0.21050700	3.26338500
C	2.15251800	-2.78624600	-2.11926000	O	1.65598700	0.06686700	1.49836500
C	1.51529800	4.61175600	-1.43263000	C	1.54230300	-2.03582700	2.62065500
C	2.76572100	2.96894200	1.47358100	C	2.11103400	-2.78507000	3.66657200
C	4.59584200	-0.86403500	0.66727800	C	0.62725600	-2.64084300	1.73706600
C	0.97656100	-3.48305000	-1.79945500	C	1.78676400	-4.13269400	3.81190200
C	0.85388700	3.03695300	-3.15658000	H	2.81797600	-2.30536700	4.34762300
C	4.71093300	2.85417300	0.02540400	C	0.29812400	-3.98226500	1.89187900
C	3.84999800	-3.15801300	0.42036900	H	0.17372200	-2.05083100	0.93945200
C	3.03845800	-3.32583800	-3.06557200	C	0.88414500	-4.72930200	2.92427400
C	0.85950800	5.63434100	-2.12360800	H	2.23560800	-4.72130700	4.61462700
C	3.55712200	3.50611900	2.49056300	H	-0.41366400	-4.45357000	1.21127400
C	5.46317400	-1.25762200	1.68812400	H	0.62870100	-5.78550700	3.03915600
C	0.68818800	-4.70177500	-2.41772600	C	3.38595000	1.14784300	-2.26385000
C	0.20396400	4.06321400	-3.84475900	C	3.49078200	-0.18734500	-2.33962700
C	5.50100100	3.37888800	1.05208400	H	3.96517000	1.79433500	-2.93286500
C	4.72002000	-3.54614700	1.44209900	H	4.17837900	-0.64894000	-3.05600900
C	2.74213300	-4.53982100	-3.68927900				
C	0.20168800	5.36332300	-3.32716400	TS2_s			
C	4.92627900	3.70603400	2.28428600	N	-3.26946600	-2.00750700	1.06261600
C	5.52597500	-2.59906200	2.08009500	S	-4.86481200	-2.45147700	1.13344000
C	1.56855900	-5.22934700	-3.36667400	C	-2.81309400	-0.76245500	1.70298900
H	2.02234900	4.83280100	-0.49226800	C	-2.43768000	-2.30638900	-0.11152100
H	1.70437700	2.79541200	1.64659500	O	-5.29546400	-2.20624200	2.51487900
H	4.55320100	0.18696200	0.38073900	O	-4.94357800	-3.79324400	0.54430400
H	0.28499400	-3.07351600	-1.06286200	C	-5.77797100	-1.33650600	0.07916600
H	0.84958700	2.02325100	-3.56529500	H	-2.98024400	-0.79153000	2.78951200
H	5.17162200	2.60311900	-0.93165000	H	-3.34527500	0.11965700	1.30030600
H	3.21911600	-3.90623600	-0.06051200	C	-1.35244400	-0.73425400	1.31394300
H	3.97079000	-2.81402400	-3.31024700	H	-2.71388300	-1.67977400	-0.97986000
H	0.86492000	6.64882900	-1.71771300	C	-1.05281700	-1.91794800	0.42930500
H	3.10086900	3.76005800	3.45026800	H	-2.52638700	-3.36484300	-0.38236500
H	6.09103900	-0.50945100	2.17803800	C	-6.27141700	-0.14064200	0.60981800
H	-0.22897600	-5.23636000	-2.15968800	C	-5.98017700	-1.66739000	-1.26442200

C	-0.36404900	0.12613000	1.61000000	C	2.78223900	-4.48900700	-2.85232200
C	0.08170900	-1.60000800	-0.53223100	C	-3.33266900	0.80507900	-2.69348300
H	-0.75824800	-2.73735100	1.10843800	C	1.51493400	4.91441600	0.51435300
C	-6.97390700	0.73056300	-0.22228100	C	6.88367800	0.10590100	-1.14812900
H	-6.12116100	0.09250700	1.66481400	C	4.04068800	-4.57566600	-0.78735100
C	-6.68697800	-0.78490600	-2.08002200	C	-4.05316400	1.83795700	-2.08769100
H	-5.60219800	-2.61237300	-1.65695800	C	2.01527500	5.65723700	-0.55900600
C	-0.47897800	1.27370000	2.52589400	C	6.90160500	1.49636600	-1.01576600
H	-0.31557700	-1.26580600	-1.49903300	C	3.50862600	-5.22052900	-1.90826000
H	0.68989300	-2.49260100	-0.72610200	H	-1.54712700	3.27845200	-0.28777400
C	-7.19669500	0.42330900	-1.57465600	H	1.61047600	3.37408200	-3.05305600
H	-7.36110100	1.66706900	0.18699500	H	3.55227200	2.09004600	-0.98106900
H	-6.85020800	-1.03947900	-3.13043700	H	2.00811900	-2.56114700	-3.41919300
C	0.47352200	1.50133100	3.53869100	H	-1.41720100	-0.14897200	-2.92535500
C	-1.54740500	2.18563600	2.40961500	H	0.68609700	3.03728700	1.16007500
C	-7.97415700	1.35815300	-2.46080600	H	5.67788800	-1.66411800	-1.34422200
C	0.37902900	2.61077000	4.37994200	H	4.26562000	-2.71461400	0.27040200
H	1.28777200	0.79071500	3.68210900	H	-3.96398500	3.53042600	-0.74238100
C	-1.64100000	3.29682000	3.24917900	H	2.43617800	5.66955100	-2.68246400
H	-2.29969300	2.03038100	1.63753600	H	5.69635800	3.29173300	-0.86931300
H	-7.93391800	2.39287800	-2.08957400	H	2.35948600	-4.98819000	-3.72733800
H	-7.59747500	1.33932000	-3.49475600	H	-3.83232800	0.11748300	-3.37921400
H	-9.03750200	1.06304600	-2.49769100	H	1.48818200	5.34382800	1.51859400
C	-0.67285600	3.52141000	4.23296800	H	7.82072900	-0.45353900	-1.20040300
H	1.13062600	2.76324600	5.15871700	H	4.60399500	-5.14202400	-0.04208600
H	-2.47432200	3.99416600	3.13041700	H	-5.11502000	1.96087700	-2.30121600
H	-0.74236700	4.39373400	4.88729200	H	2.38272800	6.67382400	-0.39896500
P	0.46942400	1.32891900	-1.20559700	H	7.85331400	2.03005500	-0.95827700
P	2.80869800	-0.69543500	-1.26494500	H	3.65772500	-6.29431800	-2.04447500
C	-1.31484500	1.53279600	-1.55259200	Co	1.23475100	-0.17671000	0.28798100
C	1.07810200	3.04386900	-0.97054500	C	3.29204100	0.67797800	1.95593200
C	4.45502000	0.12039800	-1.15534300	H	4.06956100	1.31570300	2.41338600
C	3.12906600	-2.46228100	-1.56133200	O	2.48049800	1.17654300	1.16306400
C	-2.04387700	2.57075400	-0.95085600	C	3.20992300	-0.72978300	2.26995600
C	1.57695100	3.79571100	-2.04757900	C	4.17273800	-1.39907200	3.04132300
C	4.48029400	1.52205500	-1.03025100	C	2.09662000	-1.41096500	1.70393600
C	2.58999000	-3.11580800	-2.68120800	C	4.02810000	-2.76667900	3.27004100
C	-1.96960600	0.65100500	-2.42942200	H	5.02518600	-0.84783600	3.44566100
C	1.05558700	3.61129600	0.31346500	C	1.97110200	-2.77977300	1.95608900
C	5.66827000	-0.58164900	-1.22256600	H	0.90135700	-0.74196800	1.74537100
C	3.84860700	-3.20469000	-0.60927300	C	2.92821500	-3.44699200	2.73144300
C	-3.40729400	2.71760200	-1.21453600	H	4.76659700	-3.30570800	3.86696300
C	2.04611800	5.09496000	-1.83896300	H	1.13333200	-3.34506600	1.54841700
C	5.69537500	2.20334600	-0.96416800	H	2.81611200	-4.51901000	2.91141500

C	1.16927600	0.83921500	-2.82329600	C	-0.47387300	3.33906300	4.44990700
C	2.17667800	-0.04116900	-2.84824500	H	-1.43423400	1.93207800	5.78527300
H	0.78189100	1.29461000	-3.74038100	H	0.53168800	4.48428000	2.90960100
H	2.67745000	-0.32299500	-3.78069600	H	-0.56160600	4.18163500	5.14022800
TS2_T				P	0.53772700	1.58290000	-1.28121600
N	-3.29952600	-1.62859900	0.91823200	P	2.80944100	-0.70098800	-1.46175800
S	-4.80490000	-2.24129000	1.19019200	C	-1.25492500	1.41382400	-1.57260600
C	-2.63650600	-0.71673600	1.85727500	C	0.84492000	3.39261400	-1.22137200
C	-2.42423300	-2.08397700	-0.16400600	C	4.49020100	-0.05448400	-1.13383200
O	-5.11144300	-1.97831400	2.60328600	C	3.01531100	-2.43684500	-1.98190600
O	-4.83406900	-3.60969300	0.65627400	C	-2.12810300	1.84162600	-0.55675800
C	-5.93432700	-1.26898600	0.20478800	C	-0.07041600	4.32290300	-1.73911700
H	-2.78596200	-1.05893100	2.89204500	C	4.77697800	1.28847600	-1.42937600
H	-3.01038500	0.31863100	1.79060000	C	2.89193800	-2.83456500	-3.32204900
C	-1.19259400	-0.80744700	1.42912400	C	-1.77652900	0.79170700	-2.71624600
H	-2.51738100	-1.43477900	-1.05070200	C	2.04905100	3.84313100	-0.65313900
C	-1.01763600	-1.94589000	0.45974000	C	5.44710200	-0.83644500	-0.46920800
H	-2.66869700	-3.11456100	-0.44737300	C	3.27222300	-3.40429300	-0.99475700
C	-6.41893200	-0.05792900	0.71079500	C	-3.50419000	1.66249300	-0.69511800
C	-6.31222600	-1.72420100	-1.05904900	C	0.21755000	5.68901600	-1.68556900
C	-0.16531900	0.01691700	1.72739800	C	6.00721300	1.83913100	-1.06707800
C	0.12296400	-1.68535500	-0.51646400	C	3.04081300	-4.18089500	-3.66739800
H	-0.82303000	-2.86033800	1.05048900	C	-3.15710800	0.60745200	-2.84482200
C	-7.28123600	0.70582800	-0.07227400	C	2.33212000	5.21031500	-0.60757300
H	-6.13353300	0.27169300	1.71095400	C	6.67554900	-0.27855600	-0.10611800
C	-7.18074600	-0.94748700	-1.82873400	C	3.42615300	-4.74553100	-1.34689600
H	-5.94021100	-2.68088400	-1.42797800	C	-4.02159200	1.04224300	-1.83742300
C	-0.25174600	1.16004500	2.66241900	C	1.41720400	6.13490300	-1.12131300
H	-0.24081500	-1.26233700	-1.46564100	C	6.95758600	1.05873700	-0.40073400
H	0.69618800	-2.59254400	-0.74454200	C	3.31103400	-5.13673200	-2.68473700
C	-7.67565700	0.27711200	-1.35361200	H	-1.72796000	2.31229700	0.34359600
H	-7.66419900	1.65199400	0.31917500	H	-1.00872500	3.98399600	-2.18131400
H	-7.48328900	-1.30255200	-2.81704200	H	4.03513600	1.91225600	-1.92944600
C	-0.85235600	1.00194000	3.92799400	H	2.67636900	-2.10841300	-4.10571500
C	0.25545000	2.42901700	2.32622000	H	-1.11109200	0.43876200	-3.50664000
C	-8.59293600	1.12621000	-2.19112800	H	2.74858000	3.12417400	-0.22605600
C	-0.96404600	2.07940300	4.80958600	H	5.24279100	-1.87951300	-0.22711100
H	-1.22656200	0.02041300	4.22532400	H	3.33638500	-3.11100500	0.05272800
C	0.13841100	3.50780700	3.20380000	H	-4.17819900	1.99590600	0.09650700
H	0.74466700	2.57299000	1.36667300	H	-0.50004400	6.40841100	-2.08766400
H	-8.08182200	2.04968400	-2.51309500	H	6.22070900	2.88429400	-1.30314400
H	-8.92725300	0.59277000	-3.09256200	H	2.94239500	-4.48157500	-4.71310300
H	-9.48242300	1.43508400	-1.61897800	H	-3.55709900	0.11733900	-3.73559800
				H	3.26819800	5.55405200	-0.16075300

H	7.41404200	-0.89508900	0.41157200	H	-1.72052200	-0.14294400	-0.17543300
H	3.62727200	-5.48741000	-0.57065700	C	-4.06664800	-3.33269700	0.27491500
H	-5.09671300	0.88806000	-1.93288400	H	-3.60202000	-2.58186500	-1.69708000
H	1.63690300	7.20447900	-1.07899900	C	-5.50346600	-1.94369100	1.62897000
H	7.91862100	1.49206300	-0.11374100	H	-6.17572900	-0.09699700	0.71603600
H	3.42554300	-6.18774100	-2.96033700	C	-1.99599500	4.18744800	0.98978800
Co	1.36393200	-0.26404000	0.22324600	H	0.40562700	1.78621500	-1.12679200
C	3.59455400	0.76595200	1.87946900	H	0.29657500	0.23289400	-1.96650900
H	4.39804300	1.41913800	2.27114400	C	-4.75781600	-3.12551300	1.48014200
O	2.80579800	1.21116000	1.03921400	H	-3.47861000	-4.24306100	0.13740300
C	3.48729100	-0.60144300	2.35506800	H	-6.04928800	-1.76601200	2.55925600
C	4.46052800	-1.18553700	3.18540700	C	-3.30697100	4.29987500	1.49636200
C	2.36295700	-1.32578800	1.90444900	C	-1.15668200	5.31949700	1.06759200
C	4.31212900	-2.51696500	3.56814400	C	-4.72800500	-4.15372800	2.57833900
H	5.32509700	-0.60048100	3.51069500	C	-3.76711900	5.50777800	2.02594000
C	2.21813200	-2.65015100	2.32378800	H	-3.96535200	3.43114000	1.50969800
H	1.02220000	-0.62861300	1.81555400	C	-1.61841300	6.52565600	1.59353200
C	3.19116500	-3.24448900	3.13918600	H	-0.13107700	5.24335000	0.69548700
H	5.06100200	-2.99315100	4.20471200	H	-4.64986000	-3.68090300	3.56954100
H	1.34608700	-3.23249900	2.01292400	H	-5.65907400	-4.74680000	2.57817400
H	3.07482100	-4.28645100	3.44964300	H	-3.88986600	-4.85504500	2.45469400
C	1.31353600	1.14401300	-2.87968800	C	-2.93017600	6.62712500	2.07097700
C	2.27371000	0.21253000	-2.94338000	H	-4.78674200	5.57184600	2.41452800
H	1.03023200	1.71095600	-3.77446900	H	-0.95227700	7.39142400	1.63326700
H	2.79814400	0.01534400	-3.88425100	H	-3.29419000	7.57043800	2.48546500
				P	3.06895700	0.76559500	-0.93028100
4s				P	1.62653300	-1.88053400	-0.77000000
N	-3.62181900	0.99177100	-1.69072300	C	3.18795900	-0.32377000	-2.38779900
S	-4.92439500	-0.01734000	-1.89528100	C	2.54420200	-1.49637000	-2.30962800
C	-3.57148900	1.85223400	-0.49163900	C	3.02225600	2.47316100	-1.54276600
C	-2.27410600	0.55913100	-2.09170100	C	4.64734100	0.55209400	-0.04631400
O	-4.70769300	-0.71790100	-3.16733000	C	2.83106300	-2.78985000	0.26300900
O	-6.11714000	0.80920000	-1.67705600	C	0.33919700	-3.04731300	-1.32148200
C	-4.87590400	-1.23343200	-0.58486800	C	3.43339800	3.51789800	-0.69827400
H	-4.13187100	1.39959400	0.34602200	C	5.88691700	0.78269000	-0.66430000
H	-4.01749300	2.83731300	-0.69254600	C	4.07631000	-3.18821600	-0.24999300
C	-2.09559100	1.93671700	-0.18131400	C	0.11001000	-4.26768500	-0.66818500
H	-1.89266500	1.21425600	-2.89385600	C	2.44857900	2.76871100	-2.78958200
C	-1.44456800	0.71886200	-0.80527900	C	4.60026600	0.07037000	1.27058200
H	-2.28506700	-0.46999800	-2.46844200	C	2.54861700	-2.99121200	1.62577800
C	-4.12321800	-2.39845700	-0.75844300	C	-0.44669500	-2.69392200	-2.43205900
C	-5.57227400	-0.99871600	0.60582000	C	3.27928100	4.84426800	-1.10563600
C	-1.44653800	2.95780600	0.40606100	C	7.06787900	0.52172800	0.03219200
C	0.05661100	0.74876900	-1.02611200	C	5.02350000	-3.77714900	0.58930300

C	-0.89825700	-5.12268400	-1.12088900	H	3.79599600	-0.04884900	-3.25608300
C	2.29979200	4.09841300	-3.19190200	H	2.58731200	-2.24540900	-3.10721600
C	5.78473800	-0.18879400	1.96413000				
C	3.49847500	-3.58661300	2.45872600	4 _T			
C	-1.44790400	-3.55585800	-2.88296800	N	-3.87996800	2.05047600	-1.02315200
C	2.71240700	5.13661100	-2.35130200	S	-5.37150600	1.32769800	-1.19284500
C	7.01731600	0.03239800	1.34329800	C	-3.41341700	2.41149200	0.33415500
C	4.73871800	-3.97503700	1.94399000	C	-2.75691800	1.53960000	-1.83060100
C	-1.67749900	-4.76961300	-2.22654500	O	-5.66573300	1.31934800	-2.62969200
H	3.87298400	3.29572100	0.27645900	O	-6.25848700	2.00385600	-0.23921200
H	5.92651800	1.16359000	-1.68757800	C	-5.18952200	-0.37447300	-0.67344300
H	4.31838100	-3.02716500	-1.30140200	H	-3.98427900	1.87013300	1.10766100
H	0.71871100	-4.55552500	0.19064900	H	-3.55620800	3.48687200	0.52004300
H	2.11176400	1.96392000	-3.44673400	C	-1.95621300	2.01625200	0.33242600
H	3.63786600	-0.10700300	1.75485300	H	-2.30444700	2.36576900	-2.40447100
H	1.59028200	-2.67800200	2.04125200	C	-1.77326500	1.00210100	-0.77411700
H	-0.27450600	-1.75108800	-2.95521000	H	-3.09396100	0.77667000	-2.54297100
H	3.60440000	5.65372800	-0.44771900	C	-4.80279700	-1.34185800	-1.60875600
H	8.03268100	0.69771900	-0.44944900	C	-5.39498300	-0.71360200	0.66676600
H	5.99217400	-4.07649900	0.18267000	C	-0.95291900	2.49651500	1.08628400
H	-1.07095700	-6.07193400	-0.60848500	C	-0.37422000	0.76455500	-1.28185000
H	1.85707700	4.32297700	-4.16511800	H	-2.21037900	0.05784800	-0.40503100
H	5.74281600	-0.56835600	2.98733800	C	-4.60122900	-2.65367400	-1.18480200
H	3.26962500	-3.73813100	3.51617500	H	-4.68417000	-1.07094300	-2.65855900
H	-2.05329100	-3.27505300	-3.74778800	C	-5.19398400	-2.03416700	1.07123200
H	2.59277200	6.17570300	-2.66705100	H	-5.72892500	0.04315800	1.37779900
H	7.94456900	-0.17529100	1.88284800	C	-0.97032800	3.41816200	2.22397600
H	5.48554800	-4.42947000	2.59925600	H	0.02299700	1.67754300	-1.74158900
H	-2.46574400	-5.43945800	-2.57752400	H	-0.35795900	-0.04392400	-2.03393200
Co	1.28914400	0.00626300	0.31370900	C	-4.78757100	-3.02193000	0.15960800
C	0.62826900	1.55232000	2.44898600	H	-4.30404300	-3.41226600	-1.91212300
H	0.62327600	2.37817800	3.18317200	H	-5.36383800	-2.30403000	2.11614900
O	1.37418100	1.63997200	1.45141500	C	-2.13149400	3.76155300	2.94836400
C	-0.20090800	0.39193300	2.61700600	C	0.25970700	3.96542600	2.65022800
C	-1.06908100	0.23711900	3.71517600	C	-4.53612400	-4.43693600	0.60371000
C	-0.07463100	-0.57432500	1.57437400	C	-2.06384400	4.64050500	4.03083800
C	-1.83674500	-0.91882600	3.80634500	H	-3.09342900	3.32235000	2.68623100
H	-1.12961300	1.01764600	4.47833000	C	0.32534400	4.84321400	3.73188600
C	-0.86810300	-1.72043600	1.70532500	H	1.17316600	3.69024000	2.11643000
C	-1.72472600	-1.89163100	2.80209100	H	-4.94693200	-4.62487700	1.60609100
H	-2.51854100	-1.07069200	4.64570000	H	-4.97874300	-5.16132800	-0.09774300
H	-0.84771000	-2.50339300	0.94678300	H	-3.45342800	-4.64541400	0.63646700
H	-2.32009300	-2.80305300	2.87309200	C	-0.83925900	5.18942900	4.42588200
H	-0.35722600	2.90975600	0.41862300	H	-2.97656000	4.89167300	4.57727300

H	1.28961600	5.25718900	4.03763700	H	3.13751900	-3.62305200	3.87981100
H	-0.79183900	5.87499500	5.27550000	H	-1.95860600	-3.67462300	-3.34317800
P	2.66691800	0.75140600	-1.45455500	H	1.13251200	5.25187600	-4.60542300
P	1.86061700	-2.14104900	-0.64950600	H	7.81390500	1.69149500	0.88142700
C	3.09207800	-0.63806700	-2.56702700	H	5.48025200	-4.20688100	3.24753300
C	2.78492100	-1.88960200	-2.19848900	H	-2.42518200	-5.68462500	-1.93838300
C	2.28839800	2.17376000	-2.51954600	Co	0.97970800	-0.04327900	-0.02603900
C	4.29409600	1.11886800	-0.68965600	C	1.33475900	0.46687400	2.69085900
C	3.00540000	-2.88843100	0.54786000	H	1.68271000	0.83744200	3.67327700
C	0.56608900	-3.35066900	-1.06570200	O	1.94733300	0.81214800	1.66446000
C	2.16241700	3.43496700	-1.90930400	C	0.19000200	-0.40952700	2.61436200
C	5.17185100	2.06217900	-1.24814500	C	-0.45957000	-0.87472100	3.77294400
C	4.32350300	-3.21530400	0.19383300	C	-0.21490500	-0.80489000	1.30817300
C	0.30952400	-4.48542800	-0.28344700	C	-1.51689700	-1.77055100	3.64363900
C	1.98089600	2.02595900	-3.87919200	H	-0.12196600	-0.53923500	4.75723500
C	4.69537900	0.38074100	0.43664000	C	-1.27686800	-1.70553700	1.21053200
C	2.58334900	-3.03009300	1.88230700	C	-1.91447600	-2.18488700	2.36462600
C	-0.25683600	-3.06213200	-2.16829400	H	-2.03096900	-2.15264500	4.52802700
C	1.75412800	4.53692800	-2.65968000	H	-1.62189200	-2.05630600	0.23575000
C	6.43203300	2.26674300	-0.68021700	H	-2.73451700	-2.89746900	2.26478000
C	5.20797000	-3.68873800	1.16599400	H	0.04860700	2.15722900	0.81351100
C	-0.76504600	-5.32073400	-0.60151600	H	3.67425500	-0.43622700	-3.47326500
C	1.56916800	3.13462700	-4.62587600	H	3.07586200	-2.75780600	-2.79986200
C	5.95804300	0.58496100	0.99493900				
C	3.47121700	-3.51176900	2.84552100	TS3s			
C	-1.32540100	-3.90275900	-2.48284100	N	2.22251400	0.04010000	-0.73479400
C	1.45669300	4.38834500	-4.01982700	S	2.60018000	0.72912700	-2.19840400
C	6.82731900	1.52981000	0.44033300	C	3.06111600	-1.05461500	-0.22195500
C	4.78446200	-3.83853900	2.48997200	C	1.72556000	0.87597400	0.36523700
C	-1.58441000	-5.03076700	-1.69652200	O	1.45735500	1.57950500	-2.56307800
H	2.38084400	3.55217800	-0.84454400	O	3.01454500	-0.36872800	-3.08051900
H	4.87692100	2.63755300	-2.12715900	C	4.00878300	1.78082400	-1.91723900
H	4.66762200	-3.08800400	-0.83412600	H	4.14248100	-0.84887400	-0.33216200
H	0.94382100	-4.72147600	0.57218900	H	2.83691000	-1.98083900	-0.77136600
H	2.05127700	1.04918800	-4.36177900	C	2.68114300	-1.12227900	1.23726700
H	4.02730700	-0.35501200	0.88101500	H	0.79622800	1.36530000	0.06932900
H	1.56647600	-2.75764900	2.16881100	C	1.53826000	-0.14617500	1.48769400
H	-0.06283000	-2.18039600	-2.78377100	H	2.45614000	1.65006800	0.66190800
H	1.66105100	5.51439700	-2.18085000	C	3.80942500	3.09127900	-1.46581700
H	7.10865100	3.00361800	-1.11959500	C	5.29635900	1.26436900	-2.08766000
H	6.23411000	-3.93818800	0.88623300	C	3.23654600	-1.87086000	2.20928200
H	-0.96109200	-6.20396500	0.01072900	C	0.22729300	-0.92411400	1.38349500
H	1.33287800	3.01438000	-5.68576400	H	1.64178400	0.31998700	2.47543500
H	6.26012400	0.00374000	1.86936200	C	4.91764800	3.88342200	-1.17778000

H	2.80018600	3.48551300	-1.35241900	C	-5.44842200	1.62497700	1.90455000
C	6.39443300	2.07475500	-1.79370100	C	0.52228600	4.92978000	-0.29075400
H	5.43438600	0.24846300	-2.45984600	C	0.82146900	-4.32835400	-2.54480000
C	4.32921600	-2.84689600	2.13741200	C	-6.58857200	-2.56530200	-2.13565700
H	0.25289700	-1.79208400	2.04894200	C	-6.41158100	1.82591600	0.91129300
H	0.15060700	-1.31847000	0.35623000	C	0.10016500	5.67005800	0.81707200
C	6.22623700	3.39032100	-1.33318200	H	-2.32258300	-4.05670600	-1.24260600
H	4.76726300	4.90875800	-0.82973800	H	-3.55010700	-2.49625300	-3.68951100
H	7.40348300	1.67851900	-1.93063700	H	-4.36263300	2.12552200	-1.79547000
C	4.86631600	-3.35998600	0.93643600	H	-2.37892100	3.62059300	1.93716300
C	4.88062600	-3.30986400	3.35229200	H	0.33190900	-0.95984800	-2.68167100
C	7.40870700	4.26285200	-1.01174700	H	-4.65186100	-1.06164600	0.23499500
C	5.91595300	-4.28004900	0.95724300	H	-3.35144600	1.43816300	2.35585200
H	4.45352900	-3.06549100	-0.02605000	H	0.26872600	3.13433800	-1.45602200
C	5.93079600	-4.22676300	3.37129700	H	-0.60791600	-5.76814700	-1.78881800
H	4.47239800	-2.93446400	4.29439700	H	-5.89231300	-3.23381100	-4.07404100
H	8.35805600	3.76084300	-1.24652700	H	-6.76041800	2.17230100	-1.19616400
H	7.36694000	5.20800200	-1.57749000	H	-1.28313900	5.76673900	2.47979200
H	7.41759100	4.53084100	0.05822400	H	2.03226700	-2.65486300	-3.22315000
C	6.45730500	-4.71556700	2.17084100	H	-6.99494500	-1.80579800	-0.14940800
H	6.31081200	-4.66459800	0.01341100	H	-5.75136400	1.47688900	2.94381100
H	6.33979300	-4.56378500	4.32715200	H	1.33247100	5.30176300	-0.92260000
H	7.27965400	-5.43510200	2.18102700	H	1.57596400	-5.08339400	-2.77882400
P	-2.27145000	-1.10962900	-1.37860200	H	-7.61704600	-2.89248500	-2.30707300
P	-1.90285500	1.60950400	-0.17803400	H	-7.47310800	1.83197600	1.16987200
C	-1.86729800	1.49167700	-2.00347700	H	0.58078900	6.62176400	1.05611900
C	-1.11575100	-2.39634500	-1.94513400	Co	-1.70140100	-0.41765700	0.70176400
C	-3.95413000	-1.73013800	-1.69997900	C	-2.37488700	-2.04190800	2.69252700
C	-3.68555400	1.79060900	0.23819800	H	-2.89088100	-2.83299600	3.26504700
C	-1.13605500	3.22696000	0.20096600	O	-2.22324100	-2.18227000	1.45782800
C	-1.37089000	-3.75272500	-1.68374300	C	-1.85977900	-0.86728400	3.33371900
C	-4.30508800	-2.34211600	-2.91481700	C	-2.10636500	-0.55609600	4.68472500
C	-4.65756600	1.99721300	-0.75298600	C	-1.11130500	0.00315300	2.46847200
C	-1.56171700	3.97719800	1.30993300	C	-1.63050900	0.64033300	5.20601500
C	0.11686200	-2.01253900	-2.49636100	H	-2.68690800	-1.24797100	5.30090000
C	-4.92599200	-1.54076800	-0.70636100	C	-0.64379100	1.20555500	3.04060000
C	-4.09161500	1.60410400	1.57298800	C	-0.90791400	1.51705900	4.37222300
C	-0.08808200	3.71102900	-0.60061700	H	-1.81528700	0.90395200	6.24924600
C	-0.40413300	-4.71334600	-1.98878300	H	-0.08210700	1.91639200	2.43521800
C	-5.62035300	-2.75749300	-3.12899500	H	-0.55039400	2.46811600	4.77596700
C	-6.01236800	2.01669400	-0.41527600	H	2.83480500	-1.72197400	3.21775900
C	-0.94331600	5.19100600	1.61562700	C	-2.04787100	0.27911800	-2.54218000
C	1.08030400	-2.97774200	-2.79855400	H	-2.10089200	0.11930300	-3.62443600
C	-6.24139700	-1.95777100	-0.92563300	H	-1.75419300	2.39449500	-2.61097700

TS3_T				P	-2.57159300	1.03601000	-0.55726100
N	1.86879200	0.37238300	-0.54570700	C	-2.05643900	0.55172500	-2.24414200
S	2.22645600	0.91814500	-2.08949300	C	0.28101900	-2.74986100	-1.27480900
C	2.82515600	-0.56443100	0.07623100	C	-2.59771100	-2.92321400	-1.23756900
C	1.41458000	1.37261500	0.43505000	C	-4.36765800	0.71822900	-0.47191700
O	1.07586600	1.72568700	-2.51245200	C	-2.37979100	2.85183400	-0.51950700
O	2.64400000	-0.25069100	-2.86883400	C	0.66344000	-3.56722300	-0.19359200
C	3.63408300	2.00038800	-1.93291800	C	-2.50451100	-3.99971700	-2.13502300
H	3.86742100	-0.37008100	-0.23333400	C	-5.13194300	0.44225400	-1.61508900
H	2.57649300	-1.59009300	-0.22489400	C	-3.24011600	3.65743600	0.24230100
C	2.67302100	-0.32377300	1.55854800	C	1.06349100	-2.72386900	-2.43438100
H	0.39898800	1.70056800	0.18754300	C	-3.78923500	-2.71107700	-0.52736800
C	1.50595200	0.62917800	1.77505500	C	-4.97374500	0.68318600	0.79499700
H	2.07473700	2.25753200	0.46092200	C	-1.27927100	3.43446700	-1.17064300
C	3.43869300	3.35939000	-1.65581900	C	1.81066200	-4.35491800	-0.27947500
C	4.92116400	1.46667300	-2.05080200	C	-3.59753300	-4.84832200	-2.32320500
C	3.40355200	-0.84949400	2.56048300	C	-6.48948300	0.13718400	-1.48982000
C	0.27949500	-0.20657200	2.14390400	C	-3.00584400	5.03067000	0.34590600
H	1.70632800	1.33826600	2.58830400	C	2.21766900	-3.51057900	-2.51290000
C	4.55027500	4.18072200	-1.48245200	C	-4.88039300	-3.56204700	-0.72139300
H	2.42963500	3.76792500	-1.59193500	C	-6.33292400	0.38547100	0.91400700
C	6.02171800	2.30614600	-1.87271600	C	-1.05224400	4.80948800	-1.06302000
H	5.05750000	0.41280000	-2.29628800	C	2.59170800	-4.32539100	-1.44215600
C	4.49966700	-1.82293600	2.50771000	C	-4.78743300	-4.62910300	-1.61948100
H	0.25252000	-0.42863300	3.21509200	C	-7.09156900	0.10776500	-0.22782400
H	0.31168400	-1.19911700	1.62484600	C	-1.91190600	5.61028500	-0.30467200
C	5.85743200	3.67006600	-1.58362700	H	0.05931300	-3.58324000	0.71773500
H	4.40365400	5.24306400	-1.27055400	H	-1.57789700	-4.17713900	-2.68584500
H	7.02935200	1.89425800	-1.96765300	H	-4.66918900	0.45172300	-2.60352400
C	4.84489200	-2.57845200	1.36514600	H	-4.09430900	3.21826900	0.76006100
C	5.24964400	-2.03548000	3.68516900	H	0.80424000	-2.07105400	-3.26629800
C	7.04364400	4.57715500	-1.40247700	H	-3.86180300	-1.88719200	0.18011700
C	5.89920100	-3.49247200	1.40359000	H	-4.38139900	0.88630100	1.68803800
H	4.27820400	-2.48365700	0.44195200	H	-0.59088700	2.81914600	-1.75303400
C	6.30544000	-2.94548600	3.72023800	H	2.10538500	-4.98170700	0.56524600
H	4.99069100	-1.46986100	4.58424100	H	-3.52046100	-5.68417300	-3.02294500
H	7.98945100	4.01779000	-1.43414200	H	-7.07838700	-0.08306200	-2.38339200
H	7.07277600	5.34436500	-2.19449000	H	-3.68221800	5.64971000	0.94026000
H	6.98828100	5.11262100	-0.44065500	H	2.83205700	-3.47326100	-3.41517700
C	6.63781400	-3.67919900	2.57629200	H	-5.80489200	-3.38805600	-0.16570400
H	6.14094700	-4.06880600	0.50682600	H	-6.79782500	0.36188400	1.90245300
H	6.86974100	-3.08658300	4.64551800	H	-0.19867400	5.25627400	-1.57923200
H	7.46250200	-4.39570000	2.60043200	H	3.49775100	-4.93283600	-1.50603300
P	-1.21172800	-1.73884500	-1.02258600	H	-5.64104800	-5.29477100	-1.76938100

H	-8.15287900	-0.13454700	-0.13387800	C	4.49847200	-2.72796500	2.10972700
H	-1.73113000	6.68477900	-0.22190900	H	0.29823700	-1.80594700	2.09546100
Co	-1.22248300	-0.28523500	0.83560900	H	0.14938200	-1.33240500	0.37700300
C	-2.77360800	-0.87420500	3.14612100	C	6.13853400	3.44395000	-1.41222200
H	-3.41543900	-1.33668300	3.92241200	H	4.66080300	4.93799800	-0.89105600
O	-2.46497300	-1.52327100	2.13701300	H	7.33678900	1.75166000	-2.02337000
C	-2.32862400	0.48700200	3.32183500	C	4.99375200	-3.27340300	0.90524000
C	-2.87421900	1.30618600	4.32896700	C	5.14335700	-3.09550600	3.31105600
C	-1.38458400	0.98835200	2.37236800	C	7.30993300	4.33647800	-1.10558300
C	-2.51079200	2.64562400	4.40644500	C	6.09465100	-4.13170400	0.90824800
H	-3.59975000	0.87987000	5.02747800	H	4.50644700	-3.05450200	-0.04294000
C	-1.02907100	2.34356600	2.48585400	C	6.24519200	-3.94966100	3.31183800
C	-1.59360100	3.15486300	3.47281300	H	4.76821400	-2.69297400	4.25573900
H	-2.93324400	3.29463700	5.17599900	H	8.26531900	3.84598700	-1.34020300
H	-0.32182300	2.79602300	1.79207600	H	7.25164100	5.27506600	-1.68081400
H	-1.30926800	4.20949000	3.51483700	H	7.32003200	4.61581800	-0.03858300
H	3.15993000	-0.50203100	3.57037800	C	6.73016800	-4.47023600	2.10713100
C	-1.43340600	-0.62069700	-2.44657800	H	6.45607900	-4.54431400	-0.03712100
H	-1.13814500	-0.93061500	-3.45459700	H	6.72797800	-4.21212600	4.25662900
H	-2.26059200	1.23226600	-3.07753400	H	7.59269400	-5.14114200	2.10339300
TS3_{oss}				P	-2.27596800	-1.21771700	-1.33019500
N	2.21096800	0.02963300	-0.74544600	P	-2.00091500	1.58692300	-0.21794100
S	2.54822300	0.71792700	-2.22014300	C	-1.95397800	1.38906500	-2.03420100
C	3.08485200	-1.04418900	-0.24384400	C	-1.10467400	-2.48905700	-1.89946000
C	1.72375300	0.86484000	0.36058900	C	-3.95701000	-1.86375400	-1.60181300
O	1.38199300	1.54301100	-2.56774200	C	-3.78734000	1.76961400	0.17357600
O	2.96739200	-0.37658100	-3.10406900	C	-1.25674700	3.21884500	0.12040600
C	3.94128300	1.79658600	-1.96645300	C	-1.32461200	-3.84789300	-1.61875200
H	4.15880800	-0.81899400	-0.38356100	C	-4.30771700	-2.55359600	-2.77437500
H	2.86483700	-1.97938700	-0.77943400	C	-4.72645700	2.13266000	-0.80418400
C	2.74652400	-1.10286000	1.22606800	C	-1.70325300	3.98073300	1.21336100
H	0.77711400	1.33590700	0.08751800	C	0.11280400	-2.08312700	-2.46919300
C	1.58221000	-0.15686700	1.49077900	C	-4.92943600	-1.60900400	-0.62282500
H	2.44773700	1.65219400	0.63739900	C	-4.22776100	1.44854400	1.46949100
C	3.72560500	3.10395400	-1.51340700	C	-0.19355900	3.69087700	-0.66779300
C	5.23514300	1.30202600	-2.15366900	C	-0.33861000	-4.78903100	-1.92323800
C	3.36211200	-1.80495100	2.19677900	C	-5.62274400	-2.98312400	-2.96031900
C	0.29359200	-0.95653600	1.40720100	C	-6.08647000	2.16762100	-0.48993400
H	1.68432500	0.31427800	2.47642400	C	-1.09284600	5.19998400	1.51351800
C	4.82387300	3.91513500	-1.24066200	C	1.09567800	-3.02894100	-2.76974700
H	2.71134300	3.48086000	-1.38606600	C	-6.24501000	-2.03780000	-0.81607800
C	6.32303500	2.13117200	-1.87441300	C	-5.58963800	1.48907600	1.77959700
H	5.38575600	0.28782800	-2.52564700	C	0.40758700	4.91574900	-0.36352400
				C	0.87144800	-4.38213700	-2.49730600

C	-6.59151900	-2.72513700	-1.98285000	S	3.14148100	-1.67163600	0.04173700
C	-6.52123600	1.84345900	0.79972500	C	3.77360900	0.68456500	-1.08911900
C	-0.03678200	5.67036100	0.72615400	C	1.81717400	-0.41028900	-1.95369300
H	-2.26334200	-4.16961700	-1.16234800	O	2.18652200	-2.74776500	-0.27994100
H	-3.55364800	-2.75685200	-3.53831600	O	2.99092400	-0.96253600	1.32899300
H	-4.40265200	2.37431700	-1.81816800	C	4.79798800	-2.31258300	-0.02086700
H	-2.53037700	3.62648000	1.83044000	H	4.16647000	0.77539200	-0.06451100
H	0.30219100	-1.02778700	-2.66812400	C	2.70033100	1.71509100	-1.39095700
H	-4.65842700	-1.06964400	0.28605400	H	4.62761000	0.77637800	-1.78014900
H	-3.50902100	1.15523100	2.23584300	H	1.10811900	-1.20874900	-1.70689200
H	0.18011000	3.10086700	-1.50680800	C	1.37723300	0.98603300	-1.50361100
H	-0.51517600	-5.84575200	-1.70819700	H	1.99379200	-0.43080100	-3.04035000
H	-5.89400600	-3.52106500	-3.87191900	C	5.20683800	-3.03109100	-1.15096000
H	-6.81131700	2.44372000	-1.25932600	C	5.64200500	-2.13581200	1.07461400
H	-1.44795700	5.78672400	2.36404400	C	2.84093600	3.04211400	-1.56825400
H	2.03548400	-2.68892300	-3.20786100	C	0.67499800	0.93397200	-0.12368500
H	-6.99880500	-1.83398500	-0.05212000	H	0.69661400	1.44881700	-2.22690100
H	-5.92143700	1.23406100	2.78885800	C	6.48816600	-3.57127900	-1.17374500
H	1.22860600	5.28158300	-0.98499000	H	4.53081000	-3.16096800	-1.99800500
H	1.64128900	-5.12188100	-2.73015800	C	6.92576500	-2.68525900	1.03166300
H	-7.61985900	-3.06303000	-2.13282600	H	5.29600000	-1.57785300	1.94540700
H	-7.58714200	1.86491000	1.03877500	C	4.03876800	3.88499100	-1.47401500
H	0.43733300	6.62655900	0.96026700	Co	-1.86817500	-0.17412700	-0.29748200
Co	-1.67367200	-0.43790800	0.74137700	H	1.39740200	0.63540800	0.64780500
C	-2.32319000	-1.98814600	2.87352700	H	-0.01312100	0.05514800	-0.14487900
H	-2.76744400	-2.77543700	3.50932400	C	7.36842800	-3.40869600	-0.08527400
O	-2.28180900	-2.15637800	1.63471200	H	6.81815000	-4.13351600	-2.05116300
C	-1.78067100	-0.79059900	3.44828400	H	7.59424700	-2.55005600	1.88530500
C	-1.90975000	-0.46714600	4.81350200	C	3.95679100	5.20329000	-1.97300800
C	-1.11904300	0.07882800	2.51484600	C	5.26502100	3.47355900	-0.90833500
C	-1.40470900	0.74018800	5.27997200	O	-1.69742500	0.92113800	-1.84802600
H	-2.42179900	-1.16020800	5.48653000	C	0.00649900	2.21657400	0.30122900
C	-0.61111200	1.28844100	3.03229100	C	8.75017500	-4.00057000	-0.13571200
C	-0.76354900	1.61399600	4.37894200	C	5.05225500	6.06491900	-1.93316600
H	-1.50268100	1.01326700	6.33257000	H	3.01160700	5.54681700	-2.40173400
H	-0.10200700	1.99353700	2.37522800	C	6.36046100	4.33816400	-0.86644300
H	-0.37875100	2.57108900	4.74145300	H	5.36919700	2.48128100	-0.47393800
H	2.98776000	-1.64879300	3.21459400	C	-2.17977800	1.66418500	-0.88396300
C	-2.09726700	0.15125500	-2.52580800	C	-1.32583200	2.54889200	-0.05816500
H	-2.13856400	-0.04796200	-3.60219900	C	0.72862200	3.10988400	1.10175700
H	-1.85965600	2.26707900	-2.68049700	H	9.29554600	-3.83934200	0.80513000
				H	8.70627000	-5.08485000	-0.32972300
5s				H	9.33793300	-3.55325400	-0.95482000
N	3.10813200	-0.62379600	-1.26725300	C	6.26402800	5.63436000	-1.38213400

H	4.96033200	7.07856800	-2.33152300	H	1.28837600	-4.06927500	4.69698300
H	7.29772500	3.99586200	-0.42026500	C	-5.60252400	1.20722800	-3.66896000
H	-3.24023600	1.97127800	-0.93464000	H	-3.85327600	-0.05237300	-3.53811800
C	-1.89708800	3.73308400	0.43905200	C	-6.95778500	1.36709000	-1.66572800
C	0.16279100	4.30529700	1.55305800	H	-6.27836100	0.22850600	0.03706300
H	1.75052400	2.85236000	1.38782000	C	-1.77499300	-4.15554100	-2.56585400
H	7.12464000	6.30690400	-1.34761900	H	-1.34527700	-2.56486700	-1.17110400
C	-1.16040300	4.61442200	1.22807300	C	-4.03755300	-4.22351500	-3.43784700
H	-2.93596900	3.96069100	0.18702300	H	-5.38085700	-2.68287200	-2.73431600
H	0.75091900	4.98360000	2.17565500	C	-6.71684300	1.72184800	-2.99627700
H	-1.61971000	5.53461400	1.59608900	H	-5.41227200	1.48617300	-4.70794400
P	-2.30570400	-0.71172800	1.79862000	H	-7.82704700	1.76739900	-1.13896600
C	-2.56987900	0.78956200	2.80371800	C	-2.74308700	-4.75219000	-3.38034400
C	-3.91937900	-1.57235400	1.83722000	H	-0.76245100	-4.56304100	-2.52087900
C	-1.17101700	-1.76685500	2.75227400	H	-4.79140800	-4.69030200	-4.07619400
C	-1.50012000	1.36063400	3.50983900	H	-7.39860700	2.40263000	-3.51159900
C	-3.80916900	1.44773000	2.76138300	H	-2.48738000	-5.63234900	-3.97518900
C	-4.57552000	-1.70736500	0.67760100	H	1.93206200	3.58755300	-1.84093100
H	-4.31215400	-1.96030600	2.78316700				
C	-0.03754400	-2.28551200	2.11187200	5_T			
C	-1.41746000	-2.07850600	4.10107500	N	3.33222000	-0.32764500	-1.61937800
H	-0.52879700	0.86195700	3.53508000	S	3.18104000	-1.68460200	-0.64918000
C	-1.67758200	2.57214700	4.18098200	C	3.97945100	0.86237300	-1.02466600
C	-3.98114000	2.65590400	3.44018000	C	2.15081800	0.10625700	-2.39483600
H	-4.63998000	1.01970900	2.19651700	O	2.30651500	-2.61155500	-1.39000900
P	-3.76011100	-1.05415500	-0.81491100	O	2.82311400	-1.35194100	0.74511000
H	-5.54134100	-2.21736500	0.59471900	C	4.84538900	-2.31224100	-0.63781800
C	0.84725800	-3.11141700	2.81081600	H	4.18915900	0.69027400	0.04321900
H	0.17737200	-2.03871200	1.07198300	C	2.98715700	1.99239400	-1.23950400
C	-0.53456400	-2.90733900	4.79309900	H	4.94137500	1.06449600	-1.52292100
H	-2.29296500	-1.66770200	4.60944300	H	1.40087400	-0.68907300	-2.44705900
C	-2.91669900	3.21920900	4.15065100	C	1.67744000	1.36185700	-1.66297800
H	-0.84071700	3.01565800	4.72506800	H	2.47700300	0.34659900	-3.41928400
H	-4.94952900	3.16095200	3.41004200	C	5.46417100	-2.61914300	-1.85588800
C	-4.97307200	-0.02454100	-1.68018100	C	5.48663300	-2.53310300	0.58013300
C	-3.40256000	-2.49858400	-1.86376600	C	3.18221000	3.31832900	-1.11199000
C	0.59761500	-3.42406800	4.14852100	C	0.84189600	1.00289600	-0.39787100
H	1.73066500	-3.49501600	2.29896400	H	1.09594100	2.01647300	-2.32417000
H	-0.72621000	-3.14932600	5.84125900	C	6.75054000	-3.14725700	-1.84012300
H	-3.05084300	4.16770100	4.67603100	H	4.94575700	-2.43860800	-2.79927100
C	-4.72808200	0.33833600	-3.01567000	C	6.77855600	-3.06519600	0.57489000
C	-6.08679700	0.49762400	-1.00396000	H	4.98065300	-2.28845500	1.51478900
C	-2.10318200	-3.03051100	-1.80826600	C	4.37836700	4.05703500	-0.68978300
C	-4.37189200	-3.09728700	-2.68222900	Co	-2.03061900	-0.37463500	-0.66596600

H	1.50884200	0.87437100	0.46265600	C	-1.00425700	1.65427400	4.21797000
H	0.37474900	0.02284600	-0.55398700	H	-2.74995300	0.90276900	3.19508900
C	7.42951500	-3.37833500	-0.62726700	P	-4.29958800	-0.27859800	-0.26065900
H	7.24455000	-3.38652600	-2.78545000	H	-5.57931000	-1.01267100	1.81368100
H	7.28985700	-3.23886700	1.52484400	C	0.65342400	-4.47508200	0.85525400
C	4.40848500	5.45058800	-0.91495000	H	0.19729300	-2.60333900	-0.09835500
C	5.49920200	3.47012000	-0.06389400	C	-0.64242000	-5.01075000	2.83190200
O	-1.19106600	0.37764500	-2.34258900	H	-2.09037600	-3.54085900	3.45835700
C	-0.18692700	2.04499900	-0.04790400	C	0.37399600	1.52479900	4.41312700
C	8.82342600	-3.94326800	-0.63751700	H	2.16088300	0.42597200	3.87481900
C	5.51329600	6.22125000	-0.55466200	H	-1.56141900	2.43714200	4.73811300
H	3.54504700	5.92730600	-1.38674700	C	-5.22992100	1.28440300	-0.27382600
C	6.60435600	4.24293800	0.29787700	C	-5.20435700	-1.46270700	-1.31596600
H	5.50768800	2.40666700	0.16774000	C	0.35349700	-5.34586000	1.90563800
C	-1.86583100	1.34095400	-1.85788100	H	1.43966900	-4.70949000	0.13513900
C	-1.40726700	2.21926500	-0.76645400	H	-0.87612100	-5.69143300	3.65414600
C	0.08096300	2.92306700	1.00984700	H	0.89758200	2.20509500	5.08912600
H	9.20513900	-4.09988700	0.38138600	C	-5.65508500	1.83010900	-1.49787200
H	8.85304600	-4.90751300	-1.17121300	C	-5.38106400	2.03092800	0.90501700
H	9.51639800	-3.26586500	-1.16416500	C	-4.42903000	-2.44866800	-1.94825300
C	6.62138000	5.61938900	0.05145200	C	-6.59756200	-1.45672300	-1.48190500
H	5.50993800	7.29741400	-0.74592100	H	0.89775000	-6.28795900	2.00822100
H	7.45840800	3.76414700	0.78379300	C	-6.23052700	3.10130900	-1.53551600
H	-2.79804700	1.66012800	-2.36126300	H	-5.53632400	1.26117100	-2.42312100
C	-2.30638200	3.23750300	-0.37919000	C	-5.95663200	3.30387200	0.86155400
C	-0.81446900	3.92989100	1.37692900	H	-5.04171800	1.62479400	1.86065900
H	1.01056600	2.79844700	1.56756900	C	-5.04076800	-3.42214700	-2.74066000
H	7.48871900	6.21987200	0.33656300	H	-3.34233900	-2.45603500	-1.80787100
C	-2.01753700	4.08913700	0.68081100	C	-7.20472900	-2.42852400	-2.28114600
H	-3.24449600	3.34477900	-0.92739700	H	-7.20666500	-0.69336300	-0.99279400
H	-0.57300500	4.58755100	2.21515500	C	-6.38032500	3.84180200	-0.35688300
H	-2.72567000	4.86990200	0.96573100	H	-6.56241100	3.51716000	-2.48982000
P	-1.82237100	-1.29426400	1.46376300	H	-6.07159600	3.87698500	1.78463200
C	-0.96886600	-0.22477600	2.68327100	C	-6.42928400	-3.40960000	-2.90947000
C	-3.51776300	-1.42062100	2.13358200	H	-4.43385400	-4.18750400	-3.22999800
C	-1.03778300	-2.92836700	1.65790200	H	-8.28933800	-2.42121100	-2.41352900
C	0.41726000	-0.34839000	2.87264000	H	-6.82848500	4.83767200	-0.38964100
C	-1.67545400	0.78690100	3.35212800	H	-6.90956700	-4.16681600	-3.53395200
C	-4.55658500	-0.95862300	1.42178900	H	2.33374900	3.95668600	-1.37992700
H	-3.66816300	-1.84592900	3.13226700				
C	-0.05117600	-3.27586900	0.72327800	6s			
C	-1.33166100	-3.80188600	2.71791800	N	-2.94036800	-2.42099100	0.45826800
H	0.98665300	-1.11103300	2.33769200	S	-4.48535500	-3.02403500	0.50740700
C	1.08173000	0.52645900	3.73500300	C	-2.52312000	-1.41136400	1.45102700

C	-2.25841500	-2.20023000	-0.82835900	C	1.17411200	2.45546200	-2.42231800
O	-4.77787200	-3.28720300	1.92179700	C	-1.51070900	2.02047900	-1.42625200
O	-4.54223900	-4.10052900	-0.48837100	C	1.86151800	3.84619500	0.38178900
C	-5.57405700	-1.71639200	-0.03769600	C	-0.50729900	4.20014500	0.76425900
H	-3.24479600	-0.57357200	1.50160400	C	2.28309700	1.77144300	-2.73196700
C	-1.19663200	-0.94476500	0.89546300	H	0.85159500	3.32436600	-3.00587000
H	-2.46184800	-1.85977100	2.45475200	C	-1.85404400	2.14901000	-2.78181500
H	-2.73726200	-1.39210400	-1.41456100	C	-2.52789100	1.82273600	-0.47540000
C	-0.87185100	-1.76096500	-0.33572700	H	2.67605900	3.30059700	-0.09809100
H	-2.25710100	-3.12433800	-1.41873100	C	2.16009200	4.90453000	1.24001100
C	-6.14148200	-0.85181300	0.90536300	C	-0.20196600	5.25623100	1.62713300
C	-5.82580900	-1.55780900	-1.40302100	H	-1.55029100	3.93807500	0.58823400
C	-0.34387600	0.04329000	1.22364100	P	2.79040700	0.42404400	-1.61377900
C	0.03625800	-0.96701900	-1.25977900	H	2.89984000	2.03599300	-3.59789100
H	-0.34346100	-2.67445600	-0.00329200	C	-3.19391700	2.10278200	-3.17639000
C	-6.95695700	0.18938700	0.46545300	H	-1.08231000	2.27637700	-3.54208600
H	-5.95699800	-1.00941500	1.96873800	C	-3.86417600	1.78195200	-0.87496400
C	-6.64725300	-0.51156600	-1.82398800	H	-2.27949900	1.69737400	0.57618800
H	-5.39633900	-2.25480900	-2.12384900	C	1.12827400	5.60846000	1.86992900
C	-0.37531100	0.93732200	2.38619800	H	3.20300600	5.17612300	1.42004800
Co	1.10972700	0.16887800	-0.06785600	H	-1.01224500	5.80354600	2.11419800
H	-0.53600400	-0.35604400	-1.97196900	C	4.37283300	0.99606900	-0.90261100
H	0.73277300	-1.60678600	-1.81759300	C	3.24008500	-0.97314000	-2.69157800
C	-7.21833700	0.38098900	-0.90300900	C	-4.20039700	1.92502800	-2.22482300
H	-7.40389500	0.86714400	1.19758500	H	-3.44830700	2.20567600	-4.23385100
H	-6.84900600	-0.38499500	-2.89042400	H	-4.64657300	1.62427300	-0.13084700
C	0.81398600	1.61943400	2.72243800	H	1.36165400	6.43208200	2.54879600
C	-1.51298400	1.18084500	3.18692600	C	4.48023000	1.07498900	0.49355800
O	2.02452700	-1.41072600	0.65047300	C	5.45989600	1.37400000	-1.70757700
C	-8.06836600	1.53478000	-1.36044800	C	4.18097400	-1.91619400	-2.24600200
C	0.87753500	2.49689000	3.80258400	C	2.57383900	-1.17848800	-3.90988500
H	1.69942200	1.46407500	2.09805200	H	-5.24651900	1.89124300	-2.53264700
C	-1.45513100	2.06788600	4.26418000	C	5.66229100	1.53051500	1.08433400
H	-2.45594700	0.68223700	2.96323100	H	3.63901300	0.77306400	1.11962700
C	2.07432900	-1.82253700	1.81605800	C	6.63805000	1.83081200	-1.11489400
H	-8.27319700	1.48490700	-2.43943300	H	5.38660600	1.30518200	-2.79561100
H	-9.03103100	1.55811400	-0.82467300	C	4.45491300	-3.04796300	-3.01658700
H	-7.56485800	2.49451600	-1.15327700	H	4.70414600	-1.76323900	-1.29989700
C	-0.26238100	2.72754300	4.58056800	C	2.85592400	-2.31052900	-4.67918500
H	1.81315400	3.01227200	4.03151300	H	1.83184300	-0.45674600	-4.25956200
H	-2.35169300	2.24500200	4.86411500	C	6.73991200	1.91020600	0.27974300
H	-0.22268900	3.41904400	5.42564500	H	5.74032300	1.58647900	2.17256100
P	0.23848500	2.01165800	-0.91189500	H	7.48275700	2.12528200	-1.74226900
C	0.52415600	3.48426900	0.14231700	C	3.79382800	-3.24693900	-4.23361600

H	5.18958000	-3.77660000	-2.66550000	C	-7.33675900	0.05092300	-0.83565100
H	2.33906300	-2.46123700	-5.62997800	H	-7.50808600	0.80546300	1.18538500
H	7.66488300	2.26708800	0.73906000	H	-6.97319400	-0.96204600	-2.71019000
H	4.01131700	-4.13232500	-4.83576900	C	0.71724000	1.94510400	2.54944500
C	2.78940900	-3.03117600	2.18420100	C	-1.62314500	1.57570900	3.00650600
C	2.79966700	-3.43062600	3.53385200	O	2.01778700	-1.20575500	0.93459000
C	3.45541600	-3.80389200	1.20964800	C	-8.22670900	1.10984800	-1.42720100
C	3.47160300	-4.59318100	3.90789200	C	0.74712400	2.97795700	3.48416400
H	2.27721300	-2.82437400	4.27826100	H	1.62851900	1.69715100	1.99559300
C	4.12378300	-4.96175500	1.59018100	C	-1.59775000	2.61696900	3.93690700
H	3.43269100	-3.48260400	0.16691100	H	-2.56007600	1.04658100	2.83333200
C	4.13176500	-5.35530900	2.93735200	C	2.34148500	-2.38151600	0.73177200
H	3.48172400	-4.90925300	4.95303200	H	-8.42138200	0.92657500	-2.49358200
H	4.64010100	-5.56710700	0.84193200	H	-9.19412600	1.15607800	-0.90122800
H	4.65763200	-6.26728300	3.23068000	H	-7.76360400	2.10654800	-1.33056100
H	1.55992800	-1.26931100	2.62330300	C	-0.41487700	3.32201000	4.18325000
6''_s				H	1.67702500	3.52333200	3.66138700
N	-2.97046300	-2.41939800	0.82064200	H	-2.51188500	2.87937600	4.47608500
S	-4.49120200	-3.06502200	0.96414700	H	-0.39946200	4.13546600	4.91264000
C	-2.57701300	-1.27946000	1.67196700	P	0.11676200	1.87025500	-1.09877900
C	-2.30174600	-2.34607900	-0.48898300	C	0.35991600	3.48515900	-0.26728100
O	-4.76404000	-3.15912600	2.40335700	C	1.02391300	2.10772600	-2.67685600
O	-4.51613600	-4.25943100	0.11153300	C	-1.63761500	1.75616600	-1.58863700
C	-5.62803300	-1.87385900	0.27177900	C	1.68389900	3.92166700	-0.08525800
H	-3.31795400	-0.45947500	1.61186500	C	-0.69582100	4.25159700	0.24469800
C	-1.25918700	-0.86280800	1.05801800	C	2.15465600	1.42266700	-2.89685000
H	-2.50807500	-1.59113100	2.72549100	H	0.66117700	2.85932300	-3.38619300
H	-2.80150400	-1.62800700	-1.16754700	C	-1.99608400	1.65374900	-2.94252200
C	-0.92246900	-1.82060800	-0.06407000	C	-2.64228500	1.68970000	-0.60619600
H	-2.28446600	-3.33666800	-0.95899700	H	2.51937900	3.34106500	-0.47793500
C	-6.20530700	-0.90596800	1.10181900	C	1.94519900	5.10480800	0.60587700
C	-5.90175100	-1.90347700	-1.09807600	C	-0.42743700	5.43276300	0.94147200
C	-0.41912800	0.16744700	1.25982700	H	-1.72954900	3.93568900	0.10914500
C	-0.03103900	-1.12919400	-1.08465000	P	2.73184000	0.32081400	-1.56710300
H	-0.38510300	-2.67937100	0.38000500	H	2.74637900	1.56378600	-3.80756900
C	-7.05287300	0.04815000	0.54167200	C	-3.33731800	1.51151300	-3.30863600
H	-6.00254200	-0.91594900	2.17349400	H	-1.23460400	1.67512100	-3.72293600
C	-6.75476100	-0.94148800	-1.63986500	C	-3.98034500	1.55090100	-0.97806300
H	-5.46380000	-2.67921100	-1.72759400	H	-2.38395100	1.74720700	0.44908200
C	-0.46307400	1.21534700	2.28555300	C	0.88971700	5.86065000	1.12661600
Co	1.02631200	0.15327900	-0.04925300	H	2.97841800	5.43306000	0.74148500
H	-0.62003800	-0.62853500	-1.86502200	H	-1.25676900	6.01953100	1.34308200
H	0.67410200	-1.81799600	-1.57268000	C	4.19891900	1.15415800	-0.86811900
				C	3.34716200	-1.20568900	-2.33655500

C	-4.33148900	1.46495300	-2.32902200	O	5.29233400	-2.90472700	1.97241100
H	-3.60216100	1.43590700	-4.36584500	C	4.65727400	-0.50076300	1.07405900
H	-4.75280600	1.49657300	-0.20896500	H	2.31135500	-4.20291300	0.50486800
H	1.09422800	6.78326700	1.67500500	C	1.60226400	-2.16775100	0.17001000
C	4.29626100	1.26659700	0.52813500	H	2.81458400	-3.08610200	1.77770000
C	5.19567000	1.71450500	-1.68362100	H	3.09836600	-3.10786600	-2.04390900
C	4.39440000	-1.91840300	-1.72877700	C	2.23394900	-1.40186000	-0.96752900
C	2.68138300	-1.75614900	-3.44497700	H	4.25677900	-1.76753400	-1.84779800
H	-5.37870100	1.35498500	-2.61440700	C	4.91202700	0.51168600	0.14350200
C	5.37903900	1.93660700	1.10442900	C	3.89958300	-0.24628400	2.22145300
H	3.52731200	0.82724600	1.16744000	C	0.30304400	-1.91411300	0.43762700
C	6.27307600	2.38625800	-1.10349700	C	1.13303000	-1.04663500	-1.94645600
H	5.13027600	1.62741700	-2.77053500	H	2.66233800	-0.46538000	-0.57306400
C	4.77198600	-3.16739200	-2.22837800	C	4.34597400	1.77197500	0.33828200
H	4.91750600	-1.49831000	-0.86727700	H	5.53156100	0.30599000	-0.73044800
C	3.06973800	-3.00116000	-3.94406400	C	3.35199600	1.02265400	2.40510300
H	1.85722800	-1.21447600	-3.91572900	H	3.74287000	-1.03359400	2.95989900
C	6.36453800	2.49977500	0.28910700	C	-0.58157300	-2.63379000	1.36416000
H	5.44893100	2.02043500	2.19140600	Co	-0.22317600	-0.34291900	-0.64607300
H	7.04537300	2.82450900	-1.74009900	H	0.62737200	-1.94287500	-2.33839200
C	4.11170300	-3.70993300	-3.33486900	H	1.44518800	-0.40240900	-2.77473200
H	5.58526500	-3.71699900	-1.74889500	C	3.53353800	2.04119500	1.45302600
H	2.55458200	-3.42162000	-4.81097600	H	4.53141000	2.56117000	-0.39387500
H	7.20873100	3.02829100	0.73842800	H	2.76757000	1.22971700	3.30322100
H	4.40980700	-4.68569200	-3.72565600	C	-1.61088000	-1.95893800	2.05277200
C	3.31198500	-3.08614500	1.55152600	C	-0.48581000	-4.03046600	1.55003500
C	3.62733500	-4.41934100	1.22838700	O	-0.25128200	1.08454700	0.85749600
C	3.95758500	-2.44618100	2.62911400	C	2.84441700	3.36883500	1.60968300
C	4.58175200	-5.10753900	1.97522500	C	-2.48961400	-2.63405200	2.90016000
H	3.12403700	-4.90279400	0.38756400	H	-1.74418100	-0.88990500	1.90418200
C	4.90999000	-3.13825200	3.36904000	C	-1.36479200	-4.70895900	2.39510500
H	3.70277800	-1.41235900	2.86910900	H	0.26842000	-4.59600700	1.00181400
C	5.22197500	-4.46653200	3.04197700	C	0.08653400	0.92454100	2.03766600
H	4.83014600	-6.14183600	1.72826500	H	2.77507600	3.66799700	2.66615300
H	5.41561900	-2.64929600	4.20453500	H	3.36065200	4.16233300	1.04984800
H	5.97214700	-5.00513000	3.62619500	H	1.81183500	3.30979300	1.22436400
H	1.89522100	-2.94223900	-0.10984800	C	-2.37012100	-4.01569100	3.07897800
				H	-3.27876400	-2.07704900	3.41172800
6_T				H	-1.27074500	-5.79165700	2.51266900
N	3.84603400	-2.89886700	-0.08900300	H	-3.05946300	-4.55012900	3.73714300
S	5.14520200	-2.18203400	0.70425600	P	-2.47857100	-0.80755300	-1.24441700
C	2.61981700	-3.16321000	0.69911000	C	-3.90019700	-0.27733200	-0.23054900
C	3.42233300	-2.29608800	-1.37220800	C	-2.73612600	0.01204500	-2.86154000
O	6.23910900	-2.13004300	-0.27070100	C	-2.68881900	-2.57937100	-1.60429200

C	-3.67485800	0.65773800	0.79225800	H	-2.48625200	6.18435500	0.54132000
C	-5.20219800	-0.74368600	-0.47452600	H	3.95296600	3.37818800	-5.08623100
C	-1.90317800	0.99158600	-3.24300600	C	-0.26021900	1.86759400	3.08415000
H	-3.59238100	-0.28391900	-3.47878900	C	0.11222500	1.58562500	4.41209200
C	-2.15266800	-3.08863100	-2.79950100	C	-0.97914200	3.04181900	2.78033600
C	-3.23901100	-3.45893600	-0.65903300	C	-0.22926700	2.47420700	5.42988400
H	-2.66797100	1.03389600	0.97208400	H	0.66222000	0.66798700	4.63505500
C	-4.73971200	1.11636500	1.57064500	C	-1.31457300	3.92471700	3.80026300
C	-6.26306900	-0.28497200	0.30933800	H	-1.25738800	3.24447600	1.74648600
H	-5.38725000	-1.46903600	-1.26958900	C	-0.93954900	3.64093800	5.12249100
P	-0.55462800	1.47937800	-2.11768500	H	0.05488700	2.26193500	6.46256700
H	-2.06950900	1.53691600	-4.17759400	H	-1.86800900	4.83837100	3.57270300
C	-2.18199400	-4.46190800	-3.05065000	H	-1.20551700	4.33761400	5.92120700
H	-1.70653100	-2.41193300	-3.53269900	H	0.65433700	0.02370100	2.33164500
C	-3.26551900	-4.83127300	-0.91696200				
H	-3.63585700	-3.07754400	0.28227000	TS4s			
C	-6.03340300	0.64273900	1.33208500	N	3.15157000	1.15464800	0.25616200
H	-4.55528400	1.84451200	2.36404600	S	4.70126300	1.71012800	0.37142000
H	-7.27443500	-0.65268800	0.12056700	C	2.48052100	0.46768500	1.35845900
C	-1.18434700	3.01748000	-1.32937800	C	2.23810300	1.54209900	-0.81839400
C	0.84697900	2.07233200	-3.12782700	O	5.07389200	1.61850500	1.78991600
C	-2.73863700	-5.33520300	-2.11005000	O	4.77436900	2.99022700	-0.34490800
H	-1.76708600	-4.85097800	-3.98353900	C	5.70688900	0.54340000	-0.53276300
H	-3.69361900	-5.50952800	-0.17538100	H	2.75933100	-0.59453800	1.43459900
H	-6.86677900	0.99707600	1.94360200	C	1.02255700	0.65651200	1.04609200
C	-2.55460000	3.17576600	-1.07285000	H	2.72191200	0.94396000	2.32434900
C	-0.28578700	4.00894400	-0.90173700	H	2.20540000	0.77253100	-1.60600400
C	2.11552600	2.08493200	-2.52119300	C	0.88228800	1.63968300	-0.09196900
C	0.70728500	2.53162600	-4.44543100	H	2.54911700	2.49544200	-1.26140300
H	-2.75865500	-6.40984400	-2.30663900	C	6.25547800	-0.55290100	0.13501300
C	-3.01864500	4.31079900	-0.40176100	C	5.91566200	0.73391200	-1.90250000
H	-3.26766800	2.41800600	-1.39766600	C	-0.07715800	0.09880600	1.61577100
C	-0.75422700	5.14205300	-0.23344200	C	-0.35093100	1.36505200	-0.94178500
H	0.78314600	3.90383000	-1.09146100	H	0.82304100	2.64535800	0.36313700
C	3.22622600	2.55977400	-3.21990800	C	7.02002000	-1.47257300	-0.58569200
H	2.23778600	1.71067300	-1.50229700	H	6.09463700	-0.67671600	1.20701100
C	1.82483700	2.99724000	-5.14479200	C	6.67939400	-0.19476600	-2.60592200
H	-0.26642500	2.53529500	-4.93735500	H	5.49425000	1.60625000	-2.40394600
C	-2.12176500	5.29699400	0.01839400	C	-0.11740300	-0.98882200	2.60709800
H	-4.08852900	4.42115800	-0.20921800	H	-1.23439700	3.96533900	1.02309200
H	-0.04518600	5.90581500	0.09448800	Co	-1.57115900	0.24859300	0.10969700
C	3.08260000	3.01433600	-4.53503100	H	-0.09226600	0.86261700	-1.88504400
H	4.20752000	2.56398200	-2.73995600	H	-0.90245100	2.28476100	-1.16810400
H	1.70924500	3.35018600	-6.17231100	C	7.24516000	-1.31058600	-1.96230300

H	7.45568900	-2.33028100	-0.06734400	H	-3.27058100	-0.60712100	-3.76349900
H	6.84905200	-0.04916400	-3.67608400	C	2.70114400	-1.69041500	-2.81804700
C	-1.31068300	-1.73390700	2.70295400	H	0.67098900	-1.24220200	-3.38251200
C	0.95457600	-1.35465200	3.44649400	C	3.04301700	-2.41481300	-0.53529900
O	-2.23090100	1.69085500	1.15831100	H	1.28389800	-2.51723000	0.70717200
C	-0.59671500	3.87831900	1.90436400	C	-2.77743100	-5.55491100	0.70404600
C	8.07638300	-2.29412000	-2.74047400	H	-4.60121200	-4.39516800	0.86490900
C	-1.42128300	-2.82974100	3.55571400	H	-0.82992400	-6.44918200	0.40918100
H	-2.15950300	-1.44242100	2.07845700	C	-4.77437100	-0.08153000	-0.83460800
C	0.84461400	-2.45206300	4.30549100	C	-3.40155300	2.11591400	-2.18756100
H	1.87835000	-0.77851200	3.44618400	C	3.55929500	-2.10707200	-1.79760400
C	-1.40999700	1.52122100	2.16084100	H	3.10132500	-1.44313200	-3.80392200
C	-0.58293300	2.67000000	2.61526300	H	3.71287600	-2.73616100	0.26521400
C	0.18866600	4.95230100	2.33429400	H	-3.22563900	-6.46823600	1.10235100
H	8.99476400	-1.81537700	-3.12020400	C	-5.06849000	0.09153700	0.52894300
H	8.37148700	-3.15422400	-2.12266300	C	-5.70327700	-0.71615000	-1.67530500
H	7.52590600	-2.66974900	-3.61838800	C	-4.21078900	3.05388600	-1.52629300
C	-0.33529400	-3.20042800	4.35668400	C	-2.71318600	2.48457100	-3.35441100
H	-2.35289400	-3.39921600	3.59019500	H	4.63173600	-2.18187800	-1.98051200
H	1.69065600	-2.72183700	4.94266000	C	-6.28410900	-0.36758800	1.04340500
H	-1.75106900	0.87938800	2.98994600	H	-4.34577900	0.58617100	1.18146000
C	0.21380300	2.54808100	3.76645700	C	-6.91250600	-1.17763700	-1.15184500
C	0.99461500	4.82047100	3.46810400	H	-5.48558100	-0.85631500	-2.73585500
H	0.17357700	5.89363100	1.77969500	C	-4.33543100	4.34721800	-2.03705900
H	-0.41214000	-4.06148400	5.02488500	H	-4.74386600	2.77519700	-0.61525400
C	1.00427800	3.61577300	4.18594500	C	-2.84677600	3.77926800	-3.86197500
H	0.21940500	1.60502300	4.31904200	H	-2.07007900	1.76509700	-3.86654700
H	1.61416400	5.65733400	3.79967900	C	-7.20343300	-1.00625400	0.20631600
H	1.62933900	3.51558800	5.07649300	H	-6.50954600	-0.22954700	2.10350900
P	-0.95691500	-1.62690400	-0.95492700	H	-7.63132900	-1.67451200	-1.80766400
C	-1.61883600	-3.20757500	-0.30297700	C	-3.65598100	4.71111200	-3.20460000
C	-1.76034900	-1.55886000	-2.59984900	H	-4.96828400	5.07348300	-1.52161800
C	0.80752600	-1.88152900	-1.31136000	H	-2.31496200	4.06058600	-4.77396600
C	-2.97319800	-3.22650700	0.07346900	H	-8.15008500	-1.37162400	0.61153700
C	-0.85473800	-4.37715500	-0.18954500	H	-3.75772100	5.72351700	-3.60271200
C	-2.72318900	-0.65271600	-2.81643700				
H	-1.49535100	-2.30966300	-3.35204200	TS4'' _s			
C	1.32900400	-1.57953400	-2.57965500	N	3.65011900	-0.79618800	-0.34500300
C	1.67511600	-2.29557300	-0.28680800	S	4.69349400	-0.83376300	1.00397400
H	-3.58574300	-2.32814600	-0.01589300	C	2.50774000	-1.72264500	-0.18435900
C	-3.54839700	-4.39426800	0.57336600	C	3.06550500	0.52651200	-0.63221600
C	-1.43455200	-5.54370200	0.31878300	O	5.07501700	-2.24319800	1.16872400
H	0.19122300	-4.38844800	-0.49569300	O	4.11583000	-0.12749800	2.16435800
P	-3.14716700	0.47468300	-1.45067700	C	6.07944700	0.10187100	0.40221800

H	2.26147800	-2.16482400	-1.16238700	C	-2.10884100	2.39127400	-2.28440000
C	1.36759900	-0.86684000	0.31823000	H	-1.73008300	1.19289200	-4.01048800
H	2.78322600	-2.54799500	0.48330100	C	0.86301100	-0.48539100	-3.50287100
H	2.83013400	0.55558300	-1.70667200	C	-0.02692100	-2.54811600	-2.58106700
C	1.77302600	0.58868900	0.21035600	H	-3.89732800	-0.34822200	-0.38477600
H	3.77574800	1.33384800	-0.41475700	C	-5.25358700	-1.62907300	-1.45646000
C	6.82072900	-0.39735500	-0.67533900	C	-4.39755000	-2.62073500	-3.49280300
C	6.42681200	1.29333700	1.03750100	H	-2.37155500	-2.11110900	-4.02735200
C	0.11445700	-1.17633600	0.73100600	P	-2.16673600	2.35574400	-0.46252500
C	0.63075000	1.41521200	-0.34826800	H	-2.38976700	3.29872000	-2.82871500
H	2.05403400	0.94111100	1.21732800	C	1.91596500	-1.20083900	-4.08032400
C	7.92149400	0.32642300	-1.12213000	H	0.80479700	0.59621800	-3.64241000
H	6.53450300	-1.33439900	-1.15597900	C	1.02256600	-3.25765700	-3.16679000
C	7.53776700	2.00320400	0.57619200	H	-0.77396800	-3.07834100	-1.98973200
H	5.83471600	1.65581100	1.87879800	C	-5.43713600	-2.45128100	-2.57289800
C	-0.52208700	-2.50101700	0.77330200	H	-6.06174900	-1.48659900	-0.73560800
Co	-1.04860200	0.52765000	0.17571500	H	-4.53912500	-3.25790100	-4.36894400
H	0.68596400	1.48857700	-1.44322400	C	-3.92890600	2.26102200	-0.00482800
H	0.61272700	2.42451500	0.07873600	C	-1.57368100	3.98609800	0.08974900
C	8.29926500	1.53533800	-0.50516900	C	1.99614900	-2.58650500	-3.91528500
H	8.50623100	-0.05097100	-1.96500000	H	2.67379700	-0.67189500	-4.66276700
H	7.81773500	2.93814900	1.06760800	H	1.08420200	-4.33937300	-3.02821800
C	-1.92794500	-2.55018800	0.77546200	H	-6.39221700	-2.95889600	-2.72795900
C	0.17548200	-3.72539100	0.79156600	C	-4.24119400	1.76781800	1.27386200
O	-0.99468800	0.99988900	2.00023100	C	-4.95792800	2.57617300	-0.90403600
C	9.50054700	2.29347400	-0.99906900	C	-1.99556000	4.51409300	1.32032300
C	-2.62025300	-3.75919100	0.74456700	C	-0.62618800	4.68322200	-0.67825200
H	-2.47533000	-1.60662300	0.79897700	H	2.81909300	-3.14436900	-4.36798900
C	-0.51278200	-4.93951600	0.76930800	C	-5.57551900	1.60090600	1.65091500
H	1.26303900	-3.73943100	0.82770900	H	-3.43467900	1.50920800	1.96317600
C	-0.26574200	-0.00769800	2.40248500	C	-6.29016800	2.39893300	-0.52295900
H	9.62005800	3.25043500	-0.47162500	H	-4.72563500	2.94528700	-1.90468800
H	10.42118500	1.70393900	-0.85201700	C	-1.47802800	5.72986700	1.77184500
H	9.42196600	2.49856500	-2.07923600	H	-2.73218500	3.98370800	1.92605500
C	-1.91177900	-4.96439600	0.73524300	C	-0.11664600	5.90151500	-0.22281700
H	-3.71264400	-3.75960700	0.72813100	H	-0.28266500	4.27760200	-1.63234900
H	0.05037500	-5.87615900	0.77798300	C	-6.60045600	1.91141200	0.75107300
H	-2.44537600	-5.91759900	0.71048500	H	-5.81446300	1.21945000	2.64645700
P	-1.42575900	-0.22667100	-1.90478100	H	-7.09033000	2.63885900	-1.22701100
C	-2.98040000	-1.16162200	-2.17230600	C	-0.53985000	6.42539300	1.00243700
C	-1.74553900	1.26665500	-2.91761700	H	-1.81227000	6.13616200	2.72934300
C	-0.11522100	-1.15629200	-2.75254300	H	0.61491400	6.44189500	-0.82820400
C	-4.03043200	-0.98841900	-1.25631200	H	-7.64421700	1.77107100	1.04203800
C	-3.17345800	-1.97510600	-3.29989800	H	-0.13898900	7.37757300	1.35804700

C	-0.82416400	-1.00749900	3.33996900	C	-1.26864500	-1.97776400	2.32857400
C	0.04568800	-1.93251500	3.93876600	C	0.93680500	-2.94451100	2.19465400
C	-2.19715500	-1.06510300	3.61784900	O	-1.08576900	1.41816100	1.88558300
C	-0.45327300	-2.91161400	4.79602600	C	1.22891000	3.05156400	1.60217900
H	1.11411900	-1.88710200	3.71011300	C	7.28202600	2.17324700	2.24082000
C	-2.69492200	-2.04017400	4.48291900	C	-1.72423900	-3.09156200	3.03221200
H	-2.86930500	-0.34537900	3.14978700	H	-1.95343500	-1.15281400	2.12986600
C	-1.82595900	-2.96842500	5.06703700	C	0.48377800	-4.05800200	2.90533500
H	0.22571200	-3.63498700	5.25349000	H	1.98641400	-2.89773600	1.91206000
H	-3.76519800	-2.08268900	4.69881000	C	0.06446300	0.92958400	2.26017300
H	-2.21831200	-3.73758300	5.73688400	C	1.27683800	1.78583300	2.20452800
H	0.80292300	0.19121200	2.56992600	C	2.37204400	3.85353000	1.56648800
TS4_T				H	8.28199400	2.49050000	1.89977500
N	3.00074500	-1.31983900	-1.53092000	H	6.67784400	3.08781100	2.35143600
S	4.62999400	-1.57893600	-1.75732400	H	7.39307500	1.70754800	3.23043800
C	2.38575400	-1.79293000	-0.28457400	C	-0.85093000	-4.14718200	3.31277900
C	2.38494100	-0.06939900	-1.99269900	H	-2.76569200	-3.13420900	3.35970200
O	4.93198700	-1.12243800	-3.11767600	H	1.18300600	-4.86385300	3.14194800
O	4.87756400	-2.96506600	-1.34547700	H	0.05823800	0.22413500	3.10531100
C	5.47513500	-0.50312900	-0.60845700	C	2.47433700	1.33771300	2.78562000
H	1.86664500	-2.75195500	-0.42577100	C	3.56529500	3.39776300	2.13572900
C	1.44714300	-0.68704300	0.12318500	H	2.33007600	4.83819200	1.09475800
H	3.14657100	-1.94621000	0.49923200	H	-1.20303500	-5.02511600	3.85958600
H	1.64320700	-0.29447500	-2.77516000	C	3.61305700	2.13938900	2.75088700
C	1.69158600	0.52187200	-0.74720400	H	2.50719600	0.35153000	3.25626300
H	3.13127500	0.60677400	-2.42621700	H	4.46097000	4.02337600	2.10658600
C	5.71942500	0.82938000	-0.96566300	H	4.54109700	1.78758500	3.20385600
C	5.82414500	-0.98369200	0.65662700	P	-2.22334100	-1.32412400	-0.85574700
C	0.44836300	-0.72423200	1.04681400	C	-3.71545700	-2.12951500	-0.18268200
C	0.38834400	1.25127900	-1.04826300	C	-2.84512000	-0.51816100	-2.37849500
H	2.40804800	1.17846900	-0.22105800	C	-1.08954400	-2.62208100	-1.43771000
C	6.30113900	1.68416800	-0.03308400	C	-4.42016100	-1.47527200	0.83949900
H	5.46908600	1.18488400	-1.96626400	C	-4.20145600	-3.33904100	-0.70502200
C	6.40971500	-0.11164700	1.57647200	C	-2.98902000	0.81474200	-2.39026300
H	5.65471300	-2.03141200	0.90822700	H	-3.15503100	-1.13822600	-3.22748800
C	0.05891600	-1.89428900	1.85833000	C	-0.31012000	-2.37740300	-2.58094400
H	0.28973400	3.39877200	1.16957600	C	-0.88092100	-3.79464800	-0.69364100
Co	-1.01624200	0.47936400	0.17639000	H	-4.04926900	-0.53114500	1.23905200
H	0.03531900	1.03410300	-2.06777100	C	-5.59954000	-2.02900800	1.34122200
H	0.44064100	2.33657800	-0.90951100	C	-5.37779400	-3.89155300	-0.19389200
C	6.65408600	1.23117300	1.25106900	H	-3.66317100	-3.85066100	-1.50510600
H	6.49223700	2.72522200	-0.30624600	P	-2.52051700	1.75526000	-0.90084200
H	6.68535600	-0.48346000	2.56644100	H	-3.41646800	1.34009900	-3.25052200
				C	0.66065400	-3.29771800	-2.98057200

H	-0.45660900	-1.46421800	-3.16134100	C	0.97353600	0.44050400	1.29279100
C	0.08645100	-4.71492600	-1.10390900	H	3.05577200	1.58403500	-1.05506900
H	-1.46418500	-3.98881900	0.20731300	C	1.23289200	1.44479200	0.17312300
C	-6.07651900	-3.23936100	0.82807100	H	3.26926800	2.07155000	0.64940800
H	-6.14324000	-1.51297900	2.13568200	C	5.90538900	0.22767300	-2.09880800
H	-5.75170200	-4.83539000	-0.59773800	C	6.27390500	-0.32339800	0.24544200
C	-4.07714500	1.97798900	0.02880500	C	-0.07844300	0.47038400	2.15425100
C	-1.98988000	3.40198700	-1.45963300	C	0.43197100	0.93442100	-1.01007800
C	0.85990900	-4.46856700	-2.24311800	H	0.91223200	2.45475800	0.44750700
H	1.27144600	-3.09278000	-3.86224400	C	7.20002800	0.74886800	-2.16793000
H	0.24473600	-5.62367500	-0.51891100	H	5.24873300	0.22900900	-2.96959300
H	-6.99607400	-3.67660400	1.22448600	C	7.55931200	0.20048600	0.15771700
C	-4.02721600	2.26450300	1.40362300	H	5.90540400	-0.74466200	1.18268500
C	-5.31845900	1.80685200	-0.60495100	C	-0.26359000	-0.57794700	3.19899400
C	-2.00651400	4.47670000	-0.55468000	H	0.94135900	0.11453500	-1.53471800
C	-1.44989900	3.58086500	-2.74357300	H	0.17852900	1.73089500	-1.71817000
H	1.62758200	-5.18267600	-2.54943400	C	8.04417200	0.74513700	-1.04803800
C	-5.21400400	2.38273100	2.13164700	H	7.55985100	1.16578300	-3.11171900
H	-3.06459600	2.36748200	1.90491200	H	8.20594200	0.18829600	1.03906800
C	-6.49892200	1.92207400	0.13155700	C	-1.42785700	-1.36414600	3.20806500
H	-5.37049900	1.56975700	-1.66888300	C	0.69823400	-0.78834100	4.20132700
C	-1.49773500	5.71885800	-0.93820700	C	9.43903900	1.30379600	-1.11868900
H	-2.41748600	4.34903200	0.44854500	C	-1.61219700	-2.36110800	4.16782400
C	-0.94589200	4.82815700	-3.12106100	H	-2.19067700	-1.20029800	2.44798800
H	-1.41658100	2.75109600	-3.45255300	C	0.50949500	-1.77846700	5.16942600
C	-6.44897800	2.20874500	1.49958800	H	1.59519000	-0.16639500	4.22926300
H	-5.17103000	2.60258500	3.20100600	H	10.18515000	0.52407700	-0.89164800
H	-7.46157000	1.78157300	-0.36562100	H	9.66190400	1.71268400	-2.11448200
C	-0.96731700	5.89696800	-2.22056000	H	9.57979900	2.10626900	-0.37574100
H	-1.51758500	6.55189300	-0.23165100	C	-0.64061000	-2.57346100	5.15122100
H	-0.53353800	4.96255800	-4.12380700	H	-2.51829000	-2.97151700	4.14523400
H	-7.37467000	2.29270100	2.07395300	H	1.26656500	-1.92809800	5.94311900
H	-0.57100700	6.87069100	-2.51800800	H	-0.78232300	-3.35160700	5.90509400
				P	-1.09215300	-1.76974100	-0.96758700
7s				P	-2.43250500	0.83744100	-1.71016200
N	3.09154300	-0.01379100	0.34675200	C	-1.49011900	-1.48512900	-2.73374500
S	3.81938300	-0.99898000	-0.78541800	C	-2.10638500	-0.33933200	-3.05764100
C	2.08772200	-0.58908000	1.25908100	C	0.25476800	-2.98421400	-0.92753500
C	2.75304900	1.36607100	-0.02244500	C	-2.55779300	-2.70566800	-0.39314000
O	3.20095300	-0.85535400	-2.11744000	C	-4.20732800	0.69917500	-1.30756800
O	3.89056400	-2.32557000	-0.15988400	C	-2.17358800	2.51397100	-2.36110500
C	5.45465700	-0.29921700	-0.88969700	C	0.44724700	-3.72720000	0.25196200
H	2.51833300	-0.74338100	2.25753800	C	-3.50275400	-2.02716500	0.38775700
H	1.73624600	-1.56859200	0.90528900	C	-5.10776200	0.08833100	-2.19277800

C	-2.66694900	3.61678500	-1.64434700	H	0.18801100	2.07867200	4.54069900
C	1.08377400	-3.20768100	-2.03523300	C	0.09982700	5.29739300	2.36859800
C	-2.78777100	-4.03995400	-0.76440300	H	-0.96131900	4.08363300	0.91327600
C	-4.65675400	1.17475700	-0.06364300	C	0.71461600	5.32294500	3.62323000
C	-1.40743900	2.71997500	-3.51954100	H	1.21709300	4.17153800	5.38701000
C	1.44270300	-4.70168900	0.30471400	H	0.06929400	6.20215200	1.75559000
C	-4.67136600	-2.67019300	0.80114300	H	1.16747100	6.24489300	3.99656600
C	-6.45258900	-0.03814000	-1.83617200	H	-1.88062900	1.38771300	2.85986600
C	-2.40078100	4.91173300	-2.09172600	H	-1.30843100	-2.27168000	-3.47340700
C	2.07233500	-4.19210100	-1.97640900	H	-2.45019800	-0.13114000	-4.07570400
C	-3.95678900	-4.68101900	-0.35037900				
C	-6.00363600	1.05028900	0.28115500	7 _T			
C	-1.15020000	4.01965600	-3.96369600	N	2.62273800	-1.86618300	0.72891700
C	2.24868700	-4.94183800	-0.81318800	S	3.01549500	-1.47828700	-0.85924000
C	-4.89819000	-3.99864000	0.43047600	C	1.33477500	-2.54575200	0.94083900
C	-6.90196000	0.44241000	-0.60245100	C	2.76215900	-0.86632600	1.79467000
C	-1.64430000	5.11565800	-3.25089200	O	2.26976000	-0.30789000	-1.37854900
H	-0.19104800	-3.55446700	1.12197700	O	2.89859100	-2.73607800	-1.60955800
H	-3.32078400	-0.98856700	0.66838000	C	4.72235900	-1.01544500	-0.70337500
H	-4.76753700	-0.29759200	-3.15542100	H	1.52735900	-3.42090200	1.58043800
H	-3.25073500	3.46978300	-0.73596000	H	0.90664300	-2.92100200	0.00131300
H	0.96470700	-2.61831500	-2.94515800	C	0.45056800	-1.54140600	1.66826400
H	-2.05527800	-4.57656000	-1.37131900	H	3.46793100	-0.07299600	1.51996200
H	-3.93926600	1.61737500	0.63123600	C	1.33606600	-0.34681400	2.08245000
H	-1.00225900	1.87146300	-4.07436900	H	3.16115000	-1.38098700	2.68350000
H	1.58785200	-5.27786800	1.22146400	C	5.10118600	0.30472700	-0.94228600
H	-5.40198400	-2.13089300	1.40775600	C	5.66152100	-2.00059100	-0.37583300
H	-7.15123000	-0.51731300	-2.52592500	C	-0.87671500	-1.67462000	1.92172100
H	-2.78656600	5.76587100	-1.53038200	C	1.01322200	0.90167200	1.27765600
H	2.71692300	-4.36010500	-2.84185800	H	1.20877800	-0.14406800	3.15234800
H	-4.13574300	-5.71954500	-0.63885600	C	6.45151400	0.64565500	-0.84280500
H	-6.35087600	1.42093500	1.24849000	H	4.35057500	1.05125600	-1.19975400
H	-0.55857400	4.17394700	-4.86900500	C	7.00177600	-1.64043300	-0.28128900
H	3.02787100	-5.70638600	-0.76936300	H	5.34411000	-3.03000000	-0.20043400
H	-5.81109000	-4.50673800	0.75038600	C	-1.67679600	-2.86150300	1.51668200
H	-7.95417200	0.33856100	-0.32694300	H	1.70532000	1.07437700	0.44536800
H	-1.43956800	6.13119100	-3.59811000	H	0.85506100	1.81332400	1.86534700
Co	-1.13267100	0.28031000	-0.03669200	C	7.41957300	-0.31478900	-0.51241000
C	-1.08324000	1.66270300	2.14273200	H	6.75681300	1.67861400	-1.02655900
O	-1.61938500	1.80884200	0.86360100	H	7.74479700	-2.40065600	-0.02717500
C	-0.44492400	2.94821400	2.66165500	C	-2.98171200	-2.68220700	1.01546100
C	0.16498500	2.98126000	3.92512700	C	-1.19826100	-4.17769300	1.65142700
C	-0.47815600	4.11572600	1.89055200	C	8.87498300	0.04818800	-0.40554100
C	0.74330600	4.15952600	4.40194200	C	-3.77119600	-3.77181700	0.65225000

H	-3.37742500	-1.67559000	0.88883500	H	-2.38940500	2.56287400	1.18430800
C	-1.98950100	-5.27013600	1.28735000	H	2.00606700	2.12177600	-2.58171500
H	-0.21368400	-4.35987700	2.08053200	H	-2.83604500	-5.12841700	-2.77873600
H	9.48203100	-0.55803100	-1.09806300	H	-6.04857100	1.08610800	0.35756100
H	9.04605500	1.10954200	-0.63482900	H	-3.02244600	6.58563000	-1.69778300
H	9.25478000	-0.15172300	0.61025800	H	2.82589100	5.71249200	0.77583500
C	-3.27816900	-5.07338900	0.78431000	H	1.24763000	-3.84772300	-3.38058800
H	-4.77508700	-3.60055700	0.25640300	H	-6.32555500	-0.33249500	-3.71207700
H	-1.59689500	-6.28263600	1.40891700	H	-4.15507300	4.22344400	1.73547500
H	-3.89569400	-5.92913500	0.50112200	H	4.20300600	3.27271400	-2.50964600
P	-1.78283000	-0.37809500	-1.67245600	H	-0.49322800	-5.64565000	-3.46120300
P	-0.42837300	2.41267200	-0.97355300	H	-7.41278700	0.61008500	-1.67557700
C	-1.24204800	0.74789700	-3.01173900	H	-4.48048800	6.23122700	0.29346000
C	-0.69967600	1.93654000	-2.71327400	H	4.62641500	5.05844700	-0.82129800
C	-1.44524200	-2.04912000	-2.31277000	Co	-0.62937300	0.47257700	0.28164000
C	-3.59248700	-0.12990100	-1.67585600	C	-1.67648600	-0.52868500	2.59327500
C	-1.70856400	3.64491300	-0.56899700	O	-1.81170800	0.53881800	1.70304700
C	1.15519600	3.30415000	-0.97393300	C	-1.11162300	-0.10119200	3.94322000
C	-2.41936700	-3.05809200	-2.34540400	C	-0.81531400	-1.06208000	4.92169500
C	-4.20357800	0.40581800	-0.53164700	C	-0.90735200	1.25212100	4.23442400
C	-1.88664800	4.77968500	-1.37946200	C	-0.30094700	-0.67615800	6.16114000
C	1.39616200	4.30588400	-0.01933500	H	-0.97863500	-2.12170900	4.70725900
C	-0.12471500	-2.34191500	-2.69421000	C	-0.39317100	1.64055200	5.47642000
C	-4.35993400	-0.38979900	-2.82465800	H	-1.14348300	1.99418000	3.47122600
C	-2.52601300	3.44423300	0.55349900	C	-0.08356800	0.67844700	6.44161000
C	2.17458200	2.92412600	-1.86160000	H	-0.06763100	-1.43477100	6.91276900
C	-2.07383200	-4.34592600	-2.76136000	H	-0.23149200	2.70064400	5.68928100
C	-5.57656700	0.66921200	-0.53528600	H	0.32164300	0.98061900	7.41059500
C	-2.88321500	5.70447500	-1.06699300	H	-2.68131600	-0.93475800	2.80827000
C	2.64363800	4.93102100	0.03442400	H	-1.42785000	0.45663400	-4.05188200
C	0.21320500	-3.63102000	-3.10933900	H	-0.43278300	2.65303300	-3.49797300
C	-5.73045600	-0.12640900	-2.81921400				
C	-3.51990500	4.37943700	0.86027300	TS5_s			
C	3.41653200	3.56212000	-1.80887500	N	3.22367000	-1.62882200	-0.88114700
C	-0.76006800	-4.63480100	-3.14321800	S	3.71351600	-1.09841400	0.66239700
C	-6.33977200	0.40320800	-1.67515300	C	2.94902300	-0.53171600	-1.82390000
C	-3.70096500	5.50446200	0.05220700	C	2.01276400	-2.46584000	-0.91347600
C	3.65342800	4.56299200	-0.86129400	O	3.52007800	-2.24015300	1.56690700
H	-3.44368000	-2.84601400	-2.04210900	O	3.10936700	0.20200700	1.01774600
H	-3.60367900	0.60878400	0.35790700	C	5.45123100	-0.82658800	0.39763500
H	-1.24630000	4.94263800	-2.24929900	H	3.12988600	-0.91591200	-2.84338700
H	0.60797700	4.60055000	0.67701600	H	3.62062500	0.31847200	-1.67181200
H	0.64690400	-1.57160000	-2.64504200	C	1.47523900	-0.23190400	-1.64051700
H	-3.88832700	-0.79996000	-3.72047800	H	1.94616600	-3.08414100	-0.01176000

C	0.81662700	-1.48668600	-1.09052200	C	-3.39076500	1.56356900	3.74085100
H	2.09808100	-3.13201200	-1.78539700	C	-4.84621400	-0.27987900	-1.02047600
C	6.26975300	-1.92062400	0.09205900	C	-1.52966800	-4.42511900	-0.17554000
C	5.97488100	0.45813600	0.53317400	C	1.43451800	1.48341600	4.10220800
C	0.89529400	0.97410400	-1.81674800	C	-4.11695900	3.26231700	1.62789600
C	0.12621300	-1.22659900	0.24438000	C	-6.63618800	-2.35326800	-1.58850600
H	0.09818700	-1.90726600	-1.80650100	C	-1.57342500	-4.56965200	-2.97044600
C	7.63218400	-1.70851200	-0.08836200	C	1.51434800	-0.92426300	4.36216800
H	5.84257300	-2.92016600	-0.00582600	C	-4.26805000	2.62583000	3.96490900
C	7.34645100	0.65091500	0.34754600	C	-6.11962300	0.01492000	-1.51217800
H	5.31865800	1.29272600	0.78165600	C	-0.91225900	-5.49437100	-0.83126400
C	1.68786200	2.17689400	-2.20555800	C	2.07374500	0.33653700	4.58572200
H	0.80486500	-0.71103900	0.93307500	C	-4.63247700	3.47234600	2.90994400
H	-0.17291700	-2.18048800	0.70284100	C	-7.01399100	-1.02139100	-1.79666400
C	8.19350100	-0.42183000	0.03413700	C	-0.93119500	-5.56687200	-2.22688500
H	8.28002200	-2.55548300	-0.32897300	H	-0.24824600	2.26699000	2.99680700
H	7.76411200	1.65542800	0.44968100	H	-2.81788000	2.04016100	0.40141100
C	2.68290200	2.67882600	-1.34872100	H	-5.07118700	-3.69371300	-0.93661600
C	1.42848000	2.84803300	-3.41057700	H	-2.67743600	-2.71577400	-2.90741900
C	9.66953800	-0.21942300	-0.17170300	H	-0.10836400	-2.03200800	3.46812300
C	3.40434300	3.82358900	-1.69465000	H	-3.10096300	0.90728500	4.56498200
H	2.87450300	2.16722000	-0.40276400	H	-4.14431600	0.52671100	-0.80371100
C	2.15018600	3.99340100	-3.75603200	H	-1.50461600	-4.37308900	0.91504600
H	0.65034200	2.47127500	-4.07871100	H	1.87243000	2.46939900	4.27466700
H	10.25293300	-0.84938000	0.51994900	H	-4.39177200	3.92519400	0.80497500
H	9.96564900	-0.50883000	-1.19389900	H	-7.33553800	-3.16214700	-1.81288500
H	9.96174700	0.82850300	-0.01363900	H	-1.59105500	-4.62471100	-4.06142900
C	3.13937800	4.48509800	-2.89871100	H	2.01727400	-1.82138900	4.72944100
H	4.17214800	4.20562400	-1.01687900	H	-4.66915700	2.79634400	4.96673400
H	1.93741300	4.50521100	-4.69795400	H	-6.41006000	1.05517400	-1.67659800
H	3.70119100	5.38323000	-3.16722700	H	-0.41510600	-6.27250300	-0.24738900
P	-1.76520700	-0.03859600	2.07366100	H	3.01454700	0.42659100	5.13387100
P	-2.80974900	-1.92480100	-0.11318300	H	-5.31945000	4.30239000	3.09176800
C	-2.65907800	-1.54846600	2.58915900	H	-8.00930400	-0.79213300	-2.18496400
C	-3.11202200	-2.37370800	1.63446700	H	-0.44631100	-6.40234300	-2.73737900
C	-0.32262900	0.10574200	3.16430700	Co	-1.44208300	-0.13180000	-0.06020500
C	-2.87661600	1.34992000	2.45246300	C	-0.58725700	1.13869800	-1.61203400
C	-4.46567000	-1.61401700	-0.80844500	O	-1.37736500	0.17047400	-1.95133800
C	-2.17104200	-3.42280900	-0.91880300	C	-1.19221100	2.51743000	-1.56983800
C	0.24100900	1.37186200	3.38815300	C	-0.65250200	3.55129900	-0.78790900
C	-3.23853200	2.20046300	1.39771700	C	-2.37177800	2.74590100	-2.29193800
C	-5.36530500	-2.65355200	-1.09456300	C	-1.27516400	4.79644900	-0.74365900
C	-2.18884500	-3.49816200	-2.32225400	H	0.24183200	3.36983600	-0.19093500
C	0.31648600	-1.04293100	3.65324500	C	-2.99130600	3.99881800	-2.25381700

H	-2.79726100	1.93472500	-2.88426300	H	-2.47023900	4.42013400	-0.21243700
C	-2.44405900	5.02625000	-1.48138600	H	-10.30943500	-0.53165200	0.95291000
H	-0.85302700	5.59150800	-0.12477100	H	-9.97314500	1.20706200	0.96740800
H	-3.90524200	4.17014600	-2.82761300	H	-10.12598200	0.34497600	-0.58851900
H	-2.92992600	6.00428400	-1.44571900	C	-2.25416800	4.91052900	-3.57970400
H	-0.55046100	1.03450400	0.19061500	H	-0.90683400	3.85519500	-4.90454200
H	-2.84375900	-1.73328400	3.65300600	H	-3.46637400	5.79231000	-2.01892400
H	-3.69660300	-3.26931300	1.87294200	H	-2.68667600	5.52353400	-4.37418400
8_s				P	1.34865000	-2.54585000	-0.76803900
				P	2.65967900	-0.95057400	1.51072500
N	-3.13979100	0.49809500	1.20801200	C	2.10930700	-3.47252400	0.61934000
S	-3.78556200	-0.93652800	0.59111800	C	2.67663800	-2.77666000	1.61538700
C	-2.77299600	1.53330700	0.23240600	C	-0.21955100	-3.39486900	-1.11230500
C	-2.04276700	0.42107000	2.18391800	C	2.44842700	-2.83884800	-2.18921600
O	-3.54647900	-1.96907000	1.60944700	C	4.41737000	-0.47491900	1.38507000
O	-3.34627400	-1.16073800	-0.79753700	C	2.09587700	-0.36296200	3.13708100
C	-5.52714000	-0.56713300	0.53644900	C	-0.73783200	-3.40807300	-2.41681400
H	-3.23770700	2.48620000	0.52736700	C	3.02327400	-1.71693600	-2.80538900
H	-3.12808500	1.29262300	-0.77949800	C	5.30088500	-0.54886700	2.47386900
C	-1.25844600	1.62869200	0.29203800	C	2.34378400	0.97407500	3.49504400
H	-2.05132400	-0.54055700	2.70701800	C	-0.97813700	-3.91691200	-0.05415800
C	-0.76697300	0.66068400	1.34510000	C	2.76332500	-4.12850300	-2.64428500
H	-2.18322100	1.22641000	2.92338000	C	4.88634700	-0.04095600	0.13505500
C	-6.20845700	-0.31839000	1.73405500	C	1.27821200	-1.15908800	3.95339000
C	-6.18893500	-0.55707200	-0.69018700	C	-2.00133000	-3.94991000	-2.65652600
C	-0.52249900	2.47120100	-0.47934800	C	3.91046500	-1.88252700	-3.87193500
C	-0.30058300	-0.66181100	0.72449700	C	6.64021800	-0.19081600	2.30805600
H	0.03500900	1.09260500	1.95902000	C	1.78503900	1.50144700	4.65996600
C	-7.57178200	-0.04730900	1.68791200	C	-2.24572900	-4.44799400	-0.29946900
H	-5.67510300	-0.33201700	2.68638900	C	3.64912300	-4.28895100	-3.71135300
C	-7.55924600	-0.28289200	-0.71627000	C	6.22757600	0.31500400	-0.02683700
H	-5.63730500	-0.76021100	-1.60882700	C	0.71783700	-0.62404900	5.11756400
C	-1.14062400	3.33363400	-1.53072200	C	-2.75703900	-4.46647900	-1.59898800
H	-1.07474900	-1.06877200	0.06625400	C	4.22301500	-3.16819000	-4.32375100
H	-0.13310200	-1.38509600	1.53849400	C	7.10403100	0.24138300	1.05982000
C	-8.27012000	-0.02381100	0.46418700	C	0.96824800	0.70473700	5.47131900
H	-8.11170600	0.15183400	2.61737800	H	-0.15657900	-2.99215800	-3.24276000
H	-8.08452100	-0.27004100	-1.67440100	H	2.76855100	-0.71222700	-2.45039100
C	-0.70356600	3.19597000	-2.85924300	H	4.94038200	-0.87993200	3.45050100
C	-2.14028600	4.27711800	-1.24329700	H	2.96925100	1.60375700	2.85779100
C	-9.74596900	0.26618300	0.44004500	H	-0.59002700	-3.89223800	0.96632300
C	-1.25645800	3.97713600	-3.87643000	H	2.31422000	-5.00414600	-2.16954400
H	0.07404200	2.46472900	-3.09445600	H	4.20094600	0.01613000	-0.71286100
C	-2.69319700	5.05868300	-2.26004400	H	1.07186700	-2.19668600	3.68168100

H	-2.40137600	-3.96054700	-3.67327100	C	6.24562900	0.90753400	-1.66417400
H	4.35579600	-1.00763300	-4.35128300	C	5.68750900	0.69454300	0.69943500
H	7.32622500	-0.24796200	3.15665100	C	-0.18720500	2.17632000	-0.88995200
H	1.98422000	2.54023800	4.93409000	C	0.45952000	-0.90231300	-1.79494500
H	-2.84056400	-4.83260200	0.53113100	H	0.01186600	0.64068700	-3.25779500
H	3.89328700	-5.29246600	-4.06787900	C	7.44840500	1.51811800	-1.31453100
H	6.58627100	0.65244600	-1.00210100	H	5.98529100	0.74874900	-2.71232100
H	0.08334200	-1.25017800	5.74936400	C	6.89615000	1.30745600	1.02854300
H	-3.75191900	-4.87675400	-1.78843000	H	4.99190000	0.36409500	1.47188600
H	4.91584400	-3.29910300	-5.15853400	C	-0.05345800	3.13798900	0.23637900
H	8.15259200	0.52272700	0.93574100	H	1.38378600	-1.41150000	-1.50546900
H	0.52846500	1.12087600	6.38085200	H	-0.08417000	-1.57832300	-2.49177500
Co	1.32602400	-0.44088100	-0.28491000	C	7.79350100	1.72840000	0.03240300
C	0.94684900	2.48249400	-0.36462200	H	8.13623800	1.83807300	-2.10096400
O	1.58567700	1.44008300	-0.10632200	H	7.14958100	1.46090700	2.08075400
C	1.74343000	3.71579000	-0.55492400	C	-0.82209500	2.92381300	1.39580700
C	1.19796800	5.00109600	-0.38169300	C	0.83564800	4.22590700	0.20851100
C	3.11229200	3.58439400	-0.86338200	C	9.09016200	2.39218900	0.40820800
C	2.00521500	6.12934600	-0.52254300	C	-0.68846700	3.76452600	2.50294100
H	0.14754400	5.12169600	-0.12227900	H	-1.52397300	2.08873000	1.43667300
C	3.91145500	4.71414600	-1.01661600	C	0.96449700	5.06802800	1.31497000
H	3.53521000	2.58649800	-0.98503600	H	1.41363900	4.43287600	-0.69318100
C	3.35866700	5.98954400	-0.84766700	H	8.90522400	3.34303900	0.93574700
H	1.57566100	7.12324100	-0.37892000	H	9.67487000	1.75571000	1.09241300
H	4.96886400	4.60358900	-1.26758000	H	9.70675000	2.60600300	-0.47638600
H	3.98554300	6.87658200	-0.96705500	C	0.20783100	4.83696100	2.46820700
H	0.47130300	-0.30677400	-1.49571500	H	-1.28885300	3.57614000	3.39484400
H	2.11821900	-4.56805500	0.59963000	H	1.65737800	5.91206000	1.27369100
H	3.18358800	-3.27311100	2.45056800	H	0.31157200	5.49478700	3.33446800
				P	-0.26701300	-2.60322700	0.64885400
				P	-2.99349700	-1.32145100	0.57256600
				C	-1.62576800	-3.44790100	1.54602700
				C	-2.83136300	-2.86286900	1.53933300
				C	0.67686700	-3.94358000	-0.14642600
				C	0.77703000	-1.99242800	2.02615400
				C	-3.35479000	-0.03760700	1.82266900
				C	-4.52915900	-1.50831400	-0.39508000
				C	2.04392400	-3.77270100	-0.42267200
				C	0.70624200	-0.63501800	2.37289800
				C	-4.16529400	1.06381100	1.50538700
				C	-4.43370600	-1.53206800	-1.79496300
				C	0.01168900	-5.09085300	-0.60929000
				C	1.59363600	-2.85734600	2.77056800
				C	-2.70824900	-0.08397500	3.06929200
TS6 _s							
N	3.06950500	0.85367600	-1.99567900				
S	3.86222500	-0.32394500	-1.08509200				
C	2.32815500	1.87150700	-1.23395900				
C	2.19548900	0.42190500	-3.10205900				
O	4.15397300	-1.43270500	-2.00565800				
O	3.14418000	-0.61518500	0.17226200				
C	5.37442500	0.50475400	-0.64842600				
H	2.60493400	2.86601900	-1.61645400				
H	2.57403300	1.84934000	-0.16299400				
C	0.86443000	1.57616400	-1.49649900				
H	2.50493900	-0.55808500	-3.48102900				
C	0.77851000	0.43885100	-2.49680700				
H	2.29229100	1.16092400	-3.91329700				

C	-5.78434300	-1.64471500	0.22058400	H	-2.98040600	6.11433000	-2.28699800
C	2.73531300	-4.74412500	-1.14905100	H	-5.91830900	2.94803200	-2.35238700
C	1.45055300	-0.14295000	3.44626600	H	-5.33309600	5.35954500	-2.61544900
C	-4.33090200	2.10146300	2.42583800	H	0.15272500	-0.38772000	-0.26642200
C	-5.58438400	-1.68771600	-2.57352700	H	-1.41709100	-4.36022900	2.11623200
C	0.71227000	-6.06352600	-1.32746600	H	-3.68264300	-3.26059900	2.10273900
C	2.34283500	-2.36052500	3.83981000				
C	-2.88027600	0.95425600	3.98717600	TS6_T			
C	-6.93039800	-1.80229900	-0.56034700	N	-3.47435700	1.97468800	0.11879100
C	2.07350700	-5.89100500	-1.59982500	S	-4.16192900	1.02189300	1.35225300
C	2.27392600	-1.00418600	4.17816400	C	-3.20752100	1.24106500	-1.13157500
C	-3.69138400	2.04829800	3.66814000	C	-2.19249600	2.59525600	0.49770000
C	-6.83149000	-1.82228300	-1.95696700	O	-4.22068500	1.88903000	2.53597700
H	2.56682400	-2.87994800	-0.07783200	O	-3.49615800	-0.29050400	1.48530500
H	0.06959300	0.03480100	1.79345900	C	-5.79444500	0.75265100	0.70113100
H	-4.66891100	1.11615800	0.53994400	H	-3.20569000	1.98064100	-1.95168800
H	-3.45963500	-1.41244800	-2.27391600	H	-3.99187100	0.51039300	-1.35056700
H	-1.05430200	-5.22790200	-0.40995100	C	-1.82099700	0.67098300	-0.93862500
H	1.65535800	-3.91650400	2.51145800	H	-2.13401200	2.72624100	1.58496300
H	-2.06907600	-0.93059900	3.32582300	C	-1.06383700	1.67418500	-0.07109300
H	-5.86626000	-1.61777300	1.30973100	H	-2.14442000	3.59031100	0.03286800
H	3.79517600	-4.59534300	-1.36776700	C	-6.59888200	1.85682800	0.39491100
H	1.39000600	0.91721300	3.70425900	C	-6.26424300	-0.55251000	0.55985500
H	-4.96027900	2.95625600	2.16718400	C	-1.38057400	-0.52083900	-1.37784700
H	-5.50568900	-1.69988700	-3.66312500	C	-0.20638400	1.01496600	0.98661900
H	0.19149600	-6.95823700	-1.67734200	H	-0.42192500	2.30139600	-0.71507900
H	2.98443800	-3.03571200	4.41125300	C	-7.88791100	1.63535600	-0.07839800
H	-2.37505200	0.90818800	4.95482300	H	-6.21416200	2.87066200	0.51666300
H	-7.90556200	-1.90769900	-0.07884600	C	-7.56271000	-0.75388900	0.08602200
H	2.61781500	-6.65081700	-2.16605300	H	-5.62172300	-1.39514600	0.81705600
H	2.86353400	-0.61981700	5.01422200	C	-2.22057700	-1.46200500	-2.17119500
H	-3.82271100	2.86063700	4.38675400	H	-0.78099900	0.32283800	1.61750800
H	-7.73148200	-1.94160100	-2.56514200	H	0.33671700	1.72348800	1.62794800
Co	-1.08214900	-1.01684900	-0.59970900	C	-8.39113400	0.32963800	-0.24170800
C	-1.55916000	1.77044500	-1.30066900	H	-8.52237200	2.48996600	-0.32731500
O	-1.88096800	0.56719900	-1.38518300	H	-7.93753800	-1.77347100	-0.03095400
C	-2.57530700	2.78169100	-1.65045600	C	-3.41899800	-1.97758100	-1.64936000
C	-2.25094600	4.14176600	-1.81325600	C	-1.79255000	-1.88908300	-3.43871600
C	-3.90476800	2.36022800	-1.85761800	C	-9.78938500	0.11703900	-0.75294000
C	-3.23992700	5.06090200	-2.16131000	C	-4.18769600	-2.87551300	-2.39226500
H	-1.22545700	4.48207100	-1.67624700	H	-3.73322400	-1.67910400	-0.64802000
C	-4.88945100	3.28197500	-2.20024900	C	-2.56108000	-2.79022200	-4.18003900
H	-4.14792000	1.30383400	-1.74449200	H	-0.85126000	-1.51106300	-3.84485900
C	-4.55941600	4.63542800	-2.34885700	H	-10.52871200	0.56130100	-0.06561000

H	-9.92943400	0.60579900	-1.73116700	H	6.77726700	4.16996900	-2.15095800
H	-10.02244200	-0.95152200	-0.86338800	H	0.59417600	6.39565400	-1.31606500
C	-3.76260700	-3.28305200	-3.66130100	H	0.65466600	-1.19346700	5.71768100
H	-5.11910300	-3.26495600	-1.97326200	H	6.57625900	-4.10459500	1.31401600
H	-2.21875100	-3.10961300	-5.16759100	H	4.64893900	1.16791500	-4.41174100
H	-4.36228800	-3.98884700	-4.24134900	H	0.58030600	5.56213900	2.92069600
P	2.81685600	-0.81612800	1.27938600	H	0.20263400	-3.63627300	5.49460700
P	2.78953400	2.18114700	0.04905200	H	6.94655200	-3.93054100	-1.14467900
C	3.76192200	0.54802600	2.06187400	H	6.53357700	2.78661700	-4.20937100
C	3.76530200	1.78599200	1.54030900	H	-0.08227500	7.01333100	1.00432700
C	2.08647900	-1.73645800	2.66462800	Co	1.34427300	0.38803200	-0.14135600
C	4.12569000	-1.85637500	0.55036600	C	0.05885700	-0.99279400	-1.14412900
C	3.98012800	2.40963500	-1.30487100	O	0.99051600	-0.39899100	-1.87495900
C	2.00071300	3.78461400	0.37452800	C	0.23311600	-2.46086400	-0.83580400
C	1.81838200	-3.10866100	2.53474500	C	-0.63696700	-3.10387800	0.05747900
C	4.33568100	-1.75884800	-0.83370900	C	1.27778200	-3.17985900	-1.42643700
C	5.03777700	3.32726600	-1.19203500	C	-0.47530500	-4.46009300	0.33750700
C	1.62440400	4.60209200	-0.70476900	H	-1.44044400	-2.53839400	0.53369100
C	1.65625900	-1.04810500	3.81152100	C	1.44374200	-4.53690800	-1.13866300
C	4.93860700	-2.69954200	1.32502900	H	1.94811000	-2.66837800	-2.11617100
C	3.83950200	1.63183400	-2.46428500	C	0.56519500	-5.18047500	-0.26100700
C	1.61733800	4.13261800	1.68026900	H	-1.15663700	-4.95532200	1.03296300
C	1.14704000	-3.78670400	3.55378100	H	2.26074300	-5.09344500	-1.60406900
C	5.35247300	-2.49960500	-1.44034100	H	0.69330900	-6.24273900	-0.03897100
C	5.95274700	3.45835400	-2.23711200	H	0.11201400	-0.51455100	0.16870500
C	0.88004000	5.76031700	-0.47446800	H	4.37231500	0.31547100	2.94282400
C	0.98285500	-1.73279000	4.82595200	H	4.37504800	2.57979600	1.98718600
C	5.94760400	-3.44462000	0.71144900				
C	4.75923000	1.77148200	-3.50788400	9s			
C	0.87143500	5.29333600	1.90263300	N	-2.71819700	-1.09674900	-2.31419600
C	0.72958000	-3.10264500	4.70002800	S	-3.37738600	-0.05022800	-1.14748700
C	6.15574500	-3.34518600	-0.66927100	C	-1.82752900	-2.13242000	-1.77368900
C	5.81432600	2.68064600	-3.39362200	C	-1.94033400	-0.46139900	-3.39140100
C	0.50120600	6.10672900	0.82769500	O	-3.82810300	1.13438100	-1.89008800
H	2.12591600	-3.64705800	1.63691100	O	-2.46289700	0.10872800	0.00034100
H	3.69481100	-1.11226300	-1.43473800	C	-4.78245000	-0.97425700	-0.57671600
H	5.14256500	3.93710300	-0.29153400	H	-2.08343700	-2.41293800	-0.74362700
H	1.91201300	4.33332200	-1.72392800	C	-0.42359400	-1.56686000	-1.91219000
H	1.84399500	0.02362600	3.91437300	H	-1.95140500	-3.02906600	-2.40096600
H	4.78041200	-2.77938700	2.40270400	H	-2.38180000	0.49835600	-3.67924900
H	3.01267900	0.92333200	-2.55185000	C	-0.49716100	-0.35351900	-2.84329000
H	1.90130900	3.50162900	2.52599500	H	-1.97831900	-1.14010100	-4.25698500
H	0.94298700	-4.85449800	3.44605800	C	-5.80499800	-1.28830100	-1.47985500
H	5.51156300	-2.42069200	-2.51833000	C	-4.86374900	-1.32904700	0.76927300

C	0.67075000	-2.08340100	-1.31004700	C	1.35393800	4.37676800	-1.76041800
C	-0.28783900	1.00223500	-2.13065100	C	-2.47632900	3.37890100	0.09983000
H	0.23469600	-0.45030900	-3.65921400	C	-1.75621100	2.52100700	2.24891900
C	-6.91746200	-1.98239100	-1.01664000	H	0.75865700	-6.27770700	2.08672100
H	-5.72503800	-0.99770800	-2.52890400	C	5.40269600	-3.52843600	-2.94433600
C	-5.99040600	-2.02484800	1.21493500	H	4.00226300	-5.01566100	-3.66075700
H	-4.05921600	-1.05846900	1.45370000	H	6.56188700	-1.89614500	-2.11753400
C	0.67039600	-3.26760900	-0.40931700	P	2.08191800	0.92440200	1.53193100
C	1.99627100	-1.41884700	-1.46931900	H	2.64446500	2.66058900	3.34928500
Co	1.09274600	1.15554000	-0.36284900	C	0.12647400	6.82184800	-1.18207300
H	-0.65445700	0.94670200	-1.08147400	H	-0.77108900	5.81140900	0.50187800
H	-0.86453500	1.80700000	-2.60436000	C	1.58595500	5.48448900	-2.58022900
C	-7.02926700	-2.36325000	0.33553200	H	1.83509200	3.41898500	-1.97321100
H	-7.72043300	-2.23618800	-1.71351100	C	-3.80846400	3.22414200	0.48855900
H	-6.06204100	-2.30882300	2.26760600	H	-2.24801000	3.75559700	-0.89901800
C	-0.06850300	-4.43526900	-0.66807200	C	-3.08890000	2.36853300	2.63346100
C	1.46000900	-3.21901900	0.75364700	H	-0.95976900	2.22788400	2.93570900
O	2.15332100	-0.22912500	-1.14192900	H	6.27890200	-4.06169200	-3.32128400
C	3.15931400	-2.16788400	-1.97317400	C	3.83364500	0.40445300	1.52349700
P	0.30338900	3.01611200	0.42187400	C	1.18185000	-0.20405900	2.66057200
H	0.77297200	1.33724400	-2.21293400	C	0.97138400	6.70671800	-2.29221200
C	-8.24128400	-3.11669100	0.81030100	H	-0.35337900	7.77725100	-0.95589800
C	-0.03528500	-5.50801000	0.22589000	H	2.24706900	5.39268000	-3.44537700
H	-0.65078100	-4.52505000	-1.58527300	C	-4.11808500	2.71858200	1.75330700
C	1.49152400	-4.28793600	1.64821800	H	-4.60700600	3.48098800	-0.20994100
H	2.04108100	-2.32272100	0.96576500	H	-3.32394100	1.96798600	3.62283500
C	3.00552300	-3.39494500	-2.64475600	C	4.77291300	1.32305100	1.02194300
C	4.44841200	-1.62858200	-1.79124400	C	4.25110000	-0.89436300	1.84692600
C	1.23088000	3.45118700	1.94397900	C	1.67257700	-0.60387500	3.91406100
C	0.50604300	4.48691800	-0.64723400	C	-0.08830600	-0.63172100	2.24191500
C	-1.44090700	3.03401100	0.97955000	H	1.15066500	7.57335900	-2.93330900
H	-8.19123200	-3.32869900	1.88776400	H	-5.16159300	2.59097500	2.05189400
H	-9.16213100	-2.54337500	0.61263700	H	4.45556500	2.33433500	0.75223300
H	-8.34146200	-4.07524500	0.27429400	C	6.10725000	0.94868500	0.85674300
C	0.73803800	-5.43704700	1.38902800	C	5.58691900	-1.26950200	1.67170200
H	-0.61266700	-6.40948200	0.00650700	H	3.53914700	-1.61965100	2.23976300
H	2.10117000	-4.22056800	2.55220500	C	0.90475300	-1.44172400	4.72685800
C	4.12474200	-4.06726700	-3.13311300	H	2.65387500	-0.26605200	4.25533200
H	2.00978900	-3.81500400	-2.79139600	C	-0.85390300	-1.46517500	3.05985500
C	5.56297700	-2.31036400	-2.27121200	H	-0.47704700	-0.30656800	1.27495700
H	4.55966300	-0.68493000	-1.25625700	C	6.51680100	-0.35106000	1.17843400
C	2.05605400	2.51810300	2.43623500	H	6.82976400	1.67181300	0.47059100
H	1.07662800	4.42407800	2.42390700	H	5.89826000	-2.28672600	1.92086200
C	-0.10715000	5.71723500	-0.36034500	C	-0.35616900	-1.87606800	4.29954300

H	1.29093100	-1.75644100	5.69952100	H	0.26708500	-3.71467900	-2.63313600
H	-1.83711300	-1.79966300	2.72047700	C	2.37513500	-4.11338200	0.60055700
H	7.55984900	-0.64637100	1.04153000	H	2.83695500	-2.03093000	0.40722400
H	-0.95065700	-2.53445900	4.93781000	C	3.99317200	-1.48622800	-3.39675800
9_T				C	5.02410100	0.17287600	-1.93944400
N	-1.80971600	-0.35067400	-3.00661400	C	-0.04116300	2.05915300	2.93918800
S	-2.39739200	0.49884400	-1.65843500	C	1.45086100	3.79227200	1.20940700
C	-0.93680200	-1.49092100	-2.68110800	C	-1.38553100	3.30534400	0.76260900
C	-1.02622300	0.43943400	-3.97379200	H	-7.72014700	-2.85524800	0.19649900
O	-2.59250500	1.88641400	-2.08302000	H	-8.50380800	-1.31181100	-0.23105300
O	-1.54921900	0.20223400	-0.46879200	H	-8.19540800	-2.51659000	-1.49161600
C	-3.95873600	-0.26407400	-1.32584800	C	1.66963600	-5.20512600	0.08614800
H	-1.25133000	-2.00696000	-1.76667600	H	0.36409300	-5.89442800	-1.49626500
C	0.44637900	-0.86728400	-2.58602800	H	2.97984600	-4.22065800	1.50302100
H	-1.01382800	-2.20371300	-3.51794100	C	5.18146700	-1.58613500	-4.11856500
H	-1.41991800	1.45777800	-4.05290400	H	3.12758100	-2.08970400	-3.67568900
C	0.44536900	0.38046700	-3.48093600	C	6.20766100	0.06848200	-2.66303800
H	-1.14080000	-0.05615400	-4.94867600	H	4.94662400	0.84981200	-1.08716400
C	-5.05668000	0.10197000	-2.11328100	C	-0.02364400	0.77953700	3.33691700
C	-4.07135800	-1.19914300	-0.29664500	H	-0.19938600	2.87447100	3.65518200
C	1.46723700	-1.35500900	-1.84199600	C	1.26064000	5.00212000	1.89818700
C	0.88334800	1.71989000	-2.87428100	C	2.66547400	3.55722700	0.54684600
H	1.10880800	0.16658400	-4.33586100	C	-1.43222400	4.42723300	-0.07799700
C	-6.28723000	-0.49465700	-1.86038800	C	-2.58866200	2.71598000	1.18678000
H	-4.94646800	0.84521000	-2.90464700	H	1.72441900	-6.17857800	0.57886800
C	-5.31644900	-1.78576700	-0.06223600	C	6.28690900	-0.81024300	-3.75274500
H	-3.20730200	-1.45802800	0.31395900	H	5.24829000	-2.26973800	-4.96761700
C	1.51148500	-2.68475800	-1.18031500	H	7.07530600	0.66961600	-2.38211800
C	2.66045000	-0.48388100	-1.54197600	P	0.31526400	-0.55615400	2.12042800
Co	0.52810200	0.48091500	0.11331700	H	-0.15047800	0.51135900	4.39260500
H	0.28419100	1.97860000	-1.98590100	C	2.27406200	5.96196800	1.92105000
H	0.73117600	2.51833600	-3.61630600	H	0.31559400	5.19660200	2.41118500
C	-6.43811100	-1.44776500	-0.83408900	C	3.67908600	4.52073000	0.57132400
H	-7.15310000	-0.21534200	-2.46613600	H	2.81252400	2.61372000	0.01647900
H	-5.41415000	-2.51744100	0.74221400	C	-2.66240500	4.95839600	-0.47550200
C	0.83063200	-3.80115200	-1.70517400	H	-0.50637200	4.88961000	-0.42740000
C	2.29697900	-2.87018400	-0.02569800	C	-3.81485000	3.24881100	0.78769700
O	2.54209000	0.30831000	-0.59371800	H	-2.56590400	1.82583300	1.81862900
C	3.90656000	-0.60542000	-2.30189700	H	7.21805000	-0.89012200	-4.31897300
P	0.19319900	2.46079500	1.16163900	C	1.72808600	-1.37819400	2.96461100
H	1.94339600	1.73385600	-2.59451800	C	-1.08884200	-1.71280300	2.33857200
C	-7.78083300	-2.07185500	-0.57234000	C	3.48402400	5.72255200	1.25741700
C	0.90224000	-5.04342800	-1.07188700	H	2.12075700	6.90181100	2.45735900
				H	4.62200900	4.33159300	0.05201300

C	-3.85545200	4.37314600	-0.04296500	C	5.39953400	-1.77894300	-0.03877500
H	-2.68676700	5.83426400	-1.12908300	C	2.70065800	2.93845500	-1.70026900
H	-4.74341400	2.77930100	1.12235300	C	-2.96505100	3.44008000	0.78605100
C	2.99801500	-0.81283100	2.75701900	C	-5.18834200	-1.29334400	-1.44561300
C	1.60241000	-2.50613400	3.78658500	C	3.88543200	-3.61008300	-0.51928400
C	-2.21905800	-1.39823500	3.10762400	C	2.52475700	3.60832100	0.61860700
C	-1.06428900	-2.92334600	1.62255900	C	-1.34883000	3.44795000	-1.01999500
H	4.27481100	6.47675000	1.27641700	C	-4.78056000	-3.01768700	0.20158400
H	-4.81607200	4.78881000	-0.35727600	C	5.18803500	-3.11760800	-0.38826500
H	3.10000000	0.05972000	2.10608200	C	2.79732600	3.92745100	-0.71338400
C	4.12605900	-1.37141200	3.36027200	C	-2.24590200	4.13303400	-0.19619400
C	2.73490300	-3.06717700	4.38587400	C	-5.58516600	-2.47024200	-0.80259100
H	0.62212200	-2.95550200	3.95598200	H	-0.15457800	1.13905600	2.43955000
C	-3.29852300	-2.28629200	3.17274800	H	-0.09471500	-0.02463200	3.76053700
H	-2.26490800	-0.45635900	3.65763300	H	2.09364100	-0.05200400	2.66271200
C	-2.13849100	-3.81085600	1.69549300	H	1.28233100	-1.59428900	2.36801200
H	-0.19800300	-3.17318700	1.00918200	H	-2.24066200	-0.29328600	2.64362900
C	3.99676400	-2.50385300	4.17337900	H	-1.25947500	-1.73463500	2.30485000
H	5.10997900	-0.92700900	3.19059700	H	4.48233000	0.11741100	0.44640700
H	2.62956700	-3.95016100	5.02129300	H	2.22899600	0.87627300	-2.12743600
C	-3.25886400	-3.49548900	2.47383800	H	-3.35360400	1.53092400	1.71459200
H	-4.17395300	-2.02902200	3.77408700	H	-3.69699100	0.25822200	-1.58823500
H	-2.10162900	-4.75027000	1.13848200	H	1.77137000	-3.13539100	-0.39731900
H	4.88008000	-2.94646000	4.64031400	H	1.95240700	2.07624000	2.01712000
H	-4.10079700	-4.18965700	2.52959900	H	-0.46230800	1.52086600	-1.48073300
cat's				H	-2.96738500	-2.83799700	1.34763300
P	1.50578200	-0.40321100	0.32735800	H	6.41767700	-1.39478800	0.06164100
P	-1.56911800	-0.42414200	0.30744600	H	2.91345600	3.18201600	-2.74405700
C	-0.09084000	0.06195500	2.66192900	H	-3.66953500	3.97541900	1.42746700
C	1.23483900	-0.51461700	2.15184300	H	-5.81288100	-0.85957100	-2.23049800
C	-1.33697900	-0.65085300	2.12660700	H	3.71793900	-4.65404300	-0.79543100
C	3.00469000	-1.41917600	0.05604900	H	2.59767400	4.37629900	1.39248600
C	2.05271300	1.31136300	-0.01215400	H	-0.78307300	3.98371600	-1.78584300
C	-1.87953400	1.37336200	0.12802400	H	-5.08585800	-3.93612300	0.70902300
C	-3.18466900	-1.20432300	-0.07054600	H	6.04144400	-3.77765900	-0.56190200
C	4.31282600	-0.92839000	0.18066800	H	3.08388000	4.94620500	-0.98541400
C	2.32180500	1.64249300	-1.35246400	H	-2.38773200	5.20983400	-0.31751500
C	-2.78497600	2.06521300	0.94929500	H	-6.52066200	-2.96016300	-1.08332600
C	-3.99489800	-0.66411700	-1.08422300	Co	-0.02164800	-1.20504400	-0.89205900
C	2.79731300	-2.76207800	-0.30021000	cat'T			
C	2.15771000	2.30455700	0.97082600	P	1.67258300	-0.48862200	0.14387300
C	-1.16775200	2.07185600	-0.85687700	P	-1.76107900	-0.49842200	0.13614900
C	-3.58399800	-2.39319700	0.56362900	C	-0.08221500	-0.08428400	2.40634900

C	1.25010600	-0.68593100	1.93743300	H	4.38377200	-4.42214100	-1.13741400
C	-1.35186100	-0.79824700	1.92253600	H	2.69861200	4.21753400	1.57976900
C	3.25580700	-1.41470000	0.03734600	H	-0.61146600	4.08324100	-1.31191200
C	2.18987800	1.26031300	-0.05299600	H	-5.40424500	-3.79362700	1.03046000
C	-2.04559400	1.31322000	0.08710100	H	6.51630500	-3.53827100	-0.19289900
C	-3.44239400	-1.21021900	-0.05180700	H	3.17594800	4.97324700	-0.74759600
C	4.46024000	-0.92017900	0.56242300	H	-2.43433600	5.18916000	-0.01223300
C	2.45572200	1.69679000	-1.36324500	H	-6.94785700	-2.82256900	-0.67282500
C	-3.06857800	1.93941300	0.81773300	Co	-0.03529100	-1.09157000	-1.17564800
C	-4.31555500	-0.67564800	-1.01616700				
C	3.23907400	-2.67498900	-0.57909200	I's			
C	2.28358800	2.17848900	1.00242000	N	2.30664200	-1.87942700	-0.33905500
C	-1.16910800	2.09395400	-0.67944000	S	3.20745900	-1.57248600	1.03897500
C	-3.84694300	-2.34159200	0.67579700	C	2.19227100	-0.79873000	-1.32194900
C	5.62717900	-1.68330500	0.47900100	C	1.17943600	-2.80203800	-0.26003500
C	2.81789400	3.02067700	-1.61274000	O	3.04894800	-2.75271200	1.89743700
C	-3.20578500	3.32829500	0.77891800	O	2.90072300	-0.24270200	1.60731400
C	-5.56832200	-1.25106900	-1.23637500	C	4.86819800	-1.49356600	0.40314400
C	4.40597800	-3.44069800	-0.65725100	H	2.31064400	-1.23298400	-2.33080000
C	2.63491200	3.50941500	0.74992100	H	3.03140700	-0.09738200	-1.18962000
C	-1.30482700	3.48478700	-0.71644100	C	0.91170800	-0.07763300	-1.23416400
C	-5.10169500	-2.91710200	0.45191200	H	1.50377400	-3.69071600	0.30342800
C	5.60124700	-2.94436700	-0.12829200	C	-0.10151300	-2.30174600	0.37296400
C	2.90295000	3.93307800	-0.55398800	H	0.97838400	-3.13899100	-1.28876000
C	-2.32389600	4.10223700	0.01368600	C	5.39977800	-2.61247600	-0.24964900
C	-5.96636200	-2.37371400	-0.50191000	C	5.62799000	-0.34204200	0.60636700
H	-0.13334600	0.98555500	2.14819300	C	0.09883800	0.85414600	-1.64013500
H	-0.08513800	-0.12666300	3.50778200	C	-0.20093100	-1.47116200	1.45306200
H	2.08427900	-0.28088300	2.53228700	H	-0.97950800	-2.89138300	0.08739300
H	1.25202400	-1.77582200	2.10539700	C	6.71121900	-2.56071300	-0.70962500
H	-2.21646900	-0.47383000	2.52312500	H	4.79271200	-3.50723700	-0.39910400
H	-1.24770200	-1.88658000	2.06027400	C	6.94312200	-0.30927900	0.13606000
H	4.48719200	0.06579100	1.03290300	H	5.19394400	0.51338400	1.12486600
H	2.37413300	0.98974900	-2.19422900	Co	-0.68220500	-0.12882500	-0.26579700
H	-3.76266900	1.34033300	1.41224200	C	-0.05852200	2.05934800	-2.42267000
H	-4.01823700	0.20359800	-1.59322500	H	0.68501200	-1.02251100	1.90096800
H	2.30373400	-3.05200900	-1.00312500	H	-1.11394200	-1.44675100	2.04602100
H	2.08129600	1.86882300	2.02869000	C	7.50457500	-1.41082800	-0.52579000
H	-0.36383800	1.60469400	-1.23139800	H	7.13500900	-3.42793900	-1.22255800
H	-3.18667800	-2.78432700	1.42381900	H	7.54387500	0.59051200	0.28912400
H	6.56231400	-1.29230400	0.88767700	C	-1.33072100	2.46082300	-2.87043000
H	3.02707900	3.34475400	-2.63521300	C	1.05616600	2.87456900	-2.70439700
H	-4.00401200	3.81153800	1.34782700	C	8.92032000	-1.37999200	-1.03212300
H	-6.23903200	-0.81869500	-1.98318500	C	-1.48760500	3.65098600	-3.57976200

H	-2.18835200	1.82134900	-2.66190100	H	-2.60697900	2.97457600	-0.40908800
C	0.89278600	4.07438500	-3.39502700	H	-0.77782500	-1.94341200	-2.35222100
H	2.04319900	2.56881100	-2.35336700	H	-3.84169400	-3.49133000	-0.90413200
H	9.52084900	-2.17755400	-0.56390100	H	-3.42398600	1.84393700	3.05408000
H	8.95253500	-1.55367600	-2.12054700	H	-1.31431400	4.56833300	0.49241000
H	9.40493500	-0.41604200	-0.82172000	H	-5.03574300	-1.23167800	-2.50827600
C	-0.37791300	4.46524600	-3.83381400	H	-3.25809600	-0.56676300	2.22450500
H	-2.47831100	3.95016500	-3.93033700	H	0.80111700	0.89288600	2.95733700
H	1.75947700	4.70972500	-3.59210300	H	1.66866300	1.46829000	1.01394300
H	-0.50298200	5.40522800	-4.37683100	H	-0.89393000	-3.10194600	-4.54548200
P	-2.78266800	-0.69299000	-0.63419800	H	-4.75483500	-5.07711100	0.76154400
P	-1.25717500	1.60020700	0.98255700	H	-3.44961300	1.45650200	5.48029000
C	-4.08282500	1.62747600	0.41598900	H	0.47614200	6.22833800	0.19698900
C	-4.06208200	0.63612700	-0.74511100	H	-5.14374700	-2.36089100	-4.69983600
C	-2.81692300	2.47938900	0.55117300	H	-4.20271100	-2.13838000	3.87736000
C	-2.89132600	-1.50959600	-2.27434200	H	0.76304300	0.51879300	5.38644100
C	-3.51041300	-1.90409700	0.53705800	H	3.44685600	3.14874500	0.76779000
C	-1.31482900	1.37578400	2.81083000	H	-3.08054200	-3.31018600	-5.73127300
C	0.04116800	2.89283600	0.78548300	H	-4.95137600	-4.41281200	3.15725300
C	-1.73482500	-2.04457300	-2.86254600	H	-1.36288800	0.77814300	6.67318900
C	-3.92286600	-3.18579800	0.13986400	H	2.87130900	5.54326200	0.33592300
C	-2.50038600	1.54147400	3.54516200				
C	-0.27767700	4.23901100	0.55527100	1'T			
C	-4.11978700	-1.63018000	-2.94740600	N	-2.65607300	-0.44531600	0.03260100
C	-3.60937000	-1.54304200	1.89244000	S	-3.94333300	0.61322600	-0.08874700
C	-0.14056300	1.01161700	3.49421200	C	-2.22318300	-0.93720500	1.33633100
C	1.39156700	2.51093400	0.85710700	C	-2.25038400	-1.21968300	-1.14010300
C	-1.80257700	-2.69104400	-4.09896600	O	-3.73860300	1.38017600	-1.32349400
C	-4.43858600	-4.08135100	1.08189300	O	-4.03155400	1.29760300	1.20800100
C	-2.51688500	1.32447100	4.92665000	C	-5.40482700	-0.38052100	-0.30238800
C	0.73916200	5.18540000	0.38947800	H	-2.57690600	-1.97077500	1.50455600
C	-4.18380900	-2.27394200	-4.18522000	H	-2.65692500	-0.29550300	2.11478400
C	-4.13268600	-2.43624900	2.82844300	C	-0.74892200	-0.91120500	1.45878000
C	-0.15938500	0.80109400	4.87339000	H	-3.02657000	-1.13293400	-1.91741400
C	2.40150500	3.46166200	0.70738200	C	-0.92155900	-0.77877900	-1.72466300
C	-3.02679500	-2.80662300	-4.76302000	H	-2.21238700	-2.28390300	-0.85918400
C	-4.54872600	-3.70914400	2.42469700	C	-5.94084000	-0.55252800	-1.57992300
C	-1.34912600	0.94893900	5.59409500	C	-5.97870200	-0.99699800	0.81673400
C	2.07948700	4.80161900	0.46656300	C	0.38247300	-1.05925800	1.95462100
H	-4.31231700	1.10150600	1.35329200	C	-0.59568800	0.53957100	-1.91332400
H	-4.92514800	2.31771400	0.24900600	H	-0.34879400	-1.55757700	-2.23937800
H	-5.04106000	0.14254800	-0.82713500	C	-7.06558300	-1.36524400	-1.73633200
H	-3.87593000	1.16237800	-1.69394400	H	-5.49004100	-0.04725700	-2.43493500
H	-2.97095800	3.27269900	1.29710400	C	-7.09857700	-1.80399900	0.63885000

H	-5.56191100	-0.83650700	1.81258500	C	3.07383800	0.58172700	-4.32240000
Co	0.37718400	-0.15375800	-0.06993100	C	-0.09551700	4.73413800	-2.31127800
C	1.51736500	-1.26275700	2.80951700	C	-1.74571200	3.01753800	2.88557500
H	-1.29082700	1.32321700	-1.60508300	C	2.57116500	-5.66810900	0.15328800
H	0.22616400	0.83283100	-2.56682000	C	3.50751800	-0.48968800	-5.10973100
C	-7.66012000	-2.00297900	-0.63703800	C	1.05400700	5.19648600	-2.96179700
H	-7.49254800	-1.50088500	-2.73293800	C	-1.14410000	3.84029000	3.84237800
H	-7.55548900	-2.28547700	1.50733400	H	4.11894000	1.43394700	-0.87936800
C	1.98952400	-0.19137200	3.59640400	H	5.08560900	1.36696600	0.58031800
C	2.16800100	-2.51000200	2.87769300	H	4.84405600	-0.87409200	-0.17449900
C	-8.87735700	-2.87086800	-0.80217100	H	3.86878200	-0.73113300	1.30392500
C	3.10481600	-0.36251100	4.41427000	H	3.41895800	2.98614900	1.03453100
H	1.47281400	0.76814700	3.55630400	H	3.02270300	1.56009400	1.99915500
C	3.28536600	-2.66916600	3.69755100	H	0.44836500	-3.13810900	-0.68541300
H	1.79758700	-3.34373300	2.28289200	H	3.42583300	-2.96298600	-2.76264000
H	-9.73603200	-2.44719500	-0.25473100	H	3.40294600	3.40883600	-1.26964600
H	-9.16220400	-2.97253600	-1.85899600	H	2.06169200	3.80600200	2.68127000
H	-8.70266200	-3.87858700	-0.39078500	H	4.69917400	-3.00917900	0.08775000
C	3.76221900	-1.59781100	4.45993500	H	2.40406000	1.22087900	-2.38439500
H	3.46443400	0.47365000	5.01858000	H	-0.90109500	3.44037600	-0.79505500
H	3.78794400	-3.63818300	3.73815300	H	-1.44468800	1.80979700	1.13065500
H	4.64076000	-1.72715300	5.09641100	H	0.45084200	-5.58466700	-0.27604300
P	2.46655900	-1.09552400	-0.61424300	H	3.96236000	-2.60435600	-5.15157400
P	1.31833700	1.96711500	0.38109500	H	3.21092200	5.07162200	-3.07237800
C	4.09210300	1.11776600	0.17358500	H	0.69872800	4.75849300	4.50875800
C	3.94652300	-0.40519700	0.25491500	H	4.69051900	-5.44001500	0.52328700
C	3.07245200	1.94374200	0.97005500	H	2.97115900	1.58045900	-4.75394500
C	2.57187900	-2.90184900	-0.33815200	H	-1.07935500	5.11397600	-2.59735900
C	2.88675600	-0.89538200	-2.39398700	H	-2.81382300	2.79455400	2.92237200
C	1.26288900	3.28586200	-0.90287600	H	2.57137000	-6.74281000	0.35088800
C	0.40065100	2.73618000	1.77303300	H	3.74781300	-0.33449800	-6.16435600
C	1.38322300	-3.64382100	-0.43718400	H	0.97275200	5.93599500	-3.76210500
C	3.32222200	-1.96532400	-3.19235900	H	-1.74138400	4.27047500	4.65009600
C	2.41217100	3.76500100	-1.55185500				
C	0.99703800	3.57157400	2.73115900	TS1's			
C	3.76244000	-3.56182400	0.00334500	N	3.09335100	0.86520400	1.19060300
C	2.75795800	0.37826100	-2.97770700	S	4.07899200	-0.51499500	1.17470100
C	0.00696100	3.78493400	-1.29374100	C	1.95341000	0.77623100	2.12182000
C	-0.97240900	2.46185300	1.86466200	C	2.65385900	1.31835200	-0.14742000
C	1.38274800	-5.01952900	-0.19811500	O	3.53512700	-1.56440700	0.29163100
C	3.62720400	-1.76156700	-4.54177900	O	4.33239300	-0.84843900	2.58251200
C	2.30578500	4.71124700	-2.57726400	C	5.55288400	0.13540500	0.42513000
C	0.22615800	4.11365900	3.76356700	H	1.87478700	1.72225600	2.68328300
C	3.75936600	-4.93722800	0.25083600	H	2.10974500	-0.03116200	2.84823200

C	0.71809100	0.55892100	1.31281300	C	-5.18406400	1.03799100	-0.41911700
H	2.68337100	0.48850000	-0.87098300	C	-1.47395300	3.75483300	1.04737600
C	1.23935300	1.85717400	-0.06123300	C	0.31540700	-3.16270900	-1.11159900
H	3.31828200	2.11900100	-0.50779400	C	-3.34850900	-1.99258800	0.03646800
C	5.98463500	-0.37400400	-0.79845600	C	-3.84932600	1.12646800	1.60110400
C	6.27101000	1.13015300	1.09969900	C	-2.74448700	4.64668400	-0.81728700
C	-0.27579500	-0.31567400	1.35199100	C	2.31817000	-2.34869500	-2.88552900
C	0.43818200	1.87946300	-1.28277200	C	-4.04922900	-4.00559200	-1.77197300
H	1.15131500	2.75838400	0.55444800	C	-6.27855300	0.59558800	0.33072300
C	7.15838400	0.13323600	-1.36146900	C	-1.28883100	5.04744500	1.54083500
H	5.40897500	-1.15444400	-1.29760200	C	1.47427700	-3.92681500	-1.25805200
C	7.43524100	1.62400700	0.52128000	C	-4.37917000	-2.88322900	0.34988700
H	5.91824700	1.50929200	2.06038300	C	-4.94455600	0.69192400	2.34674500
C	-0.45938900	-1.50467600	2.18007200	C	-2.55004800	5.93966700	-0.32224800
H	0.85449100	1.33415600	-2.13866200	C	2.47702700	-3.52217400	-2.14276900
H	0.01917800	2.85256400	-1.55674400	C	-4.73135700	-3.88798400	-0.55380000
C	7.89799300	1.13597600	-0.71698200	C	-6.16122700	0.41746900	1.71100700
H	7.50581300	-0.25928600	-2.32013900	C	-1.82572600	6.14247900	0.85584000
H	8.00320500	2.40221500	1.03774700	H	-3.87647700	-0.00744600	-2.76930800
C	-1.63826500	-1.72482700	2.91592600	H	-3.34576200	0.79580600	-4.24267200
C	0.55702800	-2.48270800	2.21666700	H	-1.90031400	-1.11970000	-3.92376400
C	9.15761500	1.69049400	-1.32351200	H	-0.92753600	0.32958200	-3.59351400
C	-1.79798000	-2.88969400	3.66780800	H	-3.84577300	2.50367100	-2.57369800
H	-2.42948300	-0.97439300	2.89782600	H	-2.11273300	2.52456900	-2.94295800
C	0.38358900	-3.65430600	2.95568300	H	1.05687300	-0.66263700	-3.32786000
H	1.47545300	-2.32223700	1.64901600	H	-2.48166100	-3.22702100	-3.03144900
H	10.00493300	1.59580900	-0.62473500	H	-5.29972300	1.16922600	-1.49489100
H	9.41980800	1.17388200	-2.25775200	H	-1.04473300	2.90317700	1.58019200
H	9.04493400	2.76532600	-1.54424200	H	-0.46029000	-3.48660100	-0.41673700
C	-0.79299400	-3.86331000	3.68320900	H	-3.07176200	-1.20648300	0.73231000
H	-2.71777500	-3.04314500	4.23790600	H	-2.89954000	1.32269600	2.10331600
H	1.17611000	-4.40702600	2.96500400	H	-3.31717800	4.50864300	-1.73566900
H	-0.92610600	-4.78077900	4.26167300	H	3.10019500	-2.02702100	-3.57760000
P	-1.32162300	-0.93785400	-1.58103500	H	-4.32045900	-4.79423500	-2.47787900
P	-2.45929800	1.82298500	-0.70499600	H	-7.22618300	0.38727000	-0.17150700
C	-3.05224400	0.57965500	-3.20342000	H	-0.72007100	5.19994200	2.46116900
C	-1.77887400	-0.26912800	-3.23626300	H	1.59534000	-4.83942700	-0.66977900
C	-2.91366500	1.92710400	-2.48002200	H	-4.90403100	-2.78753300	1.30284100
C	0.14951900	-1.98339100	-1.85742600	H	-4.84711600	0.56035700	3.42694000
C	-2.66408800	-2.10535900	-1.17817800	H	-2.97029800	6.79215300	-0.86127300
C	-3.95867100	1.29759300	0.21012200	H	3.38644200	-4.11809800	-2.24916300
C	-2.20738800	3.54585400	-0.13313100	H	-5.53734600	-4.58496000	-0.31143700
C	1.16276200	-1.57754000	-2.74290500	H	-7.01694000	0.06735000	2.29314300
C	-3.01761600	-3.12046100	-2.08538100	H	-1.67842800	7.15464000	1.24007000

Co	-0.73955700	0.61965300	-0.23056900	H	-1.23720100	-4.23785500	4.88809200
TS1' _T				P	-0.51634500	-0.99333000	-1.67420800
				P	-2.87789000	1.40768700	-0.80358200
N	2.88093700	1.44660700	1.57166600	C	-2.66612500	-0.04450400	-3.28405800
S	3.88526300	0.08166900	1.71329600	C	-1.18105100	-0.42864800	-3.30377700
C	1.70969200	1.36466800	2.46154300	C	-3.01170200	1.30860500	-2.64161200
C	2.44083300	1.75614600	0.19069900	C	1.15888700	-1.61458200	-2.03892600
O	3.27401000	-1.10869200	1.09038600	C	-1.51190800	-2.47668600	-1.29053200
O	4.25980800	0.00604100	3.13088700	C	-4.35901300	0.56465500	-0.13246900
C	5.27749800	0.57554300	0.72877000	C	-3.16541500	3.17129600	-0.40383000
H	1.51044300	2.36176200	2.88718900	C	1.91442100	-1.10624800	-3.11012500
H	1.89393400	0.67176300	3.29213400	C	-1.40758600	-3.65998700	-2.04050500
C	0.55833200	0.91467200	1.61660200	C	-5.31770600	-0.07605400	-0.93056400
H	2.65287200	0.91845800	-0.49032200	C	-2.35919200	3.78192200	0.56923300
C	0.94063100	2.03591100	0.19089700	C	1.72247200	-2.58943200	-1.19917400
H	2.97399400	2.64393700	-0.17993900	C	-2.44078500	-2.39894100	-0.24365100
C	5.53422900	-0.09257000	-0.46749000	C	-4.49908600	0.53614000	1.26597200
C	6.10092000	1.61214000	1.18309700	C	-4.18248800	3.91388300	-1.02586600
C	-0.34615200	-0.02511700	1.69080200	C	3.20619400	-1.58512500	-3.34619100
C	0.27003900	1.92728200	-1.10849800	C	-2.22319300	-4.75089200	-1.73552800
H	0.68629600	2.97368700	0.69963500	C	-6.39170500	-0.74627300	-0.33510700
C	6.63917800	0.29308500	-1.22891800	C	-2.56473300	5.12053000	0.91583200
H	4.87637500	-0.89753500	-0.79482000	C	3.00844100	-3.07026000	-1.44543200
C	7.19574400	1.98256600	0.40859200	C	-3.25896300	-3.49091800	0.05769200
H	5.88448800	2.11731300	2.12600200	C	-5.57457900	-0.12736000	1.85660800
C	-0.60212900	-1.14446400	2.58588300	C	-4.38088900	5.25244400	-0.68190900
H	0.85835500	1.48080200	-1.91726100	C	3.75176700	-2.57310400	-2.52049700
H	-0.32597600	2.79160300	-1.41450400	C	-3.14877600	-4.66777100	-0.68705600
C	7.48426100	1.33073400	-0.80677200	C	-6.52106100	-0.77724800	1.05551700
H	6.84751400	-0.22378800	-2.16891300	C	-3.57297300	5.85714600	0.28823200
H	7.84643000	2.79113200	0.75152700	H	-3.25412500	-0.85384400	-2.82378400
C	-1.88928000	-1.41286400	3.08665300	H	-3.00021800	0.00796900	-4.33243100
C	0.45631300	-2.01499500	2.92343200	H	-1.01672400	-1.24658900	-4.02280500
C	8.68221100	1.74053100	-1.61867700	H	-0.57022600	0.42758500	-3.62949300
C	-2.11221200	-2.51102400	3.91811200	H	-4.03132200	1.60621500	-2.92982500
H	-2.71668700	-0.75726100	2.81591700	H	-2.33606300	2.09239200	-3.02052400
C	0.22225600	-3.12020100	3.74345700	H	1.49910300	-0.34504100	-3.77196400
H	1.45357800	-1.82670400	2.52056700	H	-0.68366900	-3.73211600	-2.85578000
H	8.71940100	1.21168700	-2.58167100	H	-5.24072700	-0.06224600	-2.01784400
H	8.67452800	2.82484200	-1.81580700	H	-1.57086600	3.20602000	1.05908700
H	9.61535900	1.52171800	-1.07245300	H	1.15355100	-2.97664500	-0.35162900
C	-1.05901500	-3.37144800	4.24651500	H	-2.52233000	-1.47807500	0.33419800
H	-3.11716100	-2.70178500	4.30304500	H	-3.76109800	1.04031300	1.89529100
H	1.04912500	-3.79048900	3.99186500	H	-4.82655200	3.44787200	-1.77506100

H	3.78470900	-1.18853300	-4.18401300	C	-2.05658700	-3.06327800	1.67843900
H	-2.13699100	-5.67213000	-2.31686200	C	3.78915600	2.11658700	2.49156700
H	-7.13060500	-1.24630800	-0.96585600	C	-2.59756800	-1.13389500	3.62561600
H	-1.93447200	5.58797800	1.67615700	H	-1.25314000	0.13796100	2.52232900
H	3.43642900	-3.82746000	-0.78509800	C	-2.94725100	-3.34630200	2.71664400
H	-3.97661600	-3.41912200	0.87779600	H	-1.85450000	-3.82012300	0.91843400
H	-5.67284500	-0.14113100	2.94470600	H	4.01263700	2.14175000	3.56954000
H	-5.17267400	5.82603400	-1.16983800	H	4.50092600	2.76981600	1.96898900
H	4.75952400	-2.95014000	-2.71052900	H	2.78218900	2.54755900	2.36194000
H	-3.78290500	-5.52583600	-0.45082800	C	-3.21913800	-2.38543800	3.69629000
H	-7.35981300	-1.30409800	1.51665900	H	-2.80744200	-0.37305000	4.38120000
H	-3.73263400	6.90447700	0.55594100	H	-3.43099400	-4.32547300	2.76182200
Co	-0.81158900	0.59788800	-0.06465000	H	-3.91507300	-2.60963900	4.50838300
2's				P	-2.31753900	0.26930500	-1.22387100
N	2.28327400	-3.70715100	-0.45628800	P	0.41841900	2.24799400	-1.13391600
S	3.79780300	-3.55993100	0.27762500	C	-1.95583000	2.87867100	-2.52705800
C	1.11832700	-3.52971600	0.43316400	C	-2.52197100	1.45902400	-2.63126500
C	2.02932900	-2.91116200	-1.67440300	C	-0.43055600	2.99221600	-2.58195000
O	4.78515400	-3.65918600	-0.80237600	C	-3.13786100	-1.23445400	-1.89108100
O	3.79121500	-4.51656300	1.38848700	C	-3.42491600	0.80281500	0.13280200
C	3.89254000	-1.91399600	0.97389600	C	0.01056400	3.27520400	0.32089400
H	1.39074600	-3.64940100	1.48935600	C	2.19965400	2.55284400	-1.44876900
H	0.38478100	-4.32086500	0.20528100	C	-4.37576400	-1.09503200	-2.54768500
C	0.55173500	-2.17191900	0.05842900	C	-4.39222900	-0.07038700	0.65798900
H	1.35145200	-3.48916600	-2.32316600	C	-0.40119600	4.61384400	0.24586200
C	1.33031200	-1.63893600	-1.14327200	C	2.92463100	3.49456800	-0.70100000
H	2.96398600	-2.72999300	-2.21685100	C	-2.59624500	-2.51784200	-1.73428500
C	4.48470800	-0.88670700	0.23416900	C	-3.24782300	2.06559600	0.72416700
C	3.29337100	-1.65485800	2.21209000	C	0.05519400	2.63774500	1.57476600
C	-0.50645400	-1.46665200	0.49837100	C	2.85512200	1.83875500	-2.46848900
C	0.37717200	-0.82257600	-1.99116200	C	-5.04428900	-2.21540600	-3.04301500
H	2.13335100	-0.97212700	-0.78861800	C	-5.17988900	0.32339900	1.74092200
C	4.45487000	0.41554500	0.73379200	C	-0.76474800	5.29956700	1.40847600
H	4.96233800	-1.10634900	-0.72161000	C	4.27660400	3.72162100	-0.97317700
C	3.26607900	-0.34698600	2.69220900	C	-3.26870300	-3.63806500	-2.23085200
H	2.86604200	-2.46797600	2.79954600	C	-4.04052300	2.45571700	1.80548500
C	-1.42539300	-1.80599500	1.59055000	C	-0.30079100	3.32577600	2.73529100
H	-0.37798400	-1.44594200	-2.48450100	C	4.20698500	2.06604300	-2.73379800
H	0.86448000	-0.18720600	-2.74061100	C	-4.49152300	-3.49087200	-2.88831100
C	3.83852200	0.70968000	1.96170400	C	-5.00884800	1.58592300	2.31598200
H	4.91752000	1.21909000	0.15895700	C	-0.71619800	4.65854000	2.65126700
H	2.80102300	-0.14280900	3.66021500	C	4.92145100	3.00911600	-1.98756700
C	-1.72078000	-0.84664900	2.58043900	H	-2.34566800	3.38863900	-1.63397600
				H	-2.35677900	3.43996900	-3.38613000

H	-3.60323200	1.52467700	-2.81566300	H	-2.16095700	1.44158100	-0.57537400
H	-2.07891400	0.93701700	-3.49580700	C	-5.24470900	0.63690500	-2.53366400
H	-0.11730100	4.04265200	-2.68057800	H	-4.69152500	2.37770600	-1.37931200
H	-0.03399100	2.45835500	-3.46094600	C	-6.23216900	-1.19091000	-1.30466500
H	-4.84119100	-0.11499400	-2.66237600	H	-6.42772700	-0.89363200	0.83604700
H	-4.52647500	-1.06443300	0.23258200	C	-0.31316700	-1.32012600	2.28152300
H	-0.44178100	5.12746300	-0.71630900	H	0.02244000	2.81489700	1.11559300
H	2.43621100	4.05762500	0.09507500	H	-0.13472400	2.83899200	-0.66808200
H	-1.64970300	-2.64619200	-1.21511200	C	-5.80718700	-0.65312400	-2.52932500
H	-2.48276600	2.74548300	0.35419900	H	-4.92001900	1.07727300	-3.47986000
H	0.37599900	1.59272700	1.64089400	H	-6.67850800	-2.18817200	-1.28076100
H	2.31288000	1.10623200	-3.06837500	C	-1.03075400	-2.51757900	2.08304000
H	-6.00469500	-2.08955700	-3.54843600	C	0.72522000	-1.31388500	3.23720400
H	-5.92420400	-0.36754200	2.14300900	C	-5.90884700	-1.44961800	-3.80086300
H	-1.08755800	6.34127800	1.34349500	C	-0.72179100	-3.66362400	2.81832600
H	4.82740500	4.45957200	-0.38518600	H	-1.81810000	-2.54747700	1.32830200
H	-2.83079400	-4.63024900	-2.09841200	C	1.02411300	-2.45720700	3.97979400
H	-3.89345400	3.44160100	2.25197600	H	1.29440500	-0.39458700	3.40048800
H	-0.26174200	2.81975900	3.70245100	H	-6.69534500	-2.21571400	-3.73598500
H	4.70307500	1.50408600	-3.52862600	H	-6.11689500	-0.80309100	-4.66680700
H	-5.01643200	-4.36696700	-3.27667300	H	-4.95636200	-1.97058500	-4.00392700
H	-5.62492700	1.88928000	3.16587500	C	0.30560200	-3.63976300	3.76815900
H	-1.00374900	5.19948600	3.55593000	H	-1.28315400	-4.58481900	2.64256100
H	5.97930700	3.18573000	-2.19564500	H	1.82671500	-2.42942800	4.72112200
Co	-0.30715900	0.17509900	-0.46973200	H	0.54712500	-4.53921900	4.33966300
2'T				P	2.59385100	1.73766400	-0.75661000
N	-3.70471400	1.70083000	1.74480500	P	1.26439700	-1.28583900	-1.12100300
S	-5.32566600	1.71858800	1.37837800	C	2.72227100	0.20101000	-3.14265700
C	-3.06606900	0.38619700	1.97883700	C	2.54267700	1.61952800	-2.59314700
C	-2.77518100	2.65111500	1.09623800	C	1.57180100	-0.77433000	-2.87173400
O	-5.68037200	3.11873100	1.11936600	C	2.76982400	3.51308000	-0.38011000
O	-5.99741100	0.95217100	2.43406700	C	4.15949900	0.96809000	-0.23219900
C	-5.52682700	0.80040700	-0.14731100	C	2.58238300	-2.45257600	-0.64972900
H	-3.65893200	-0.42503100	1.52127700	C	-0.26057600	-2.28720500	-1.26435100
H	-2.98079500	0.16179000	3.05370400	C	3.30730800	3.88996900	0.86296300
C	-1.72471100	0.53457700	1.30670600	C	4.11967400	0.03366200	0.81380200
H	-2.28761700	3.26714100	1.87076700	C	3.63355600	-2.79882300	-1.51123700
C	-1.74420600	1.73739400	0.40635000	C	-0.27187400	-3.68434900	-1.15382000
H	-3.31808000	3.32280100	0.42069700	C	2.30882100	4.50298400	-1.26226100
C	-5.10690500	1.36906900	-1.35613800	C	5.38202400	1.26380400	-0.85677300
C	-6.09217000	-0.47570200	-0.11361600	C	2.55115300	-2.98886200	0.64958100
C	-0.56815800	-0.13244400	1.46153300	C	-1.46999600	-1.59822200	-1.45280900
C	-0.30914100	2.23732500	0.23635200	C	3.38984100	5.23860300	1.21213400
				C	5.29025000	-0.60240500	1.23445100

C	4.64684400	-3.65623100	-1.07212100	O	-5.25326700	3.59041600	0.19413200
C	-1.48345700	-4.38055300	-1.21617100	C	-5.30246600	1.05861400	-0.53803700
C	2.39320600	5.85251400	-0.90607700	H	-3.04677400	2.27122200	1.11376100
C	6.54794500	0.61913800	-0.44138000	H	-2.15119200	3.74120700	0.67789100
C	3.55575200	-3.85567100	1.07790500	C	-1.22973800	1.88977300	-0.01842800
C	-2.67619800	-2.29466300	-1.51563500	H	-1.85029600	2.86184200	-2.60661400
C	2.93253700	6.22279300	0.32857900	C	-1.50615500	1.14291700	-1.30146700
C	6.50241800	-0.31384300	0.60250200	H	-3.13375600	1.63669400	-2.74121300
C	4.61152500	-4.18511300	0.22041700	C	-5.43841600	0.12407900	-1.57075600
C	-2.68538400	-3.68881100	-1.38952200	C	-5.50637400	0.68902900	0.79527500
H	3.67809600	-0.21351800	-2.78904300	C	-0.00960600	1.81146400	0.53539200
H	2.81797300	0.28759100	-4.23688900	C	-0.14713500	0.83433500	-1.90778300
H	3.33032400	2.27805800	-2.98981300	H	-2.07914400	0.21913800	-1.09738900
H	1.57436300	2.03976000	-2.90916600	C	-5.75562700	-1.19636600	-1.25459200
H	1.70332400	-1.69691900	-3.45841000	H	-5.31837600	0.43410300	-2.60964800
H	0.61769700	-0.33009700	-3.19963100	C	-5.82465700	-0.63639200	1.09177600
H	3.66978700	3.12797900	1.55748800	H	-5.43546200	1.43749800	1.58540000
H	3.16562200	-0.21084700	1.28987200	C	0.38343900	2.59137200	1.72130100
H	3.67642400	-2.40597800	-2.52706400	H	0.28590200	1.77493100	-2.27277900
H	0.65968300	-4.23217000	-1.00431900	H	-0.18096900	0.13430900	-2.75168900
H	1.88418200	4.23150600	-2.23014700	C	-5.94281500	-1.60169500	0.07806700
H	5.42205700	1.99466500	-1.66825300	H	-5.87142000	-1.92735600	-2.05829500
H	1.74157800	-2.72579200	1.32935600	H	-5.98552200	-0.92705500	2.13264900
H	-1.47182100	-0.50941300	-1.53589700	C	-0.01962700	2.20695300	3.01710400
H	3.81486800	5.52286400	2.17773400	C	1.13030200	3.77762500	1.59056300
H	5.25056200	-1.33299200	2.04462400	C	-6.21843500	-3.04193100	0.41158400
H	5.46608100	-3.91193200	-1.74815100	C	0.34092000	2.95788000	4.13822900
H	-1.48511800	-5.46905500	-1.12145500	H	-0.64797400	1.32406500	3.14187700
H	2.03520400	6.61687100	-1.59995700	C	1.48926000	4.52995600	2.71114400
H	7.49740800	0.84401200	-0.93308600	H	1.41321500	4.11784800	0.59604400
H	3.51714300	-4.26780600	2.08885100	H	-6.77395600	-3.14007700	1.35592100
H	-3.61067500	-1.74859700	-1.64773700	H	-6.78835600	-3.54057600	-0.38666100
H	2.99785400	7.27822600	0.60341300	H	-5.26931000	-3.59474800	0.52709500
H	7.41733100	-0.81861500	0.92185400	C	1.10650100	4.11935100	3.99205000
H	5.40561100	-4.85429700	0.56006300	H	0.01272100	2.63817700	5.13101900
H	-3.63190400	-4.23357900	-1.42624400	H	2.06968500	5.44665700	2.57897300
Co	0.83874100	0.60247000	0.32246100	H	1.39019200	4.70719900	4.86859700
3's				P	2.67662000	0.83375100	-1.07064900
N	-3.17296300	2.80100600	-0.95464000	P	1.09473700	-1.94273000	-1.21999900
S	-4.83373100	2.74200600	-0.92736200	C	2.91619100	-0.99864500	-3.25265300
C	-2.43159400	2.73670600	0.32523200	C	2.81255100	0.48369700	-2.88267100
C	-2.43979700	2.12000100	-2.04221400	C	1.68319700	-1.86707700	-2.97234900
O	-5.28141700	3.01724500	-2.29737500	C	3.08644600	2.61063900	-0.93593500
				C	4.17532400	0.01878000	-0.37927900

C	2.24746600	-3.07274800	-0.35429100	H	3.96052700	6.39734800	-0.62155700
C	-0.48313100	-2.89049500	-1.36289000	H	7.41848700	-1.65883700	1.00217200
C	3.94536000	3.05745700	0.08042400	H	4.76083000	-5.28148000	1.66785200
C	5.37841100	0.08262800	-1.10768700	H	-3.93173200	-4.72046400	-1.61516300
C	3.41154500	-3.56974200	-0.96092400	Co	0.75659200	0.18570700	-0.28208100
C	-0.69084500	-4.11861700	-0.71511500	C	0.71994000	-0.84535000	2.62096500
C	2.54233200	3.54059300	-1.83763100	H	1.32426600	-0.85970700	3.54892400
C	4.16269400	-0.64199200	0.85588000	O	1.23422900	-0.37200700	1.60720200
C	1.99289500	-3.40786300	0.98770800	C	-0.60843800	-1.43725600	2.71675400
C	-1.53585500	-2.34195600	-2.11874500	C	-0.96928100	-2.05977500	3.92814100
C	4.26043600	4.41405900	0.18849600	C	-1.50934900	-1.44463200	1.63421300
C	6.53537600	-0.51988200	-0.61283100	C	-2.20561100	-2.69210700	4.04833900
C	4.31007400	-4.35606200	-0.23481600	H	-0.26788700	-2.04803500	4.76654300
C	-1.92460300	-4.76976800	-0.80513500	C	-2.73815400	-2.08098100	1.75611300
C	2.85580000	4.89622500	-1.72157900	H	-1.26088300	-0.94938100	0.69842100
C	5.32558900	-1.23886400	1.35125500	C	-3.08688000	-2.70588700	2.96112300
C	2.88422400	-4.20245500	1.70830800	H	-2.48359400	-3.17771700	4.98605400
C	-2.76471800	-2.99742700	-2.21162100	H	-3.42666700	-2.09020700	0.91278300
C	3.71610600	5.33605100	-0.70920200	H	-4.05525800	-3.20391700	3.05156600
C	6.51174200	-1.18557700	0.61770900				
C	4.05436100	-4.66992000	1.10168600	3'T			
C	-2.96788100	-4.21093900	-1.54745800	N	3.56350000	-2.50797300	-1.35220100
H	3.80486900	-1.42645200	-2.76799500	S	5.21201700	-2.23503500	-1.32575500
H	3.10881000	-1.05279500	-4.33633300	C	2.85765800	-2.62621700	-0.05017200
H	3.70656900	1.01524300	-3.23942600	C	2.74915200	-1.71274400	-2.29821500
H	1.95228200	0.95595600	-3.37331600	O	5.66915800	-2.33011800	-2.71616600
H	1.85661100	-2.89951100	-3.31174200	O	5.75356500	-3.11754400	-0.28612400
H	0.82443200	-1.49257900	-3.54817800	C	5.44941800	-0.54249400	-0.79317000
H	4.37052600	2.34811300	0.79182600	H	3.52928600	-2.35973000	0.77961500
H	5.42504500	0.61004900	-2.06164700	H	2.53144200	-3.66371700	0.12533200
H	3.63731000	-3.34801000	-2.00279800	C	1.69109600	-1.67369800	-0.18921900
H	0.10772500	-4.58217000	-0.13768700	H	2.08373500	-2.39219500	-2.85679000
H	1.87491700	3.21369200	-2.63641900	C	1.93100400	-0.79183500	-1.37483000
H	3.24368800	-0.68816100	1.43171200	H	3.38758900	-1.19535700	-3.02419500
H	1.07646300	-3.07046700	1.46736100	C	5.44720600	0.48354500	-1.74281000
H	-1.40228500	-1.40309100	-2.65352400	C	5.57070300	-0.25731800	0.57157000
H	4.92790200	4.75076400	0.98506700	C	0.50811500	-1.59919000	0.45569400
H	7.46119800	-0.46546700	-1.19053600	C	0.59597600	-0.25656500	-1.85491400
H	5.21659300	-4.72306800	-0.72153300	H	2.59298400	0.04062500	-1.06982100
H	-2.06510800	-5.72434100	-0.29238200	C	5.53821700	1.80832700	-1.31361000
H	2.42869200	5.61180800	-2.42807400	H	5.38992000	0.24634000	-2.80579200
H	5.29618500	-1.75440200	2.31347800	C	5.66752600	1.07137700	0.98118000
H	2.66326800	-4.45469600	2.74822800	H	5.60729500	-1.06959800	1.29861200
H	-3.56503100	-2.55359900	-2.80656100	C	0.18880100	-2.35436600	1.67795900

H	0.04223100	-1.04543800	-2.38789900	C	-2.69769600	-5.68486600	-1.11422400
H	0.67304000	0.61549100	-2.51532600	C	-6.78106500	0.24172000	0.69206400
C	5.64251800	2.12575700	0.05063000	C	-4.58458100	3.91220800	1.56080400
H	5.54285600	2.61137400	-2.05463400	C	1.78860000	5.31914200	-1.47496700
H	5.77185500	1.29555900	2.04540300	H	-4.05700700	1.16962400	-2.79949500
C	1.11880000	-2.42002000	2.73730300	H	-3.26372200	0.97301100	-4.34960500
C	-1.06575900	-2.96814800	1.86755300	H	-3.65684300	-1.22015000	-3.42263000
C	5.71211500	3.55519800	0.51390200	H	-1.91337800	-0.94836100	-3.43627200
C	0.81632900	-3.09219200	3.92404000	H	-2.29715300	2.87860000	-3.15641400
H	2.08152300	-1.91571600	2.63372900	H	-1.08724700	1.63310300	-3.47332500
C	-1.36722900	-3.64293800	3.05009600	H	-4.65033100	-3.07906200	-0.10294900
H	-1.80708300	-2.91703800	1.07302000	H	-5.52289600	-0.88966400	-2.26567400
H	6.49882400	3.69090000	1.27258900	H	-4.27755500	2.69971600	-1.60307200
H	5.91049700	4.24213200	-0.32094700	H	-1.58214000	4.81744100	-1.56993700
H	4.76008000	3.86093200	0.98085000	H	-0.90320400	-3.02780400	-2.26504700
C	-0.42781800	-3.70927400	4.08638800	H	-3.47681400	-0.11115600	1.45683200
H	1.55499100	-3.12583200	4.72926100	H	-1.31123700	2.96618200	1.52753900
H	-2.34477700	-4.11873300	3.16450300	H	1.60472300	1.96223000	-0.95968300
H	-0.66680000	-4.23317700	5.01526200	H	-4.56704300	-5.55374500	-0.03320300
P	-2.74262600	-1.04755400	-1.17862200	H	-7.65743900	-0.17232100	-1.24351600
P	-1.38191600	1.92668900	-1.14169900	H	-5.94724500	3.72199100	-0.10833300
C	-3.10773900	0.86949300	-3.26333600	H	0.09095800	6.62957700	-1.77255100
C	-2.85568800	-0.61212800	-2.97634100	H	-0.83712100	-5.49688400	-2.20571700
C	-1.99364000	1.85460700	-2.88800100	H	-5.63242900	0.56734200	2.49628600
C	-2.79171500	-2.87952700	-1.20057300	H	-2.99441900	3.98826200	3.03012900
C	-4.35082700	-0.54615800	-0.46783300	H	3.26746500	3.77246900	-1.14945800
C	-2.67839100	2.73899500	-0.13693100	H	-2.65785200	-6.77605600	-1.07478900
C	-0.10831800	3.25558300	-1.25654000	H	-7.72704700	0.55463200	1.14081600
C	-3.81667100	-3.60349100	-0.57233400	H	-5.32835400	4.36211900	2.22278100
C	-5.53462900	-0.56116400	-1.22494000	H	2.52528100	6.12199700	-1.55696200
C	-3.98401000	2.97122300	-0.59091600	Co	-0.63764000	-0.15059900	-0.27195800
C	-0.51921800	4.58043400	-1.48647700	C	-0.86275700	0.37688800	2.74559600
C	-1.71894600	-3.57387000	-1.78774400	H	-1.48383800	0.06721800	3.60850900
C	-4.39699400	-0.13951200	0.87467800	O	-1.33463000	0.24690300	1.61172800
C	-2.33189300	3.11680200	1.17239300	C	0.45223600	0.91072400	3.04951900
C	1.26174700	2.97937200	-1.13847200	C	0.90955800	0.86640300	4.38057200
C	-3.76611200	-5.00014200	-0.52939400	C	1.27681900	1.44280000	2.04002600
C	-6.74205600	-0.16297600	-0.64680600	C	2.18566700	1.32988600	4.69242100
C	-4.93147600	3.55368000	0.25641800	H	0.26214500	0.45034200	5.15626800
C	0.42386300	5.60388500	-1.59618700	C	2.54450800	1.91486400	2.35684500
C	-1.67652800	-4.96806200	-1.74788200	H	0.91919600	1.49077700	1.01385300
C	-5.60867200	0.24677100	1.45228700	C	3.00129600	1.85217000	3.68085600
C	-3.27781900	3.69884800	2.01521200	H	2.54853600	1.28746500	5.72135500
C	2.20520400	4.00556600	-1.24621200	H	3.18134000	2.33236500	1.57717000

H	4.00078700	2.21928700	3.92625400	H	-0.82087700	-4.79678000	4.65612100
TS2's				P	-1.30045200	-1.51654000	-1.19114600
				P	-2.34829500	1.60672800	-1.05978700
N	3.89480600	-0.34187200	0.13294600	C	-2.35792800	0.04346800	-3.41196200
S	5.27371900	-1.08673700	-0.43426100	C	-1.41349600	-1.08279400	-2.98797400
C	3.02471900	-1.08117300	1.07754300	C	-2.00042100	1.42652200	-2.86537600
C	3.13411200	0.50473100	-0.80351600	C	-0.01557100	-2.83521300	-1.28579800
O	5.10541400	-1.49772400	-1.84207500	C	-2.81083600	-2.47431100	-0.80044400
O	5.63624600	-2.09620900	0.56996500	C	-4.17885800	1.40284400	-1.03208000
C	6.46795300	0.23581900	-0.40952900	C	-2.14907900	3.39958700	-0.73958300
H	3.38692400	-0.96276000	2.11232300	C	-0.32596400	-4.19240900	-1.10621400
H	2.99866400	-2.15822000	0.86065300	C	-3.80894000	-2.73983300	-1.74898800
C	1.68352600	-0.43061100	0.86671700	C	-4.79732200	0.28605200	-0.45483600
H	2.94842700	-0.01630500	-1.75695400	C	-1.19938600	4.17130200	-1.42751300
C	1.82916500	0.76837500	-0.03538900	C	1.31116400	-2.47915900	-1.57370200
H	3.69070300	1.42729100	-1.02588000	C	-2.95337400	-2.97766900	0.50516400
C	6.93066400	0.78091300	-1.60902400	C	-4.97375400	2.35713300	-1.69685900
C	6.92417300	0.70382100	0.82567900	C	-2.92572300	4.00423400	0.26209500
C	0.46442800	-0.74940400	1.33079200	C	0.67700800	-5.16312600	-1.18688000
C	0.54579000	0.98914800	-0.83096200	C	-4.94114600	-3.47902500	-1.39269300
H	2.02248900	1.63109500	0.62420300	C	-6.18554700	0.12635400	-0.53319700
C	7.86238100	1.81778000	-1.56338300	C	-1.02557600	5.52209500	-1.10921400
H	6.56415500	0.39168200	-2.55959500	C	2.31546300	-3.44573400	-1.64611300
C	7.85587000	1.74029800	0.85124000	C	-4.07921200	-3.72293900	0.85449200
H	6.55820500	0.26080100	1.75374500	C	-6.35668100	2.19506400	-1.77326600
C	0.14858000	-1.84641700	2.26199000	C	-2.75303300	5.35246500	0.57329900
H	0.60888300	0.48076800	-1.80191400	C	1.99975700	-4.79346800	-1.44400200
H	0.39694100	2.05768500	-1.03867700	C	-5.08107300	-3.96839100	-0.09159000
C	8.33878100	2.31418200	-0.33791500	C	-6.96719500	1.07814600	-1.18931000
H	8.22962000	2.25005000	-2.49789200	C	-1.79942200	6.11528900	-0.10884900
H	8.21965200	2.11105300	1.81264100	H	-3.40014200	-0.20095700	-3.15582200
C	-0.55965400	-1.61007400	3.45710900	H	-2.32270900	0.09875600	-4.51193600
C	0.53092600	-3.17142800	1.97336200	H	-1.65927000	-2.01569900	-3.51722000
C	9.34450100	3.43296600	-0.31036900	H	-0.38159300	-0.83144400	-3.27803900
C	-0.90433400	-2.65935200	4.31008200	H	-2.58776100	2.20226500	-3.37853600
H	-0.82574500	-0.58844200	3.72928600	H	-0.93766400	1.64571400	-3.03842000
C	0.18521100	-4.22149500	2.82602500	H	-1.34748100	-4.50214400	-0.88945100
H	1.09234900	-3.38173900	1.06630500	H	-3.72050300	-2.37459700	-2.77189400
H	8.95135000	4.32859700	-0.81947100	H	-4.20175300	-0.46565100	0.05339800
H	9.61249200	3.71204800	0.71859800	H	-0.58999700	3.73293300	-2.21860700
H	10.26756500	3.14430900	-0.84005700	H	1.57063000	-1.43778300	-1.74103600
C	-0.54423000	-3.97372400	3.99267900	H	-2.17792600	-2.79227700	1.24705800
H	-1.45436500	-2.44876400	5.23090200	H	-4.51122400	3.23337600	-2.15568200
H	0.48537600	-5.24094400	2.57069900	H	-3.66617200	3.41706700	0.80680600

H	0.41917700	-6.21457900	-1.03849600	C	-1.43315000	2.99221300	0.04943300
H	-5.71549600	-3.67206500	-2.13887200	C	-0.03366800	0.56342700	-1.18288200
H	-6.65018200	-0.75192500	-0.07949500	H	-1.81038000	-0.15662800	-0.18169000
H	-0.28353700	6.11236500	-1.65225900	C	-4.35972900	-3.28743000	0.50841000
H	3.34241800	-3.13397100	-1.84713300	H	-3.91850900	-2.68167900	-1.51943900
H	-4.17372300	-4.11214800	1.87103000	C	-5.67500800	-1.74006100	1.81278200
H	-6.96121800	2.94367500	-2.29110500	H	-6.27031000	0.08497400	0.80780600
H	-3.36157700	5.80765300	1.35801700	C	-1.94992500	4.26931900	0.55826400
H	2.78394800	-5.55291400	-1.49233600	H	0.33748600	1.56975500	-1.42350100
H	-5.96670800	-4.54603500	0.18444700	H	0.14597300	-0.06812300	-2.06361500
H	-8.05113100	0.95285500	-1.24902500	C	-4.99913100	-2.96877500	1.71714800
H	-1.66244900	7.17096400	0.13745900	H	-3.82696900	-4.23664500	0.41273500
Co	-1.00410000	0.28157400	0.22283200	H	-6.18140700	-1.47668800	2.74515100
C	-2.80433300	0.46451400	2.37498400	C	-3.21992300	4.42345100	1.15196300
H	-3.65248900	0.23721400	3.04564900	C	-1.11297100	5.40280100	0.48364200
O	-2.53544400	-0.31182700	1.44763400	C	-4.97759500	-3.91753900	2.88433600
C	-2.01257200	1.65560800	2.55773700	C	-3.64613800	5.67076300	1.61417500
C	-2.34323700	2.66003700	3.48048800	H	-3.87052200	3.55961200	1.28887000
C	-0.88985400	1.76350300	1.69347100	C	-1.54076400	6.64788700	0.94310000
C	-1.55322400	3.80459900	3.54548100	H	-0.11621100	5.29468000	0.05084500
H	-3.21888800	2.54043900	4.12327700	H	-4.67543300	-3.40305500	3.81044000
C	-0.11603600	2.92466100	1.77893500	H	-5.98245800	-4.33578200	3.06513200
H	-0.19144100	0.60909600	1.57244700	H	-4.28997600	-4.75771700	2.71113300
C	-0.45085000	3.93349700	2.68979800	C	-2.81422100	6.78963900	1.50611900
H	-1.79510800	4.60272700	4.25007300	H	-4.63391700	5.76642700	2.07233300
H	0.75049900	3.06530200	1.13467300	H	-0.87560000	7.51189400	0.86583800
H	0.15980700	4.83848200	2.73112900	H	-3.15149900	7.76343400	1.86965700
4's				P	2.96951500	0.97369600	-0.88297200
N	-3.73395900	0.88090100	-1.71635500	P	1.69465300	-1.99279000	-0.83675300
S	-5.09366500	-0.06202400	-1.83491100	C	3.55539600	-0.97424300	-2.82425100
C	-3.61198900	1.81409300	-0.57941000	C	3.25080300	0.51185200	-2.63783400
C	-2.42027900	0.36542100	-2.13451200	C	2.37091500	-1.90202100	-2.55478100
O	-4.94630000	-0.84437500	-3.06851500	C	2.78970200	2.79638200	-0.91794400
O	-6.23389600	0.84082500	-1.63863600	C	4.55802000	0.69146700	-0.02676300
C	-5.07696600	-1.20045600	-0.45626500	C	2.99810500	-2.72874800	0.20863800
H	-4.10734800	1.40940100	0.32273100	C	0.44941900	-3.31763200	-1.07694900
H	-4.07828000	2.78177900	-0.81145500	C	3.22504800	3.55616900	0.18042600
C	-2.11866500	1.91675400	-0.38003900	C	5.79786100	0.86343800	-0.66361200
H	-2.05887700	0.92247600	-3.01604300	C	4.14202000	-3.34976000	-0.31800100
C	-1.52704600	0.62511700	-0.90707600	C	0.58076800	-4.57435800	-0.46667400
H	-2.48025200	-0.69585600	-2.40438600	C	2.16388500	3.44554300	-1.99482000
C	-4.39746700	-2.41510800	-0.57877300	C	4.52325800	0.29291500	1.31772700
C	-5.72267100	-0.85538800	0.73653400	C	2.84146400	-2.64433400	1.60273700
				C	-0.64971400	-3.06915000	-1.91514200

C	3.04738600	4.94033100	0.19545400	C	-0.18742300	-0.75438700	1.41388200
C	6.98235000	0.62523200	0.03594700	C	-2.15772100	-1.12103600	3.47286500
C	5.11806100	-3.86289300	0.53974200	H	-1.78201000	0.95038000	3.99267200
C	-0.38207100	-5.56405000	-0.68493000	C	-0.82543600	-1.98588500	1.60937100
C	1.98772200	4.83249600	-1.97565500	C	-1.78216800	-2.16695600	2.61861000
C	5.70977200	0.06057300	2.01764800	H	-2.91875700	-1.27930300	4.23976700
C	3.81308300	-3.17010200	2.45610800	H	-0.60281600	-2.83770200	0.97080700
C	-1.59962100	-4.06613600	-2.14309400	H	-2.24743500	-3.14740600	2.73632500
C	2.42943700	5.58288100	-0.88291200	H	-0.34529500	2.94504000	-0.00857400
C	6.94016800	0.22245900	1.37564100				
C	4.95701600	-3.77335100	1.92597000	4'T			
C	-1.47239300	-5.31377000	-1.52318700	N	-3.97663600	1.61546700	-1.47371200
H	4.42049400	-1.26320800	-2.20840200	S	-5.43803600	0.81947700	-1.56757800
H	3.86033500	-1.13096600	-3.87121600	C	-3.57877100	2.23759700	-0.19541100
H	4.06096400	1.13667900	-3.04205200	C	-2.80549600	1.00602200	-2.12060700
H	2.33374400	0.77903700	-3.18514600	O	-5.67147900	0.55649900	-2.99165500
H	2.61938100	-2.93719200	-2.83406600	O	-6.38336600	1.61627000	-0.77712700
H	1.51259500	-1.61397800	-3.18264300	C	-5.23594900	-0.76363300	-0.76050600
H	3.70871500	3.06448800	1.02603400	H	-4.21496000	1.88108800	0.63084000
H	5.84362300	1.18271500	-1.70660600	H	-3.70152000	3.33070800	-0.24680300
H	4.28066000	-3.44326500	-1.39544500	C	-2.13049300	1.84072300	-0.01009200
H	1.42871600	-4.78148400	0.18791400	H	-2.33679600	1.73607300	-2.80219300
H	1.81157600	2.88124100	-2.85918000	C	-1.86442100	0.67707800	-0.94581800
H	3.56523800	0.15774600	1.82132900	H	-3.09015100	0.12620200	-2.71101000
H	1.95479400	-2.16787200	2.02569500	C	-4.82603700	-1.87147800	-1.51217000
H	-0.77216400	-2.09556600	-2.39116300	C	-5.46181600	-0.87201300	0.61430200
H	3.39357700	5.52036100	1.05432400	C	-1.22328300	2.40499900	0.80684500
H	7.94377200	0.75556800	-0.46660300	C	-0.45227600	0.37368700	-1.38843400
H	6.00817000	-4.33817600	0.12099500	H	-2.29107800	-0.21126500	-0.44744900
H	-0.27400600	-6.53744500	-0.20055800	C	-4.63119900	-3.09233200	-0.87005500
H	1.50136500	5.32587900	-2.82042600	H	-4.68555100	-1.77768700	-2.58975200
H	5.67077400	-0.25529400	3.06242800	C	-5.26259600	-2.10394300	1.23976900
H	3.67882700	-3.09987000	3.53800900	H	-5.81018300	-0.00836700	1.18216100
H	-2.44224400	-3.86763400	-2.80916400	C	-1.37695500	3.45728700	1.81702500
H	2.28961400	6.66633500	-0.86940600	H	-0.10654700	1.15263600	-2.08014800
H	7.86946400	0.03396900	1.91866200	H	-0.42741000	-0.59651200	-1.91621100
H	5.72365700	-4.17538900	2.59259600	C	-4.84623600	-3.23056200	0.51281700
H	-2.22080900	-6.09042000	-1.69727200	H	-4.31949900	-3.96183800	-1.45367000
Co	1.21386700	-0.08554300	0.20464300	H	-5.44429500	-2.19379100	2.31338200
C	0.18215100	1.49286200	2.17747500	C	-2.61490900	3.94783600	2.28527500
H	0.00681000	2.36694200	2.82914900	C	-0.20235600	3.99436500	2.38915400
O	1.06608500	1.56611300	1.29950300	C	-4.62773800	-4.55942500	1.18298200
C	-0.55677200	0.27503800	2.33321500	C	-2.66771800	4.95129000	3.25504300
C	-1.53394200	0.11390800	3.33371800	H	-3.55055700	3.53315900	1.91492200

C	-0.25618600	4.99610800	3.35750500	H	2.35474900	3.37947700	0.37463700
H	0.76518200	3.61459900	2.05696200	H	4.67354100	2.73756900	-2.25104800
H	-4.89891700	-4.52658500	2.24767300	H	4.79013600	-3.13922400	-1.26837400
H	-5.22518100	-5.34898900	0.69871300	H	1.61035200	-4.50317900	1.06889300
H	-3.57173300	-4.86667800	1.10551100	H	1.23653200	2.51789000	-3.71315600
C	-1.49252100	5.48604900	3.79212600	H	3.91194200	-0.08423300	0.93029400
H	-3.63985100	5.31333600	3.59934600	H	2.28457500	-2.21592100	2.13966500
H	0.67083300	5.39557000	3.77681000	H	-0.28424800	-2.79415300	-2.42840500
H	-1.54022100	6.27150100	4.55035600	H	1.43710800	5.67494200	0.13586900
P	2.42747400	1.08496900	-1.35890900	H	7.01510300	2.97007100	-1.47733000
P	2.00691300	-2.14592700	-0.72730600	H	6.65894800	-3.66644400	0.25644600
C	3.44298300	-1.00025800	-2.95502200	H	-0.15080000	-6.23061900	1.16625700
C	2.71227800	0.34658300	-3.02154300	H	0.32277800	4.80404700	-3.94269500
C	2.58086400	-2.17263100	-2.48113700	H	6.25077900	0.14744100	1.70044300
C	1.86011700	2.79439700	-1.64999600	H	4.15873900	-2.77535600	3.66175300
C	4.13209400	1.29961500	-0.71566200	H	-2.02319600	-4.53455300	-2.33353500
C	3.40249100	-2.64804800	0.33041200	H	0.41371000	6.39350800	-2.02336000
C	0.79752900	-3.52419400	-0.68756300	H	7.81713800	1.67690600	0.50011500
C	1.91270800	3.69483000	-0.57295200	H	6.36086200	-3.48862600	2.72510900
C	5.01628500	2.16360200	-1.38680500	H	-1.98227900	-6.26143500	-0.52942400
C	4.63831100	-3.05717300	-0.19134800	Co	0.94314800	-0.11688500	-0.03227100
C	0.81801900	-4.50001600	0.31980700	C	1.20019300	0.55333200	2.65928900
C	1.28544400	3.20115900	-2.86385400	H	1.49513700	1.01227100	3.62154600
C	4.58676600	0.57990900	0.39741800	O	1.81502100	0.87769900	1.62566300
C	3.24000600	-2.54374300	1.72435800	C	0.12291700	-0.40356700	2.61519300
C	-0.23750800	-3.54671800	-1.63944000	C	-0.52917500	-0.82056000	3.79193400
C	1.39766000	4.98382500	-0.70890800	C	-0.22602400	-0.90722200	1.32735900
C	6.33504200	2.29618700	-0.95063400	C	-1.54086600	-1.77121000	3.70481300
C	5.69729600	-3.35553300	0.67124000	H	-0.23122800	-0.40124800	4.75665500
C	-0.17972500	-5.47711300	0.37554200	C	-1.25024200	-1.85411100	1.27690000
C	0.76839300	4.49420500	-2.99439200	C	-1.89212800	-2.28341400	2.44815300
C	5.90894600	0.71516800	0.83204900	H	-2.05703900	-2.11710400	4.60277800
C	4.29647600	-2.85481000	2.58088700	H	-1.56660100	-2.28177700	0.32420300
C	-1.22845200	-4.52840100	-1.58442200	H	-2.67962800	-3.03461100	2.37914400
C	0.82124400	5.38514100	-1.91939200	H	-0.20077800	2.03728200	0.72124100
C	6.78423300	1.57065400	0.15945500				
C	5.52984400	-3.25593000	2.05507300	TS3's			
C	-1.20538900	-5.49487100	-0.57364000	N	2.14337300	0.32169200	-0.64936400
H	4.35071100	-0.90893400	-2.33809000	S	2.41939800	0.94150900	-2.16480600
H	3.78932300	-1.24367400	-3.97177500	C	3.07416400	-0.69563600	-0.12775900
H	3.30095700	1.06996700	-3.60594500	C	1.67475500	1.18966700	0.44006800
H	1.73537300	0.23551400	-3.51829200	O	1.38039700	1.95863200	-2.39245000
H	3.09767900	-3.13166700	-2.64002300	O	2.53540000	-0.20894100	-3.07111400
H	1.66085900	-2.21311600	-3.08382700	C	3.99565600	1.76230300	-2.09808500

H	4.13182800	-0.42144000	-0.30011800	C	-1.22037700	-4.09482600	-0.76536400
H	2.89045800	-1.65987000	-0.62062600	C	-3.79968000	-2.81410400	-2.86106900
C	2.76811500	-0.71437300	1.35044200	C	-4.79734600	1.88149600	-0.99954800
H	0.71105600	1.63242300	0.18327700	C	-2.28205000	3.91178100	1.37877000
C	1.57227100	0.19320700	1.59448300	C	0.56537900	-2.77908300	-1.74653400
H	2.39455200	1.99482200	0.67382700	C	-4.57180100	-1.83261600	-0.78247200
C	4.06327300	3.08092400	-1.62952100	C	-4.33569300	1.13779700	1.25760000
C	5.15196100	1.05629800	-2.44023700	C	-0.39890000	3.91981900	-0.14329400
C	3.41342000	-1.37456200	2.33049600	C	-0.35222000	-5.18194100	-0.64753700
C	0.32488600	-0.67896700	1.50130300	C	-5.09015000	-3.27912700	-3.11804400
H	1.64227500	0.68928700	2.57022500	C	-6.16720900	1.75214000	-0.75596700
C	5.31051900	3.68610700	-1.49854800	C	-1.86055900	5.13563900	1.90386700
H	3.15170000	3.62758500	-1.38431600	C	1.42838400	-3.87272100	-1.62837300
C	6.39216500	1.68177900	-2.30215400	C	-5.86384400	-2.29998600	-1.04135300
H	5.07927600	0.03645200	-2.81994700	C	-5.70537500	1.01824400	1.50043700
C	4.56254500	-2.28299900	2.25503000	C	0.02022600	5.14292200	0.38710500
H	0.36706200	-1.47918400	2.24584600	C	0.97483000	-5.07435500	-1.07745200
H	0.32901000	-1.16957200	0.51530000	C	-6.12430600	-3.02062200	-2.20953100
C	6.49383600	2.99848300	-1.82679900	C	-6.62524600	1.31697900	0.49089600
H	5.37053700	4.71651300	-1.13874900	C	-0.70558100	5.75271800	1.41441100
H	7.29921700	1.13594500	-2.57283600	H	-3.31076400	0.51947900	-2.96448900
C	5.07477600	-2.82911600	1.05776400	H	-2.08850400	1.12091800	-4.07856000
C	5.19877100	-2.64108700	3.46378100	H	-1.52193300	-1.19238400	-3.72533300
C	7.83064500	3.66894500	-1.66674700	H	-0.33770200	-0.25616700	-2.79915700
C	6.17975500	-3.68190300	1.07568400	H	-2.39279400	2.82004100	-2.36454400
H	4.60070700	-2.61432000	0.10218600	H	-0.77719700	2.11139900	-2.24693500
C	6.30451300	-3.49007800	3.47962500	H	-2.25223100	-4.18631900	-0.42273000
H	4.81183600	-2.23694600	4.40297900	H	-2.99607600	-3.02405800	-3.57118600
H	8.64849600	3.03508000	-2.03790800	H	-4.46773300	2.22992200	-1.97814000
H	7.85918300	4.62731000	-2.21037200	H	-3.18351500	3.44439900	1.77533600
H	8.02811400	3.89693700	-0.60566100	H	0.94995800	-1.85013800	-2.16895900
C	6.80384300	-4.01390800	2.28235900	H	-4.36978800	-1.26647000	0.12622200
H	6.55358700	-4.09549400	0.13557000	H	-3.62967000	0.89289500	2.05034700
H	6.77857000	-3.74632000	4.43051300	H	0.18635000	3.46562000	-0.94362400
H	7.66887000	-4.68154000	2.29014400	H	-0.71480300	-6.11901100	-0.21771500
P	-1.86739800	-1.42060700	-1.33663000	H	-5.29179200	-3.84602600	-4.03027800
P	-2.05189300	1.63792800	-0.29475700	H	-6.87962200	1.99399300	-1.54818200
C	-2.23883800	0.75608100	-3.04990700	H	-2.44046200	5.60836500	2.70023700
C	-1.40447000	-0.51281800	-2.86798200	H	2.46087100	-3.78132500	-1.97443800
C	-1.84622700	1.89917800	-2.11002800	H	-6.66667900	-2.09551500	-0.32933100
C	-0.76969400	-2.88484000	-1.32015600	H	-6.05227400	0.68456700	2.48129200
C	-3.53422100	-2.08261200	-1.69100700	H	0.91813900	5.62203700	-0.01108400
C	-3.86510300	1.56477400	0.00140700	H	1.65283400	-5.92627500	-0.98477800
C	-1.55191700	3.28685400	0.35492300	H	-7.13418600	-3.38431400	-2.41487900

H	-7.69712500	1.21378300	0.67598400	C	5.84652500	3.82401700	-1.68255700
H	-0.37621100	6.70919600	1.82749400	H	4.43506400	5.39331100	-1.20190000
Co	-1.57278400	-0.34931100	0.65299800	H	6.97080200	2.05668300	-2.21832600
C	-2.26750300	-1.86212700	2.74007800	C	5.09016700	-2.38909700	1.22727700
H	-2.77389100	-2.64460700	3.33222800	C	5.31235300	-2.12460800	3.61881200
O	-2.03285700	-2.07131800	1.52810700	C	7.05142800	4.71500400	-1.55440600
C	-1.86011300	-0.62133200	3.32626300	C	6.20453800	-3.22968400	1.22544000
C	-2.18056400	-0.25457800	4.64738300	H	4.57801300	-2.21118400	0.28499200
C	-1.13417800	0.24447000	2.43510500	C	6.42693300	-2.96215800	3.61456300
C	-1.79055100	0.99164200	5.12049900	H	4.96073400	-1.69534100	4.56076300
H	-2.74505800	-0.94652900	5.27820600	H	7.98734700	4.14221700	-1.62041300
C	-0.74792100	1.49443400	2.96454400	H	7.05959300	5.47485700	-2.35433900
C	-1.07810900	1.85813600	4.26813000	H	7.04153100	5.25933400	-0.59640300
H	-2.03088700	1.29994100	6.13990500	C	6.88175400	-3.51864800	2.41431300
H	-0.19628600	2.20329000	2.34987900	H	6.54303500	-3.66745000	0.28282800
H	-0.78154600	2.84485600	4.63372100	H	6.94295100	-3.18364300	4.55222800
H	3.04759900	-1.19962900	3.34823300	H	7.75369800	-4.17720300	2.40632800
TS3'_T				P	-1.07490000	-1.77343900	-1.21540100
N	1.93165100	0.51065800	-0.48452300	P	-2.58658600	1.20055400	-0.56477600
S	2.16452800	1.12413400	-2.01742100	C	-2.25231000	-0.09101900	-3.13983000
C	2.94205500	-0.41664200	0.05965300	C	-1.04795700	-1.00618600	-2.88912700
C	1.45716200	1.42249400	0.56848600	C	-2.22619300	1.24031200	-2.37825400
O	0.98631000	1.96088700	-2.29732300	C	0.42302400	-2.82011400	-1.12196200
O	2.48330200	-0.01408700	-2.88581200	C	-2.45129100	-2.97838500	-1.34693700
C	3.58873200	2.18698800	-1.93750400	C	-4.37541300	0.83615500	-0.41489000
H	3.97225800	-0.11064800	-0.20003500	C	-2.42828300	2.97304400	-0.10796400
H	2.77598800	-1.42226600	-0.34864700	C	0.64734200	-3.52834400	0.07390200
C	2.73610200	-0.33395100	1.55429400	C	-2.27888900	-4.21034500	-1.99996800
H	0.44495300	1.76392000	0.33031500	C	-5.24614900	0.82675700	-1.51584100
C	1.51707000	0.53932400	1.81754200	C	-3.37195100	3.61226900	0.70961900
H	2.11623000	2.30082300	0.68903600	C	1.36993800	-2.89909000	-2.15314400
C	3.42591000	3.53438800	-1.59134400	C	-3.71351000	-2.64069700	-0.83655400
C	4.85799700	1.64767200	-2.16883200	C	-4.87884500	0.51373600	0.85761200
C	3.46191800	-0.91773000	2.52681900	C	-1.28246200	3.68221900	-0.51232300
C	0.31052100	-0.38029800	1.97978300	C	1.80010100	-4.29748700	0.23457100
H	1.63666400	1.14903900	2.72193200	C	-3.35721300	-5.08670900	-2.14132600
C	4.55533000	4.33970900	-1.46690000	C	-6.59125200	0.48686200	-1.34534300
H	2.42822200	3.94710200	-1.43718500	C	-3.17356800	4.93368000	1.11908500
C	5.97650500	2.47167600	-2.03677600	C	2.52374400	-3.67315600	-1.98820600
H	4.96630500	0.60295300	-2.46282400	C	-4.79262000	-3.51583800	-0.98702600
C	4.62080300	-1.81148000	2.42785000	C	-6.22528000	0.18685800	1.02661600
H	0.24755900	-0.78207700	2.99551800	C	-1.08847300	5.00270900	-0.09965500
H	0.40768900	-1.26229600	1.30610800	C	2.74292200	-4.37042300	-0.79758000
				C	-4.61633600	-4.74015300	-1.63774600

C	-7.08373900	0.16469700	-0.07730500	TS3' _{oss}			
C	-2.03121700	5.63241400	0.71936600	N	2.09564300	0.43189000	-0.58206600
H	-3.19002300	-0.63765000	-2.95008200	S	2.36486800	1.12953000	-2.06713500
H	-2.26041100	0.15474700	-4.21367000	C	3.05385800	-0.58186500	-0.10488200
H	-1.02712400	-1.81613900	-3.63411600	C	1.63311600	1.25573000	0.54468600
H	-0.10823500	-0.44307700	-2.97990700	O	1.27064000	2.09199200	-2.27344800
H	-2.93264600	1.95512300	-2.82673600	O	2.56508600	0.02843800	-3.01777000
H	-1.22509300	1.68421800	-2.46834900	C	3.88686400	2.04034100	-1.93364900
H	-0.08497200	-3.47668700	0.88383000	H	4.10428600	-0.26805000	-0.25572300
H	-1.29983000	-4.48932900	-2.39605200	H	2.89946500	-1.52308600	-0.64808400
H	-4.88753200	1.07944700	-2.51393500	C	2.74601600	-0.68406400	1.36985900
H	-4.26666200	3.08194300	1.03735000	H	0.66553300	1.70618300	0.31383500
H	1.23248100	-2.34326300	-3.07931300	C	1.55553500	0.21970000	1.66603200
H	-3.85445500	-1.69540300	-0.31722100	H	2.35420500	2.05330300	0.79976300
H	-4.21363500	0.52434900	1.71978100	C	3.86581300	3.33901300	-1.40842300
H	-0.53028600	3.20783900	-1.14438300	C	5.08980500	1.42245000	-2.28633200
H	1.96772200	-4.83609400	1.17017500	C	3.35939500	-1.43567100	2.30472600
H	-3.21388200	-6.04457000	-2.64763700	C	0.33355200	-0.66960200	1.55909100
H	-7.25799200	0.47574400	-2.21094600	H	1.62743000	0.68153100	2.65887900
H	-3.91808700	5.41701500	1.75641100	C	5.07100300	4.01303100	-1.22973200
H	3.25809800	-3.72126300	-2.79596100	H	2.91879400	3.81782200	-1.15738300
H	-5.77104200	-3.23879300	-0.58732900	C	6.28671000	2.11643900	-2.10056100
H	-6.60201900	-0.05741700	2.02273400	H	5.08655000	0.41785900	-2.71111500
H	-0.19461100	5.54224300	-0.42304700	C	4.46400500	-2.39074100	2.17447900
H	3.64985000	-4.96527400	-0.66806900	H	0.31864400	-1.44131400	2.33251100
H	-5.45815700	-5.42800200	-1.74988900	H	0.31363300	-1.15455700	0.56934400
H	-8.13566800	-0.10180500	0.05051100	C	6.29929200	3.41462000	-1.56714600
H	-1.87750000	6.66505200	1.04191300	H	5.06190500	5.02870800	-0.82586400
Co	-1.18895900	-0.28145600	0.63928900	H	7.22983800	1.64017800	-2.37921900
C	-2.65505800	-1.29389100	2.88433300	C	5.00524800	-2.82997100	0.94588200
H	-3.23076000	-1.91012900	3.60380000	C	5.01607400	-2.92249900	3.36071400
O	-2.34814400	-1.76313900	1.77948100	C	7.58805000	4.16148300	-1.35892800
C	-2.28529700	0.05260900	3.24435500	C	6.05199400	-3.75263600	0.91414900
C	-2.82478400	0.68453500	4.38149200	H	4.60191500	-2.47134400	0.00164600
C	-1.39731500	0.73220300	2.35237300	C	6.06408200	-3.84134100	3.32724400
C	-2.51105000	2.01128600	4.65093600	H	4.60716100	-2.60192100	4.32256000
H	-3.50379400	0.12424700	5.03044400	H	8.45409700	3.58296800	-1.71032700
C	-1.08361800	2.06615500	2.66714400	H	7.57514400	5.12522900	-1.89399400
C	-1.64307900	2.69359500	3.78189100	H	7.73844200	4.39107000	-0.29069400
H	-2.93038000	2.51784800	5.52244400	C	6.58936600	-4.26185800	2.10079400
H	-0.41453800	2.64512000	2.03257100	H	6.44920600	-4.07995200	-0.05005000
H	-1.39495800	3.73981200	3.97868400	H	6.47166400	-4.23394600	4.26225500
H	3.15959400	-0.68882600	3.55450900	H	7.40907900	-4.98376400	2.06969500
				P	-1.64066900	-1.51831800	-1.34903500

P	-2.20084500	1.59761600	-0.38985000	H	-7.00690500	1.72444600	-1.76853000
C	-2.26900200	0.59129200	-3.09210800	H	-2.84525300	5.58952800	2.52344400
C	-1.30088500	-0.57866600	-2.89401700	H	2.78804800	-3.56342200	-2.39826100
C	-1.96736700	1.80504100	-2.20730500	H	-6.45583300	-2.45722500	-0.66562200
C	-0.35540400	-2.82055600	-1.29388600	H	-6.22017900	0.44431700	2.27849200
C	-3.19997500	-2.40784700	-1.69561700	H	0.63949700	5.65883500	-0.02215300
C	-4.01604100	1.43973200	-0.14170500	H	2.46298700	-5.47953600	-0.83181400
C	-1.79077400	3.27017800	0.24691200	H	-6.57487500	-4.20186800	-2.44674900
C	-0.53719300	-3.90545900	-0.41606100	H	-7.84174600	0.90080800	0.43322800
C	-3.26982300	-3.39115900	-2.69694400	H	-0.77071800	6.73303100	1.73545300
C	-4.93595200	1.71249200	-1.16664900	Co	-1.57217200	-0.34362900	0.63205500
C	-2.58385200	3.88438100	1.22922100	C	-2.34710000	-1.77954200	2.83329100
C	0.84929800	-2.70549600	-2.00446200	H	-2.80185400	-2.55222200	3.47965900
C	-4.35125400	-2.07953200	-0.96578900	O	-2.15798000	-2.03265200	1.62345900
C	-4.49643700	0.98430800	1.10024000	C	-1.95692600	-0.50725300	3.36539000
C	-0.62704300	3.92199400	-0.19982800	C	-2.21622100	-0.12610900	4.69675500
C	0.47027500	-4.85686600	-0.25521100	C	-1.29094400	0.35754800	2.42946600
C	-4.48039000	-4.03247200	-2.96390100	C	-1.82265700	1.13229900	5.13411000
C	-6.30375500	1.51607600	-0.95866000	H	-2.73304600	-0.81899200	5.36641000
C	-2.21759800	5.12369400	1.75986000	C	-0.88533800	1.61446600	2.92569400
C	1.85414200	-3.66541600	-1.84019000	C	-1.15752700	1.99381300	4.23919800
C	-5.56325900	-2.72162100	-1.23749700	H	-2.01996000	1.45189300	6.15938200
C	-5.86470100	0.79827400	1.30792900	H	-0.36379800	2.31820900	2.27889300
C	-0.26526600	5.16105000	0.33565700	H	-0.85083900	2.98684600	4.57891000
C	1.67133700	-4.73827000	-0.96483600	H	2.98557400	-1.32272100	3.32829700
C	-5.62866600	-3.69748500	-2.23541500				
C	-6.77174600	1.05622000	0.27576600	5's			
C	-1.05616900	5.76422500	1.31841000	N	-3.26511500	1.79676800	-1.37123800
H	-3.30943200	0.25242100	-2.96440200	S	-4.88567800	1.96886300	-1.77783700
H	-2.18536600	0.92682400	-4.13792800	C	-2.87024800	2.18716600	0.00204600
H	-1.35349000	-1.28157300	-3.73948900	C	-2.62034600	0.51769800	-1.71924200
H	-0.26823000	-0.20517100	-2.83708300	O	-4.98190300	1.69638000	-3.21498200
H	-2.56829900	2.67454100	-2.51409600	O	-5.30172900	3.25903300	-1.21831800
H	-0.91183300	2.08156900	-2.33579200	C	-5.73622300	0.65948200	-0.90809200
H	-1.46475900	-3.99313300	0.15199300	H	-3.75369900	2.32850700	0.64437900
H	-2.37508100	-3.65948600	-3.26439900	H	-2.32279400	3.13819500	-0.00675700
H	-4.59672800	2.07678600	-2.13635300	C	-2.01402000	1.04414200	0.48699600
H	-3.49000200	3.39625400	1.58897700	H	-1.66612900	0.71072700	-2.23639200
H	1.03535600	-1.86116300	-2.66749300	C	-2.37629000	-0.15602700	-0.36190900
H	-4.30166900	-1.31985400	-0.18586300	H	-3.24823400	-0.07705600	-2.39371500
H	-3.79869900	0.77179800	1.91031600	C	-5.89777200	-0.57964000	-1.53422200
H	0.00848800	3.46780800	-0.96100500	C	-6.10445200	0.84088300	0.43121900
H	0.31979000	-5.69346600	0.43153700	C	-1.03670800	1.11441900	1.40725400
H	-4.52953100	-4.79776400	-3.74245800	C	-1.42963600	-1.36246200	-0.41919500

H	-3.36508400	-0.50134100	-0.01114300	C	6.31994500	-2.86582200	-1.21807000
C	-6.39200400	-1.65611500	-0.79597600	C	1.53373600	-5.43445200	0.73314800
H	-5.64064700	-0.69575700	-2.58772300	C	-0.63503900	4.33960800	-1.44395300
C	-6.59307500	-0.24620600	1.15287500	C	5.47567900	2.15125200	1.51788300
H	-6.01413900	1.82233500	0.89829600	C	6.12583400	-1.57416700	0.82092800
C	-0.57694900	2.27422000	2.18129200	C	-0.00724100	-5.09035300	-1.09717100
H	-0.37949100	-1.04011000	-0.31998100	C	-0.18039500	5.40921600	-0.66692700
H	-1.50585600	-1.79033100	-1.43016500	C	6.48625200	2.46414400	0.60281200
C	-6.72716700	-1.51503400	0.56004800	C	6.90968500	-2.29394000	-0.08409100
H	-6.51798700	-2.62633900	-1.28260300	C	0.45981800	-5.88103900	-0.04449800
H	-6.87522700	-0.10993400	2.20014600	H	4.01336900	-0.18278400	-2.76799700
C	-1.38724000	3.37568900	2.51871500	H	2.99254800	-0.16138700	-4.20363300
C	0.76371600	2.28653700	2.61172300	H	2.76729500	2.01345400	-3.10849800
C	-7.21019200	-2.68672900	1.37016300	H	1.24149600	1.13759700	-3.00224700
C	-0.86178700	4.45151100	3.23817100	H	2.62571300	-2.31343000	-3.16652200
H	-2.44276100	3.38453600	2.24825800	H	1.16513300	-1.35125800	-2.87984200
C	1.28958100	3.35651800	3.33105100	H	2.66892000	4.01205400	0.57362500
H	1.40473500	1.44187700	2.34838500	H	4.71906900	2.18845700	-2.29545800
H	-6.49021300	-2.92762700	2.17034600	H	4.50371700	-3.16989200	-2.33542200
H	-8.17070600	-2.46172300	1.86152100	H	2.96585500	-3.85990000	1.07918800
H	-7.34134500	-3.58327200	0.74753000	H	-0.29045700	2.32040600	-2.08554100
C	0.47596500	4.45011700	3.64499200	H	3.41819900	1.56356800	1.77611900
H	-1.50798000	5.29601600	3.49006000	H	4.14142300	-0.84554200	1.28127100
H	2.33785300	3.34298200	3.63894700	H	0.19955300	-3.24825400	-2.18663000
H	0.88043400	5.29414700	4.20873600	H	1.36907700	6.11009000	0.67007100
P	2.19263300	1.40590600	-0.82529200	H	6.99029600	2.70956400	-1.48608200
P	2.36334500	-1.71624400	-0.82263500	H	6.93011400	-3.43328900	-1.92518400
C	2.96405500	-0.16048900	-3.10197800	H	1.90795200	-6.04884000	1.55570700
C	2.28596300	1.13460900	-2.65418300	H	-1.56755900	4.42031100	-2.00749100
C	2.23797000	-1.42738100	-2.64239600	H	5.68725600	2.14255800	2.58982400
C	1.28966500	3.01237600	-0.76611300	H	6.57986300	-1.12453700	1.70699600
C	3.90051500	1.84420000	-0.31309700	H	-0.84526700	-5.43141000	-1.70963500
C	4.16106100	-1.97822500	-0.55086900	H	-0.75326500	6.33858800	-0.62323900
C	1.66108800	-3.39669200	-0.58862600	H	7.49281400	2.70089100	0.95601100
C	1.74219600	4.09315200	0.00517500	H	7.98181900	-2.41164700	0.09194200
C	4.91722200	2.16949700	-1.22306300	H	-0.01160700	-6.84288500	0.17038100
C	4.95191500	-2.71296600	-1.45046000	Co	1.40508300	-0.22853600	0.38810400
C	2.13035900	-4.20117000	0.46411900	C	0.20974400	-2.37358200	2.18817000
C	0.09173700	3.14787600	-1.48670200	H	0.52706800	-2.84481600	3.13816300
C	4.19685200	1.83137100	1.06041700	O	0.95546700	-1.49117000	1.74876300
C	4.75709800	-1.41601400	0.58556100	C	-1.05360600	-2.89805800	1.67819900
C	0.58818100	-3.85489200	-1.36792200	C	-1.55145400	-3.96327100	2.47085600
C	1.00803800	5.28105600	0.05710800	C	-1.79722200	-2.47068200	0.54212000
C	6.20450600	2.46892400	-0.76593300	C	-2.74416200	-4.60663100	2.17502600

H	-0.96683800	-4.28078400	3.33735000	H	-8.93624700	0.86175900	0.69749400
C	-3.00266200	-3.13646700	0.27210100	H	-9.29171500	1.16173000	-1.01163100
C	-3.47739300	-4.18288200	1.06235400	H	-9.41477900	-0.49327400	-0.36397500
H	-3.10064300	-5.42723700	2.80058200	C	0.55301400	3.19843100	4.01032600
H	-3.58698500	-2.82318700	-0.59619500	H	-1.22639900	3.97185300	3.05677200
H	-4.42050800	-4.67050100	0.80449900	H	2.19795100	2.12435800	4.92076200
H	-0.48166900	0.19498800	1.61318500	H	0.96078800	4.18619900	4.23754000
5'T				P	0.74671400	2.30000200	-0.68491600
N	-2.27299800	-1.04641800	-0.31150000	P	1.54684200	-0.79539700	-1.77935400
S	-2.98244100	-0.46451200	-1.70568500	C	1.22253900	1.47439900	-3.42381400
C	-2.17901700	-0.16049500	0.85722700	C	0.46697200	2.44805300	-2.51071000
C	-2.63600300	-2.38479700	0.17829500	C	0.83566700	-0.00658700	-3.29191800
O	-2.89455900	-1.53943300	-2.70111400	C	-0.31183400	3.67655400	-0.06879600
O	-2.34991000	0.83741900	-1.96839900	C	2.45474900	2.89661300	-0.37069500
C	-4.69962100	-0.18344000	-1.33663300	C	3.35985900	-0.67134600	-2.04938700
H	-3.17552300	0.21270700	1.16866500	C	1.22357800	-2.58752500	-1.98433700
H	-1.54781700	0.71142100	0.63818900	C	0.21800900	4.85205500	0.48340500
C	-1.59984600	-1.07746000	1.90866100	C	3.23888300	3.57262200	-1.31621100
H	-2.42603500	-3.14164400	-0.58550500	C	3.95501200	-1.04412900	-3.26661000
C	-1.75386700	-2.51746300	1.43111400	C	2.12518400	-3.51890700	-1.43918800
H	-3.70668200	-2.42979500	0.45165000	C	-1.70801500	3.52530800	-0.14320000
C	-5.61389900	-1.22461500	-1.52216800	C	3.00470000	2.60788700	0.89214300
C	-5.10580700	1.05488100	-0.82421000	C	4.16619500	-0.16972800	-1.01802900
C	-0.91630100	-0.70764700	3.00651600	C	0.01714600	-3.04678900	-2.53689200
C	-0.38334100	-3.15136400	1.07071000	C	-0.63237800	5.85690000	0.95566800
H	-2.25733500	-3.14575400	2.18039800	C	4.55184900	3.94345000	-1.00709100
C	-6.95132000	-1.01832400	-1.18213800	C	5.33221000	-0.90538100	-3.44743900
H	-5.28449000	-2.17638400	-1.94105700	C	1.82977000	-4.88334100	-1.45637800
C	-6.44564300	1.24042000	-0.49148100	C	-2.55440400	4.53048600	0.32889800
H	-4.38540300	1.86430100	-0.70106400	C	4.30805900	2.99440500	1.20582800
C	-0.48808200	0.64548700	3.38290000	C	5.54633800	-0.03308100	-1.19859600
H	0.18311300	-2.44414000	0.46189800	C	-0.27210200	-4.41483000	-2.55569100
H	-0.58475100	-4.02806000	0.43753900	C	-2.01916900	5.69915300	0.88271500
C	-7.38897600	0.21079600	-0.66290500	C	5.08820700	3.65738100	0.25153500
H	-7.67150800	-1.82678800	-1.32930000	C	6.12994800	-0.39744100	-2.41433700
H	-6.77024800	2.20655300	-0.09663800	C	0.63049400	-5.33686100	-2.01733400
C	-1.18625300	1.81945800	3.03513900	H	2.31042800	1.59217100	-3.29490600
C	0.72624100	0.78401900	4.09009400	H	1.00881500	1.78134100	-4.46071000
C	-8.83416300	0.43889400	-0.31481100	H	0.68563900	3.48804000	-2.79895100
C	-0.67022300	3.07876500	3.34591700	H	-0.61676400	2.30170200	-2.63084600
H	-2.15292900	1.75684400	2.53720000	H	1.16837500	-0.56898000	-4.17758400
C	1.24646700	2.04276700	4.38916700	H	-0.25783400	-0.10696800	-3.22657700
H	1.27326100	-0.11423100	4.38669600	H	1.29862500	4.98633900	0.55178200
				H	2.83521100	3.81208800	-2.30136200

H	3.34141300	-1.44547200	-4.07690200	C	1.14499800	-1.94568200	-0.15718100
H	3.06156700	-3.17472100	-0.99412000	H	1.56434000	-2.75116800	-2.88075000
H	-2.13251300	2.61956800	-0.58135000	C	1.57679500	-1.15601400	-1.37311400
H	2.40471700	2.07100400	1.63278300	H	3.07505200	-1.81821400	-2.89076000
H	3.71113000	0.12105100	-0.07093600	C	5.20177800	-0.52722100	-0.66394600
H	-0.72246100	-2.34680800	-2.92591400	C	4.88166600	-1.82553900	1.36814800
H	-0.20608200	6.76711000	1.38495100	C	0.11585800	-1.47755300	0.56228400
H	5.15802000	4.45942500	-1.75573600	C	0.38236700	-0.39275900	-1.91641100
H	5.78737400	-1.19417200	-4.39818100	H	2.34248600	-0.43335800	-1.04138000
H	2.53996300	-5.59642400	-1.03009700	C	5.46028600	0.60280900	0.11155600
H	-3.63796700	4.40147100	0.26374700	H	5.24621400	-0.47850800	-1.75291000
H	4.71903400	2.76861400	2.19293500	C	5.13402100	-0.68333600	2.12697500
H	6.16213700	0.36526800	-0.38884900	H	4.68778500	-2.78364000	1.85163800
H	-1.21439600	-4.75778400	-2.99083500	C	-0.38904700	-2.04424300	1.81983800
H	-2.68182000	6.48430900	1.25501900	H	-0.21199500	-0.99660600	-2.61536800
H	6.11430700	3.94894600	0.48864300	H	0.66851700	0.54138200	-2.41993800
H	7.20741800	-0.28714200	-2.56038200	C	5.42250100	0.54804400	1.51591100
H	0.40086600	-6.40515100	-2.03183000	H	5.70431100	1.54592000	-0.38181000
Co	0.86253800	0.19544400	0.16396600	H	5.11944400	-0.75202400	3.21775200
C	2.26716800	-1.84891900	2.19136200	C	-0.54619300	-1.20827500	2.94692000
H	3.29040100	-1.66986300	2.58353600	C	-0.77610400	-3.39415000	1.94251000
O	1.80199800	-1.02548600	1.40545100	C	5.66747300	1.77583000	2.34911900
C	1.62880300	-3.05425300	2.71874100	C	-1.07298500	-1.69724100	4.14384200
C	2.32069600	-3.64294900	3.80248300	H	-0.24824900	-0.15915800	2.87607000
C	0.41827500	-3.63691200	2.25381800	C	-1.31497200	-3.88002600	3.13553700
C	1.82786300	-4.76643100	4.45401700	H	-0.67268300	-4.05930700	1.08551200
H	3.25671400	-3.18622500	4.13369700	H	6.17543300	1.52352600	3.29237400
C	-0.04537700	-4.78149500	2.91827300	H	6.27403200	2.51700400	1.80996100
C	0.63236700	-5.33731700	4.00475000	H	4.71247800	2.26211200	2.60969000
H	2.36959600	-5.20004600	5.29705800	C	-1.46956000	-3.03574700	4.24070200
H	-0.96396300	-5.25611600	2.56351700	H	-1.18044500	-1.03019000	5.00323100
H	0.23149000	-6.22818100	4.49437600	H	-1.62236400	-4.92710400	3.20027600
H	-0.51847800	-1.50710600	3.63709700	H	-1.89279900	-3.41937700	5.17225600
6's				P	-2.46685600	-1.11152100	-0.94000200
N	2.84701400	-3.16101800	-1.26119600	P	-1.58051400	1.96493600	-1.34128200
S	4.49858800	-3.17765200	-1.00690500	C	-3.42776400	0.68204000	-3.03746100
C	1.97956300	-3.20621700	-0.06051500	C	-3.05923600	-0.75789300	-2.65979000
C	2.28231200	-2.20954200	-2.24258400	C	-2.28493100	1.69880300	-3.01901300
O	5.12349900	-3.02349800	-2.32654000	C	-2.33995000	-2.94689300	-0.98098100
O	4.76938000	-4.35866500	-0.17943100	C	-3.89917200	-0.81750600	0.16686900
C	4.90589200	-1.73666900	-0.02732900	C	-2.92853000	2.60636000	-0.29618200
H	2.57687600	-3.27815600	0.85957100	C	-0.44949500	3.39202700	-1.53330100
H	1.35041800	-4.10971800	-0.10303800	C	-3.25904000	-3.76438900	-0.30649900
				C	-3.70997600	-0.96755000	1.55099800

C	-3.91336200	3.49089100	-0.76131900	Co	-0.67062900	0.08825700	-0.32743300
C	-0.44149900	4.43238200	-0.58937800	C	1.00007000	1.99302400	1.18162700
C	-1.29778700	-3.55057300	-1.70410700	O	0.84158600	1.21730000	0.23679800
C	-5.17426400	-0.48152600	-0.31200400	C	2.08946800	2.95382700	1.23584200
C	-2.94838400	2.18772200	1.04289400	C	2.17277800	3.82939100	2.33430600
C	0.48472100	3.41560600	-2.58385600	C	3.00730400	3.06139300	0.17367900
C	-3.12664500	-5.15605700	-0.34056700	C	3.16045300	4.81194000	2.36548400
C	-4.76938900	-0.77934100	2.43769200	H	1.45263600	3.73941300	3.15125800
C	-4.90839600	3.94386800	0.10736400	C	3.98989200	4.04369900	0.21072100
C	0.47817800	5.47878700	-0.69882700	H	2.92212300	2.38104100	-0.67360600
C	-1.16421800	-4.93913700	-1.73344100	C	4.06440000	4.92009100	1.30208600
C	-6.23083400	-0.27599800	0.58043600	H	3.22667900	5.49686000	3.21341100
C	-3.93652100	2.65131000	1.91383000	H	4.69979300	4.13833700	-0.61350800
C	1.39923000	4.46529100	-2.69054300	H	4.83627900	5.69326400	1.32408000
C	-2.07580600	-5.74735000	-1.04520300	H	0.28121600	2.00276200	2.02546400
C	-6.03263300	-0.42333100	1.95553000				
C	-4.91899500	3.52742700	1.44397500	6'T			
C	1.40022000	5.49818700	-1.74733000	N	3.40130500	-2.60988500	-1.21329100
H	-4.24645100	1.04973700	-2.40207900	S	5.06156300	-2.55573600	-1.06743700
H	-3.83106300	0.65099000	-4.06250000	C	2.60323700	-2.77341400	0.02602000
H	-3.91966500	-1.42315400	-2.82967100	C	2.73180100	-1.66489900	-2.13234800
H	-2.25310300	-1.12509600	-3.31509400	O	5.59283900	-2.42151300	-2.42888400
H	-2.62580800	2.66667500	-3.41644200	O	5.43094600	-3.69428000	-0.21909100
H	-1.45075300	1.36229600	-3.65451900	C	5.46573900	-1.06092100	-0.17139100
H	-4.07773300	-3.32246100	0.26068300	H	3.23371600	-2.67415600	0.92313900
H	-2.73046300	-1.23814600	1.94033000	H	2.15741000	-3.77822300	0.05847900
H	-3.90449400	3.82806700	-1.80014700	C	1.56454500	-1.67613500	-0.06974700
H	-1.15524700	4.43066400	0.23613200	H	2.05322200	-2.23000000	-2.79396800
H	-0.57524700	-2.94171800	-2.24169500	C	1.93801700	-0.74600600	-1.18903200
H	-5.36544900	-0.38357300	-1.37969100	H	3.46765500	-1.15371000	-2.76424800
H	-2.19270100	1.47989300	1.39638400	C	5.67186100	0.12935300	-0.87418400
H	0.50334700	2.61390200	-3.32521100	C	5.52631700	-1.08975800	1.22702300
H	-3.84772800	-5.77786700	0.19539400	C	0.40933500	-1.47245700	0.59162600
H	-4.60244200	-0.90655000	3.50990800	C	0.68550500	-0.05019200	-1.69979800
H	-5.67904100	4.62669300	-0.25832300	H	2.64918500	0.00262100	-0.79199400
H	0.47700500	6.27818500	0.04581500	C	5.93075900	1.30205300	-0.16266800
H	-0.34083200	-5.38936900	-2.29307600	H	5.64888900	0.13243800	-1.96483000
H	-7.21612800	-0.00558400	0.19349300	C	5.77957700	0.09209400	1.92012000
H	-3.94905600	2.31549700	2.95262100	H	5.39660000	-2.03206900	1.76077800
H	2.11789100	4.47354900	-3.51362500	C	-0.11663200	-2.29929100	1.69469100
H	-1.96727000	-6.83444800	-1.06224000	H	0.11258300	-0.70663700	-2.37454100
H	-6.86168400	-0.26454100	2.64928200	H	0.88994500	0.89509200	-2.21821900
H	-5.69998000	3.88403600	2.11985800	C	5.98732500	1.30521800	1.24058500
H	2.12260400	6.31360900	-1.82760200	H	6.10525100	2.23279700	-0.70815000

H	5.83060000	0.07214300	3.01193700	H	-4.19811400	0.90928900	-2.42799300
C	-0.49135800	-1.71104800	2.92122800	H	-3.71832500	0.49066000	-4.06671500
C	-0.29940300	-3.69080800	1.55575000	H	-3.91180700	-1.58565700	-2.84943100
C	6.28274400	2.56355700	2.00968700	H	-2.21436900	-1.31094900	-3.22741400
C	-1.02522800	-2.47616700	3.95981700	H	-2.42668300	2.42455900	-3.45329900
H	-0.36430400	-0.63849500	3.05598700	H	-1.30615200	1.05360200	-3.49796500
C	-0.83733200	-4.45542700	2.59205300	H	-3.86750500	-3.77018700	0.17056500
H	-0.03347400	-4.17418100	0.61698700	H	-2.87446900	-1.50019700	1.95666100
H	7.21144900	2.45350000	2.59421400	H	-3.51244700	3.96415900	-2.06198200
H	6.40072400	3.42787100	1.34153500	H	-1.27394300	4.23567500	0.43422700
H	5.47604900	2.78695300	2.72592500	H	-0.43537000	-2.72387300	-2.23827800
C	-1.20769300	-3.85341300	3.79877100	H	-5.49373900	-0.85651700	-1.42600600
H	-1.30433900	-1.99212200	4.89941500	H	-3.07657000	1.24438000	1.26507200
H	-0.97678700	-5.52997200	2.44931300	H	0.32067900	2.75916000	-3.30624700
H	-1.63416400	-4.45272100	4.60696600	H	-3.32148600	-6.16794200	-0.10478200
P	-2.55308400	-1.28447700	-0.87615900	H	-4.81766200	-1.34492500	3.48653800
P	-1.62803600	1.86147900	-1.24202300	H	-5.61023100	4.83038500	-1.07427200
C	-3.36230900	0.51222600	-3.02398800	H	0.22063700	6.20175000	0.29049000
C	-3.05525100	-0.93125900	-2.62575900	H	0.09722900	-5.12087400	-2.52552600
C	-2.17183300	1.47315000	-2.96304400	H	-7.42069300	-0.66791600	0.10747300
C	-2.19619300	-3.07939600	-1.02340300	H	-5.17062600	2.11328100	2.25329600
C	-4.04855100	-1.18995800	0.16111400	H	1.82118200	4.71648300	-3.43274900
C	-3.15381400	2.53068900	-0.46978300	H	-1.33746500	-6.86040400	-1.44914400
C	-0.57760900	3.35115600	-1.41786200	H	-7.10077900	-0.90850000	2.56831400
C	-3.00093400	-4.05857500	-0.42580200	H	-6.45275200	3.91022900	1.08731000
C	-3.87226600	-1.32469700	1.54946200	H	1.78567000	6.44915700	-1.63773000
C	-3.87528400	3.54942200	-1.11892200	Co	-0.61179900	0.02977200	-0.15117600
C	-0.59718400	4.33613100	-0.41576100	C	-0.23986600	2.02370200	2.27411800
C	-1.08062600	-3.47494200	-1.78124400	O	-0.77599200	1.15780700	1.57724800
C	-5.33231800	-0.96027000	-0.35237100	C	0.98798400	2.73618000	1.96740700
C	-3.62834900	2.02466100	0.74752000	C	1.38143400	3.78017500	2.82631100
C	0.29865200	3.50052700	-2.50598300	C	1.74976000	2.44433100	0.81949600
C	-2.69046100	-5.41330500	-0.58046600	C	2.51504300	4.53432200	2.52905300
C	-4.96611900	-1.23324000	2.40975900	H	0.78293600	4.00045800	3.71404200
C	-5.05580900	4.04069300	-0.56140000	C	2.88297800	3.19271000	0.53127000
C	0.24488000	5.44551500	-0.49741200	H	1.43016900	1.64752500	0.15278700
C	-0.77625900	-4.82735200	-1.93831400	C	3.26139700	4.24153300	1.38197500
C	-6.42440500	-0.85553200	0.51488900	H	2.81823700	5.35197600	3.18615900
C	-4.81049800	2.52097500	1.30633200	H	3.47061500	2.97158400	-0.36047700
C	1.14484900	4.61068300	-2.58108000	H	4.14571100	4.83692200	1.14537500
C	-1.57950500	-5.80118900	-1.33345600	H	-0.73654800	2.29973300	3.22538600
C	-6.24489800	-0.99120000	1.89407200				
C	-5.52710900	3.52501200	0.65259200	TS4's			
C	1.12191000	5.58341800	-1.57753600	N	3.03338300	-1.42063500	-0.96893800

S	4.60119300	-1.83777700	-1.29407100	C	-2.23904700	-1.14354400	-2.86061900
C	2.50348400	-1.57443100	0.38886200	C	-3.06868600	1.28256100	-2.75351500
C	2.36868900	-0.35962000	-1.73547100	C	-0.46494100	-2.77648400	-1.25566200
O	4.73258300	-1.86338800	-2.75517700	C	-3.20888900	-2.34102100	-0.45569900
O	4.89036600	-3.02560200	-0.48195900	C	-4.33009300	1.74758700	-0.13186700
C	5.57473800	-0.47807300	-0.66841900	C	-2.14427800	3.44133000	-1.03999100
H	3.24117800	-1.26529000	1.15672400	C	-0.26351100	-3.66971100	-0.18906100
H	2.21990500	-2.61394000	0.59835700	C	-4.09252000	-1.66271500	0.39490800
C	1.34583400	-0.62307600	0.42292400	C	-5.55245600	1.75898900	-0.82087500
H	1.74427900	-0.79748000	-2.52736300	C	-2.41384400	4.30181400	0.03684400
C	1.51427900	0.37956600	-0.68927000	C	0.35164100	-2.87740500	-2.39297400
H	3.09601000	0.31122300	-2.21274500	C	-3.50225700	-3.66043400	-0.83889200
C	5.81546800	0.62853600	-1.49033200	C	-4.33284200	1.73114700	1.27607200
C	5.97770300	-0.47982300	0.67179400	C	-1.33829400	3.90256200	-2.09500000
C	0.25855000	-0.58567100	1.22961000	C	0.75669800	-4.61967300	-0.24957800
C	0.17051400	0.91980400	-1.16875900	C	-5.24868700	-2.28896900	0.86683800
H	2.13447800	1.19928900	-0.28523000	C	-6.75752600	1.75121800	-0.11282700
C	6.43870500	1.75252600	-0.94941700	C	-1.88520300	5.59398200	0.05778500
H	5.52405200	0.60337800	-2.54109500	C	1.38277000	-3.81894800	-2.44214800
C	6.60429300	0.65204200	1.19260000	C	-4.65540200	-4.28776200	-0.36282600
H	5.80731600	-1.36061400	1.29222900	C	-5.53989400	1.73389600	1.97774300
C	-0.08070500	-1.54842500	2.28851700	C	-0.81278000	5.19710600	-2.07086400
H	-0.06527400	0.57384400	-2.18432300	C	1.59284700	-4.68703200	-1.36928900
H	0.15278400	2.01496800	-1.15812800	C	-5.52895900	-3.60554300	0.49206500
C	6.83520800	1.78778000	0.39785700	C	-6.75484000	1.73924700	1.28483300
H	6.62313600	2.62132800	-1.58646700	C	-1.08087200	6.04531400	-0.99303700
H	6.92028800	0.65564400	2.23884000	H	-4.25786200	-0.50317000	-2.35839300
C	-1.44100000	-1.75334300	2.59024100	H	-3.79498300	-0.26518100	-4.03971800
C	0.87512500	-2.27919700	3.02188200	H	-2.48177400	-2.12562600	-3.29354000
C	7.51458100	3.00259000	0.96879900	H	-1.36944300	-0.74907200	-3.40797400
C	-1.84197900	-2.68802700	3.54367800	H	-3.85969200	1.95593500	-3.11520600
H	-2.19197000	-1.18561500	2.03998200	H	-2.15957000	1.53749000	-3.31756500
C	0.47604100	-3.21424700	3.98018000	H	-0.90255600	-3.62460500	0.69217300
H	1.93936200	-2.11476600	2.85353200	H	-3.88478300	-0.63616100	0.68611100
H	7.28129000	3.13098700	2.03638900	H	-5.57860100	1.76948200	-1.91110800
H	8.61162200	2.90871100	0.88468200	H	-3.03775300	3.96938300	0.86592300
H	7.22339400	3.91679000	0.43062400	H	0.20327300	-2.21184100	-3.24311100
C	-0.88148800	-3.43115500	4.23882500	H	-2.82775800	-4.20419700	-1.50327200
H	-2.90629700	-2.84067900	3.73916800	H	-3.38580600	1.70922200	1.81856000
H	1.23393200	-3.77661800	4.53153400	H	-1.10764700	3.25832500	-2.94389500
H	-1.18841000	-4.16757700	4.98533200	H	0.90668400	-5.30075300	0.59130000
P	-1.73437600	-1.46784600	-1.11173600	H	-5.92616500	-1.74440700	1.52843100
P	-2.71850300	1.70157600	-1.00059600	H	-7.70344400	1.75480800	-0.65951100
C	-3.42463500	-0.18569000	-3.00581300	H	-2.10427600	6.25105900	0.90276100

H	2.03596100	-3.85803500	-3.31633100	H	5.73396800	0.71755800	-2.36881200
H	-4.87271500	-5.31649700	-0.66010800	C	6.52582600	0.29716900	1.41359000
H	-5.53009000	1.72455600	3.07027400	H	5.70895700	-1.69840000	1.20752400
H	-0.19100700	5.54136200	-2.90077800	C	0.04207900	-1.69566700	2.04239600
H	2.41160300	-5.40922800	-1.40148000	H	-0.01548000	0.44460000	-2.18423700
H	-6.42849300	-4.10211000	0.86390700	H	0.39448100	2.03879700	-1.48114000
H	-7.69917400	1.73264100	1.83433900	C	6.82569900	1.51753100	0.78188800
H	-0.66787100	7.05666400	-0.97379500	H	6.77820800	2.58550400	-1.09678900
Co	-1.23732200	0.38416900	0.08283300	H	6.76335600	0.16820000	2.47281200
C	-0.07041900	1.31125700	2.00460900	C	-1.30910000	-1.82091500	2.42508100
O	-1.10587700	1.77855600	1.37362900	C	0.97140200	-2.57620000	2.63096100
H	-0.24404900	0.82727500	2.97898500	C	7.43918700	2.64654700	1.56315200
C	1.21427000	2.04952300	1.90948000	C	-1.72805700	-2.81613600	3.30674900
C	2.34202400	1.60458400	2.61933000	H	-2.04721100	-1.13940300	2.00367400
C	1.30647000	3.19653200	1.10700400	C	0.55444200	-3.57215000	3.51704700
C	3.55566300	2.27718400	2.49726700	H	2.03374300	-2.48272800	2.41137600
H	2.26548500	0.71263200	3.24628800	H	6.80370900	2.91945200	2.42186400
C	2.52275700	3.87646600	0.99549400	H	8.42082500	2.35610100	1.97292400
H	0.41878600	3.54546000	0.57820600	H	7.57944100	3.54142200	0.94018500
C	3.65012300	3.41212500	1.67875500	C	-0.79687000	-3.70639700	3.85083200
H	4.43514000	1.91962400	3.03668700	H	-2.78704900	-2.89870500	3.56332100
H	2.58936600	4.76820300	0.36762400	H	1.29502200	-4.24834300	3.95152000
H	4.60507900	3.93354100	1.58088500	H	-1.11950200	-4.49145500	4.53884300
TS4'_T				P	-2.07197900	-1.50840800	-0.95103800
N	3.11402200	-1.47976200	-1.26075400	P	-2.51810700	1.85870900	-0.95230500
S	4.71524200	-1.84832000	-1.50364100	C	-3.50180000	0.01876800	-2.89777800
C	2.50491200	-1.76546300	0.04214100	C	-2.51310200	-1.13335600	-2.71227000
C	2.52451900	-0.30697900	-1.92118300	C	-2.89960000	1.41465800	-2.69333900
O	4.95991600	-1.69418100	-2.94158000	C	-0.87569800	-2.88512300	-1.11620600
O	4.94707300	-3.12678500	-0.82220300	C	-3.61180300	-2.25930000	-0.30575700
C	5.62842900	-0.57906500	-0.64192000	C	-4.12057800	1.95942600	-0.07324100
H	3.24269000	-1.67577400	0.86110700	C	-1.90209000	3.57928000	-1.00723000
H	2.08939400	-2.78213700	0.08625900	C	-0.83812900	-3.92732400	-0.17440100
C	1.46312700	-0.69683300	0.20463600	C	-4.39300700	-1.53716600	0.60673900
H	1.89353700	-0.62701500	-2.76470600	C	-5.32876500	2.11831200	-0.77135200
C	1.68316300	0.38032600	-0.82349000	C	-2.08410600	4.42115300	0.10282400
H	3.30008600	0.35981400	-2.31989800	C	0.08226200	-2.86164300	-2.14398200
C	5.94142900	0.61225400	-1.30315600	C	-4.05695400	-3.51577300	-0.75164600
C	5.92979300	-0.75044600	0.71518400	C	-4.14242500	1.87123500	1.33067000
C	0.41662100	-0.64494800	1.07301600	C	-1.16455700	4.04622500	-2.10920500
C	0.35366800	0.96133400	-1.28447000	C	0.13386200	-4.92548600	-0.26746000
H	2.30630300	1.16205900	-0.35428100	C	-5.60102900	-2.06026600	1.07568900
C	6.53423200	1.65163600	-0.58447400	C	-6.53920700	2.17420100	-0.07592100
				C	-1.53555200	5.70508300	0.10987100

C	1.05527400	-3.85967700	-2.23176900	H	0.32293200	3.39613500	0.62970200
C	-5.26077000	-4.03955500	-0.27703000	C	3.61258000	3.48703400	1.53508000
C	-5.35518500	1.94034800	2.02020500	H	4.58628700	2.03886500	2.81482200
C	-0.61835600	5.33223300	-2.09607600	H	2.37733900	4.77471100	0.30998000
C	1.08438800	-4.89427500	-1.29328800	H	4.51900300	4.07943100	1.38878900
C	-6.03403400	-3.31423900	0.63735800				
C	-6.55592300	2.08488000	1.31913700	7's			
C	-0.79949500	6.16354600	-0.98688000	N	3.22295500	-0.41288300	0.30397200
H	-4.38606400	-0.12553100	-2.25706200	S	3.94955200	-1.27573100	-0.92720600
H	-3.87073200	-0.02588100	-3.93453600	C	2.15477900	-1.08030900	1.07822700
H	-2.92389000	-2.06410000	-3.13216900	C	2.91626400	1.00880400	0.07866400
H	-1.58212400	-0.91675400	-3.25564400	O	3.22090600	-1.15423000	-2.20682800
H	-3.56303700	2.19257900	-3.09970200	O	4.19404800	-2.61857200	-0.38367500
H	-1.94961500	1.49081100	-3.24390300	C	5.49224400	-0.40370100	-1.10308200
H	-1.56449400	-3.96007700	0.63716200	H	2.55179500	-1.45616300	2.02796800
H	-4.06304200	-0.55654900	0.94527800	H	1.73851800	-1.94243600	0.53850100
H	-5.34052200	2.19763300	-1.85898300	C	1.10596200	-0.00248000	1.28019100
H	-2.65127300	4.07849700	0.96836900	H	3.23309000	1.33357000	-0.92134700
H	0.08879700	-2.05836100	-2.88038500	C	1.39866400	1.10646300	0.27080000
H	-3.46231800	-4.08989300	-1.46519900	H	3.44526500	1.62451200	0.82447500
H	-3.20972900	1.73831900	1.87961300	C	5.78499300	0.24706400	-2.30060500
H	-1.00767900	3.41489900	-2.98437700	C	6.40064600	-0.41563600	-0.03795300
H	0.15252700	-5.72658000	0.47509900	C	0.07481900	-0.00636300	2.16543600
H	-6.20010900	-1.48438300	1.78469700	C	0.60480700	0.75067700	-0.97753500
H	-7.47393500	2.29004000	-0.62952300	H	1.10698600	2.09426600	0.63950500
H	-1.68413800	6.34911200	0.97968600	C	7.00911500	0.90820300	-2.42796500
H	1.80630400	-3.81215100	-3.02291800	H	5.06199800	0.23482100	-3.11717200
H	-5.59807000	-5.01956000	-0.62318300	C	7.61379700	0.24966500	-0.18292100
H	-5.36018100	1.87191200	3.11060400	H	6.15671800	-0.93762400	0.88911200
H	-0.05010100	5.68466000	-2.96015500	C	-0.22694800	-1.15227900	3.06645000
H	1.85322000	-5.66799200	-1.35471900	H	1.06546800	-0.08806900	-1.51842400
H	-6.97522000	-3.72909300	1.00633000	H	0.49991100	1.60258000	-1.65961500
H	-7.50477400	2.12848000	1.85913500	C	7.93801900	0.92331800	-1.37697100
H	-0.37083800	7.16845600	-0.97886500	H	7.24631100	1.42249000	-3.36251900
Co	-1.06269700	0.46345600	0.05729400	H	8.32917100	0.24810700	0.64363700
C	0.08473400	1.10938000	2.06997900	C	-1.53013300	-1.68058400	3.08146200
O	-1.06987100	1.56031700	1.65480500	C	0.73299600	-1.71392700	3.92431100
H	0.08284900	0.52829800	3.00484300	C	9.25245100	1.64284900	-1.50685700
C	1.29909500	1.94848400	1.89255100	C	-1.85450300	-2.77021300	3.88980400
C	2.50022600	1.57463100	2.51763000	H	-2.29236800	-1.24484300	2.43306500
C	1.25980100	3.10735300	1.10386400	C	0.40688200	-2.79962800	4.74201200
C	3.65199100	2.33712600	2.33579900	H	1.73833700	-1.29201600	3.96702900
H	2.52822300	0.67148700	3.13306600	H	10.09565200	0.96375800	-1.29961800
C	2.41429900	3.87453700	0.92798400	H	9.38627000	2.06370400	-2.51356300

H	9.32054000	2.46784000	-0.77777700	H	1.19200800	-2.84976000	-2.51675200
C	-0.88273500	-3.33907300	4.72006700	H	-2.69030400	-4.06253300	-2.25253600
H	-2.86825900	-3.17731200	3.86792100	H	-3.69818700	1.55128000	0.92488600
H	1.16662600	-3.22359800	5.40319500	H	-0.35438500	3.07339400	-3.14926900
H	-1.13264900	-4.19251300	5.35489700	H	0.36225400	-5.24860200	1.76915800
P	-1.24653500	-1.67491700	-1.22921600	H	-5.62334200	-1.79000500	1.08040600
P	-2.24407700	1.38553200	-1.57084300	H	-7.08612800	0.91964500	-2.66939000
C	-2.24288200	-0.60721600	-3.63211700	H	-2.51240400	5.99249800	0.25276000
C	-1.17458600	-1.54254700	-3.05960600	H	2.69616500	-4.66967000	-1.81652700
C	-2.01517100	0.87525100	-3.31993300	H	-4.93316900	-4.99007500	-1.73822600
C	-0.10923700	-3.03058500	-0.78535700	H	-6.12067100	1.46715700	1.50223700
C	-2.89265200	-2.39112200	-0.88064100	H	0.29635200	5.43489100	-2.97674200
C	-4.03171300	1.31362000	-1.19728200	H	2.29806400	-5.88555500	0.32188200
C	-1.81080300	3.16481600	-1.53089400	H	-6.40288400	-3.86623700	-0.06766800
C	-0.32730000	-3.71131400	0.42614300	H	-7.81927500	1.12863000	-0.29531100
C	-3.72237200	-1.76448300	0.05676000	H	-0.76510700	6.91903500	-1.27248600
C	-4.99047500	1.13454800	-2.20605700	Co	-1.06530100	0.25135900	-0.10938800
C	-2.41173400	4.00960100	-0.58261500	C	-0.82914200	1.25135700	2.31932100
C	0.98155300	-3.38544100	-1.59213700	O	-1.41774400	1.59044300	1.10339300
C	-3.33281100	-3.55898900	-1.52603800	C	-0.06346100	2.41414700	2.94634600
C	-4.44894800	1.43096900	0.14129600	C	0.62139300	2.24274100	4.15912600
C	-0.83455600	3.69456300	-2.39250900	C	-0.05537300	3.67091100	2.33122200
C	0.53635600	-4.73186000	0.82244500	C	1.30903800	3.31005000	4.74093600
C	-4.98249300	-2.29181300	0.35239600	H	0.61761500	1.26673200	4.65148000
C	-6.34742700	1.06527600	-1.87777300	C	0.63333700	4.74098100	2.91348400
C	-2.03751000	5.35109400	-0.49319600	H	-0.59396600	3.79636300	1.39232200
C	1.83818800	-4.41473600	-1.19273600	C	1.31872100	4.56458100	4.11848900
C	-4.59242500	-4.08297000	-1.23331800	H	1.83990600	3.16362800	5.68530000
C	-5.80591900	1.37356800	0.46016400	H	0.63257500	5.71657900	2.41988300
C	-0.46262600	5.03838300	-2.29826000	H	1.85736400	5.39926200	4.57427600
C	1.61903000	-5.08836800	0.01034900	H	-1.61780800	0.96913300	3.04197200
C	-5.41767100	-3.45121800	-0.29369900				
C	-6.75758100	1.18432500	-0.54735600	7'T			
C	-1.05867000	5.86920000	-1.34632600	N	3.28926300	-0.92681800	0.50487100
H	-3.24356400	-0.92821500	-3.30313600	S	3.50804200	-1.03581300	-1.15284500
H	-2.23143900	-0.71494500	-4.72786800	C	2.26467300	-1.79432000	1.11706100
H	-1.28531100	-2.55620800	-3.47213500	C	3.22390600	0.39159300	1.14200000
H	-0.16810700	-1.18523300	-3.32685500	O	2.43980400	-0.35140700	-1.92192700
H	-2.66698500	1.51526600	-3.93392800	O	3.73588100	-2.45813400	-1.43696300
H	-0.97904100	1.14277700	-3.57396000	C	5.01529600	-0.11862900	-1.36068700
H	-1.17054600	-3.44315200	1.06343200	H	2.75737100	-2.41815600	1.87649600
H	-3.38701200	-0.84815300	0.54495700	H	1.81355800	-2.47803400	0.38381400
H	-4.69409400	1.04960700	-3.25184800	C	1.25540200	-0.84633000	1.75036500
H	-3.17201600	3.62519100	0.09419200	H	3.61983700	1.17906200	0.48914500

C	1.74167400	0.59059600	1.52192700	C	0.76098000	-3.22044300	-2.02553400
H	3.84073700	0.36821300	2.05506500	C	-3.60336000	-2.16299500	-2.68572000
C	5.02013500	1.03807500	-2.13865500	C	-4.04973300	2.00434000	0.12694600
C	6.18111800	-0.59778100	-0.75095200	C	-0.13844900	4.57348400	-1.48408900
C	0.11419500	-1.17626300	2.39714400	C	-0.62082800	-5.25591600	-0.69711000
C	0.98229300	1.30413200	0.42591900	C	-5.17524000	-1.41814400	-0.49117100
H	1.66007000	1.16988800	2.44697100	C	-5.61684200	2.55047900	-2.12452100
C	6.21974900	1.73572400	-2.29819100	C	-0.97889800	5.56640800	0.99316800
H	4.09814900	1.38397100	-2.60765200	C	1.32099100	-4.49667500	-1.92173100
C	7.36433500	0.11336900	-0.91895800	C	-4.98045500	-2.38553700	-2.70426500
H	6.15633100	-1.50900000	-0.15078500	C	-5.43899400	2.07458800	0.24276000
C	-0.35923900	-2.57418600	2.57490600	C	0.33899800	5.80433700	-1.02060700
H	1.32398400	1.08186600	-0.59774300	C	0.63466500	-5.51587500	-1.25754100
H	0.82323600	2.37282500	0.60536700	C	-5.76748100	-2.01432600	-1.60649200
C	7.40410500	1.29069500	-1.69166500	C	-6.22457600	2.34110200	-0.88267100
H	6.23459000	2.64453800	-2.90441800	C	-0.07762500	6.30292800	0.21567300
H	8.27967900	-0.24809300	-0.44331100	H	-2.60544100	0.46502300	-3.52385200
C	-1.71861300	-2.87585800	2.35623400	H	-1.33116200	0.75391000	-4.69853100
C	0.49184600	-3.61641700	2.98345800	H	-0.90595200	-1.42808500	-3.88983400
C	8.69504600	2.04489100	-1.85344800	H	0.33411100	-0.40967400	-3.13788400
C	-2.20371300	-4.17281100	2.52050500	H	-1.53462900	2.80742800	-3.52626300
H	-2.39951300	-2.08713100	2.03330300	H	-0.02756000	2.06474100	-2.97370700
C	0.00559600	-4.91545700	3.15004300	H	-2.16289900	-3.79316200	-0.35791400
H	1.53860900	-3.40813700	3.20537800	H	-3.33341300	-0.70694600	0.39127400
H	9.46938000	1.40432000	-2.30702400	H	-3.76589700	2.68226100	-3.21719900
H	8.56807600	2.93402600	-2.48698700	H	-2.15342500	3.76969300	1.15615200
H	9.08383700	2.37041200	-0.87419900	H	1.32264200	-2.43458600	-2.52663300
C	-1.34255800	-5.20082400	2.91634600	H	-2.99370100	-2.46473100	-3.54076900
H	-3.25918500	-4.38225700	2.32978600	H	-3.44069600	1.75278200	0.99916100
H	0.68509700	-5.70737900	3.47454700	H	0.20383000	4.20463000	-2.45168500
H	-1.72098600	-6.21755200	3.04644100	H	-1.16429100	-6.04566700	-0.17389800
P	-1.20023800	-1.26586800	-1.49697200	H	-5.78560500	-1.12227800	0.36459200
P	-1.61361500	2.16245700	-1.19534800	H	-6.22750000	2.75670200	-3.00679200
C	-1.52182800	0.63340400	-3.62032500	H	-1.30981100	5.94836100	1.96192500
C	-0.74807800	-0.61174900	-3.16871900	H	2.30902600	-4.67913100	-2.34812200
C	-1.12399700	1.95918100	-2.95687300	H	-5.44347800	-2.85324000	-3.57655100
C	-0.49431900	-2.95335100	-1.45934700	H	-5.91058500	1.90181200	1.21301900
C	-3.00402800	-1.55715000	-1.56820700	H	1.04057300	6.37457800	-1.63433300
C	-3.43517600	2.22898000	-1.11693300	H	1.07693200	-6.51157700	-1.17291400
C	-1.04392300	3.83254200	-0.70912900	H	-6.84566400	-2.19121800	-1.62417300
C	-1.18410000	-3.98328600	-0.79711900	H	-7.31287400	2.38075600	-0.79392800
C	-3.79659800	-1.18629000	-0.47315400	H	0.29816000	7.26404800	0.57451500
C	-4.22556700	2.50285700	-2.24387700	Co	-0.78216400	0.43940300	0.16587600
C	-1.45662400	4.33776000	0.53698500	C	-0.85092200	-0.07851800	2.91496900

O	-1.45827300	0.59780600	1.85695500	C	-1.43519700	-2.05797400	-3.89111900
C	-0.21030600	0.88313800	3.91252600	C	-9.82256600	0.47175800	0.17354700
C	0.47975700	0.39305900	5.03077600	C	-3.37425200	-3.42021300	-2.41302500
C	-0.32812700	2.26728800	3.73874000	H	-2.87444600	-2.05704500	-0.80483000
C	1.05728800	1.27355700	5.94864200	C	-2.13244400	-3.12286500	-4.46741400
H	0.57202700	-0.68610400	5.18052600	H	-0.67073400	-1.53149900	-4.46747700
C	0.25066900	3.15044900	4.65604000	H	-10.34638200	0.96732600	1.00764600
H	-0.86180100	2.64067600	2.86488700	H	-10.14899900	0.97482100	-0.75198500
C	0.94751000	2.65717300	5.76273600	H	-10.15435000	-0.57535100	0.13130300
H	1.59602600	0.87943800	6.81432600	C	-3.10344900	-3.80746900	-3.73002400
H	0.15884300	4.22891200	4.50095900	H	-4.12827500	-3.95403500	-1.82878000
H	1.40144100	3.34554100	6.48007500	H	-1.91483700	-3.42003600	-5.49636000
H	-1.63684000	-0.60834600	3.48337100	H	-3.64644500	-4.64241300	-4.17988500
TS5's				P	1.54517000	-0.36752800	2.18074000
N	-3.33927800	1.77041600	-0.52968900	P	2.68891400	2.05997800	0.24625800
S	-3.80504000	0.94393300	0.88720000	C	3.23316700	1.77376000	3.00156800
C	-3.03521000	0.87383800	-1.65741400	C	2.02055500	0.92408100	3.39805800
C	-2.15150600	2.63241700	-0.41177100	C	2.92665700	2.80654500	1.91185600
O	-3.53936000	1.85810500	2.00757000	C	0.06538600	-1.16529300	2.90365600
O	-3.24329800	-0.42019800	0.92898400	C	2.87178200	-1.62287100	2.20932700
C	-5.56132500	0.79588100	0.64691500	C	4.37162500	1.63878200	-0.32338800
H	-3.22265900	1.43565900	-2.58950200	C	2.13661600	3.42381300	-0.83270600
H	-3.68437800	-0.00630600	-1.66867900	C	-0.16441400	-2.53139400	2.67148000
C	-1.55335500	0.58443500	-1.52381900	C	3.08491800	-2.37129500	1.03981300
H	-2.10442100	3.09507600	0.57990000	C	5.37587000	2.61109500	-0.46149100
C	-0.93116500	1.72698800	-0.74081900	C	2.39250800	3.34009000	-2.21259000
H	-2.25578400	3.42941400	-1.16371400	C	-0.90523100	-0.40918100	3.57863000
C	-6.33996800	1.95868000	0.60260700	C	3.68291600	-1.85008900	3.33258400
C	-6.13719200	-0.46946300	0.54770800	C	4.66072100	0.29874600	-0.61721400
C	-0.93840400	-0.54339500	-1.94170200	C	1.34504600	4.47552300	-0.34342000
C	-0.24348000	1.25439800	0.54134300	C	-1.34406000	-3.13022300	3.11666000
H	-0.21334300	2.27896800	-1.35997300	C	4.09214000	-3.33752300	0.99142500
C	-7.71659200	1.83838500	0.44807100	C	6.65287600	2.23831100	-0.88393800
H	-5.87122100	2.94086500	0.68456800	C	1.86536300	4.29369800	-3.08457500
C	-7.52252100	-0.56942800	0.39260000	C	-2.08855700	-1.01142700	4.01286800
H	-5.51014300	-1.36037900	0.59347500	C	4.69262100	-2.81383800	3.27896400
C	-1.70126500	-1.66093500	-2.57167100	C	5.94014300	-0.07376500	-1.03731400
H	-0.93000400	0.63716300	1.13383600	C	0.81864500	5.42753500	-1.22122300
H	0.04355500	2.13104700	1.14291900	C	-2.30926700	-2.37121800	3.78718300
C	-8.33131000	0.57484400	0.34066800	C	4.89956400	-3.55662700	2.11099300
H	-8.33347500	2.74008400	0.41139300	C	6.93651100	0.89670300	-1.17073100
H	-7.98190900	-1.55754300	0.31180600	C	1.07449100	5.33776400	-2.59231800
C	-2.67770600	-2.35578100	-1.83675300	H	4.07845100	1.13168200	2.70213500
				H	3.56738000	2.31846100	3.89818100

H	2.18566300	0.41917300	4.36177400	C	2.48730600	0.66064100	-1.71188800
H	1.14050900	1.57173500	3.52938000	O	3.54587500	-2.00043800	-1.25958900
H	3.73447400	3.55009800	1.83170600	O	4.02921600	-1.29604300	1.14391000
H	2.00713500	3.35159500	2.17178700	C	5.81643100	-0.78690900	-0.72480400
H	0.57781300	-3.13056900	2.14001100	H	3.49988700	2.22012200	0.59056200
H	2.44971600	-2.20031200	0.16937300	H	3.06964100	0.75747200	1.50052400
H	5.15644100	3.65974700	-0.24611400	C	1.46487400	1.52997300	0.24663100
H	2.99889500	2.52258300	-2.60577400	H	2.53804800	-0.18080500	-2.41064300
H	-0.76437700	0.65881100	3.74862700	C	1.10873600	0.80396700	-1.03030400
H	3.53220900	-1.28359500	4.25340300	H	2.76118800	1.58540100	-2.24672200
H	3.88144300	-0.45656500	-0.51426200	C	6.24580800	-1.05112100	-2.02619900
H	1.12422600	4.55772400	0.72155700	C	6.69841400	-0.30193600	0.24657200
H	-1.51102300	-4.19479600	2.93523800	C	0.63628700	2.28360400	1.00993300
H	4.24366900	-3.91369300	0.07634800	C	0.52653700	-0.58147000	-0.72937700
H	7.43197100	2.99680400	-0.99224800	H	0.41812400	1.38337200	-1.65560600
H	2.07122700	4.21950000	-4.15514200	C	7.58030600	-0.81110600	-2.35901500
H	-2.84640900	-0.40565900	4.51436500	H	5.54774600	-1.44554400	-2.76593500
H	5.32138400	-2.98664300	4.15559500	C	8.02599800	-0.06945500	-0.10492200
H	6.15373000	-1.12187500	-1.25994200	H	6.34840600	-0.11853800	1.26368200
H	0.20536000	6.24238600	-0.82905600	C	1.05492400	2.93119900	2.28708300
H	-3.23670500	-2.83986500	4.12502700	H	1.21869400	-1.13527300	-0.08555100
H	5.69204700	-4.30811500	2.07570000	H	0.43186200	-1.13653500	-1.67690900
H	7.93810800	0.61038200	-1.50092100	C	8.48897000	-0.31587000	-1.41066900
H	0.66053300	6.08164500	-3.27730400	H	7.92369500	-1.01713100	-3.37586500
Co	1.34095700	0.23666100	0.10884700	H	8.72199800	0.30745700	0.64921200
C	0.54469600	-0.69925100	-1.77026700	C	0.33095500	2.64205000	3.45696500
O	1.30111000	0.34041900	-1.83198500	C	2.13721700	3.82283200	2.36602800
C	1.20611300	-2.02602100	-2.02665600	C	9.92828400	-0.05973400	-1.76696100
C	0.68944600	-3.23860600	-1.54055900	C	0.68572200	3.22165500	4.67706100
C	2.42459500	-2.02847300	-2.72135300	H	-0.51298800	1.94891100	3.40770400
C	1.37580200	-4.43149500	-1.75688300	C	2.49142200	4.40318100	3.58579500
H	-0.23599400	-3.24311600	-0.96517900	H	2.69193000	4.08437900	1.46289600
C	3.10789500	-3.22681900	-2.94494800	H	10.60045500	-0.69244700	-1.16348300
H	2.83149600	-1.08291600	-3.08118800	H	10.12552900	-0.26614200	-2.82864300
C	2.58526600	-4.43012700	-2.46395300	H	10.20532400	0.98740500	-1.56107500
H	0.97131900	-5.36745500	-1.36492500	C	1.76807300	4.10385500	4.74503400
H	4.05251000	-3.21853200	-3.49391500	H	0.11520300	2.98211600	5.57777500
H	3.12101400	-5.36741000	-2.63280200	H	3.33281300	5.09918200	3.62941800
H	0.48394500	-0.98612500	0.07034700	H	2.04585100	4.56008000	5.69831700
8's				P	-1.28022300	-2.63754600	0.43375900
				P	-2.35002600	-0.56140100	-1.86655100
N	3.40581700	0.46692100	-0.58466900	C	-2.42437500	-3.36631200	-2.08688900
S	4.10265300	-1.03174400	-0.30048200	C	-1.36352400	-3.73571800	-1.04607100
C	2.93133100	1.27933500	0.54322500	C	-2.11676700	-2.08368600	-2.86896500

C	0.03887100	-3.40223100	1.44272100	H	-6.33987400	0.80466500	0.70286500
C	-2.84685600	-2.89832700	1.33896100	H	0.25957000	1.66812500	-5.48239300
C	-4.15928100	-0.39784800	-1.64064900	H	2.93563500	-4.85016500	3.61434600
C	-1.89206800	0.82825100	-2.96394500	H	-6.24378500	-3.26088300	3.21697200
C	-0.18701200	-3.74595800	2.78508300	H	-7.98405400	0.01850900	-1.00312600
C	-3.38266200	-1.81419100	2.05543500	H	-0.62340500	3.94037300	-4.94948300
C	-5.08873300	-0.83483400	-2.59839300	Co	-1.19437300	-0.49043400	0.12778500
C	-2.39163200	2.11035100	-2.67485200	C	-0.78863800	2.40073700	0.63732400
C	1.31761700	-3.58564500	0.88926100	O	-1.42888900	1.42033600	0.20563500
C	-3.54550600	-4.11577700	1.30959600	C	-1.51336300	3.68415000	0.75103800
C	-4.62274100	0.19152600	-0.45412000	C	-0.83287100	4.91532200	0.74099100
C	-0.93483300	0.68020300	-3.98024600	C	-2.92168900	3.67403300	0.77997200
C	0.85157300	-4.27082700	3.55853300	C	-1.54895000	6.11170000	0.76200200
C	-4.59866200	-1.94446500	2.72949400	H	0.25524600	4.93817900	0.69617800
C	-6.45774900	-0.68505700	-2.36638000	C	-3.63253200	4.87078100	0.81487800
C	-1.93817800	3.22171800	-3.38626600	H	-3.44781900	2.71935000	0.77753800
C	2.35406300	-4.10079600	1.67014200	C	-2.94697600	6.09213300	0.80529500
C	-4.76167100	-4.24273500	1.98424700	H	-1.01385900	7.06363200	0.74367500
C	-5.99254000	0.34666800	-0.22627900	H	-4.72429800	4.85525200	0.84704600
C	-0.48456100	1.79654400	-4.69243000	H	-3.50534900	7.03109700	0.82899500
C	2.12330900	-4.44769500	3.00416300	H	-0.49222700	-0.50777800	1.43935500
C	-5.29073700	-3.15816300	2.69248400				
C	-6.91190700	-0.09461900	-1.18142100	TS6's			
C	-0.98009800	3.06900800	-4.39499100	N	3.09633700	0.95601400	-1.86840600
H	-3.41699500	-3.29958200	-1.61212600	S	3.96049100	-0.20470000	-1.00640100
H	-2.48582300	-4.19617900	-2.80837200	C	2.34412800	1.93073500	-1.06556400
H	-1.51650500	-4.76220900	-0.67979600	C	2.22041000	0.52566800	-2.97359200
H	-0.35999000	-3.71483500	-1.49978000	O	4.29673600	-1.26363200	-1.96769200
H	-2.73601500	-2.01303200	-3.77506800	O	3.27989500	-0.56141400	0.25431000
H	-1.06780500	-2.09714500	-3.20239800	C	5.43665700	0.68968600	-0.56955000
H	-1.17355100	-3.60258100	3.22957700	H	2.59597700	2.94453100	-1.41273900
H	-2.84095000	-0.86515500	2.09562800	H	2.59993300	1.87338800	0.00180700
H	-4.74969400	-1.29337800	-3.52940400	C	0.88567400	1.61407800	-1.32448100
H	-3.13119800	2.24457200	-1.88413200	H	2.54289200	-0.44453600	-3.36731000
H	1.52894100	-3.30834900	-0.14413700	C	0.80456300	0.51032600	-2.35999700
H	-3.14320000	-4.97072900	0.76301000	H	2.29830400	1.27585400	-3.77679500
H	-3.90783800	0.53039400	0.29634000	C	6.28542400	1.13482300	-1.58665200
H	-0.52513300	-0.30210700	-4.21891700	C	5.74178300	0.89866300	0.77716800
H	0.66565000	-4.53889600	4.60156400	C	-0.16723000	2.19199500	-0.70246100
H	-5.00699300	-1.09485600	3.28173400	C	0.50079200	-0.85725500	-1.71286200
H	-7.17455800	-1.03154600	-3.11481300	H	0.03539500	0.73502500	-3.11245100
H	-2.33269900	4.21238700	-3.14734600	C	7.45495300	1.80862300	-1.23993200
H	3.34831800	-4.21035700	1.23338700	H	6.03363500	0.95926200	-2.63419600
H	-5.29962600	-5.19331500	1.95639900	C	6.91687400	1.57493900	1.10394300

H	5.06533300	0.53395700	1.55113400	C	-2.83881400	0.82982000	4.00396400
C	-0.02572600	3.14922700	0.42853600	C	-6.87467000	-0.87089200	-1.11849800
H	1.43322500	-1.32610200	-1.38239100	C	2.74818500	-5.15914100	-2.24079800
H	0.05057900	-1.53839300	-2.46650000	C	1.94342200	-1.58507200	4.33903600
C	7.78970000	2.04059400	0.10604600	C	-3.56928300	1.99151900	3.73345200
H	8.12453400	2.16203900	-2.02789200	C	-6.61838200	-0.95813400	-2.49172800
H	7.16299000	1.74384500	2.15556200	H	-1.98078000	-3.11841200	2.84323100
C	-0.73548900	2.89715200	1.61578100	H	-2.89250100	-4.57818100	2.49236900
C	0.81719800	4.27266800	0.37265100	H	-0.72407200	-4.92579000	1.51263100
C	9.04948300	2.77353200	0.47893000	H	-1.83309300	-4.63455800	0.16260500
C	-0.59515300	3.73927000	2.72133400	H	-4.36230000	-2.66123700	2.08154900
H	-1.39373500	2.02972300	1.67661200	H	-4.02305700	-3.51439500	0.56746700
C	0.95332900	5.11595000	1.47703800	H	2.74481200	-2.91836600	0.32527400
H	1.35364000	4.50443800	-0.54876800	H	0.05028900	-0.27917400	1.82278400
H	8.81453300	3.71719000	0.99953900	H	-4.51707100	1.30791000	0.53695900
H	9.66562200	2.17329200	1.16823100	H	-3.23344800	-1.34590300	-2.38939000
H	9.65526400	3.01314900	-0.40649100	H	-0.59505200	-4.75754100	-1.71670700
C	0.25066100	4.85012500	2.65689700	H	1.39008900	-4.33839900	2.40398500
H	-1.15084100	3.52216000	3.63538800	H	-2.12767300	-1.05584600	3.26089000
H	1.60923200	5.98769800	1.41374900	H	-6.03506000	-0.89365400	0.86782700
H	0.35916100	5.50952500	3.52141000	H	4.30985900	-4.13963000	-1.14339100
P	-0.24066000	-2.82767700	0.43477500	H	1.19546100	0.40461600	3.91948600
P	-3.09544400	-1.31615200	0.50246700	H	-4.72415400	3.06675300	2.25184800
C	-2.44031100	-3.69003800	2.02177800	H	-5.10436400	-1.21186500	-4.01753600
C	-1.36633600	-4.16567800	1.04308700	H	0.97830900	-5.98556200	-3.17646100
C	-3.56684300	-2.89724700	1.35813700	H	2.53764200	-3.66193300	4.49132900
C	0.96799100	-3.78532700	-0.55881400	H	-2.35851500	0.69551000	4.97617900
C	0.64524100	-2.34598700	1.96852400	H	-7.89750900	-0.73231100	-0.75979800
C	-3.32692100	-0.01513200	1.77505700	H	3.44159900	-5.69320100	-2.89520700
C	-4.50571400	-1.13105800	-0.65282600	H	2.45370200	-1.29045200	5.25950300
C	2.35194500	-3.61517900	-0.41443700	H	-3.66693400	2.76885900	4.49486100
C	0.59857000	-1.01617300	2.41002800	H	-7.44115600	-0.88362400	-3.20704500
C	-4.04318700	1.16207000	1.50616400	Co	-1.09560700	-1.07822300	-0.58529200
C	-4.25763700	-1.22754200	-2.03060900	C	-1.53361000	1.79111100	-1.13592400
C	0.48088400	-4.63491000	-1.56864200	O	-1.85593500	0.58949900	-1.23733100
C	1.34267000	-3.29759200	2.73220000	C	-2.52986700	2.81220100	-1.52121900
C	-2.71273200	-0.16468900	3.03171800	C	-2.19181200	4.17319500	-1.64795900
C	-5.82525600	-0.96271100	-0.20171700	C	-3.84539500	2.40223100	-1.82082300
C	3.23558400	-4.30007900	-1.25331500	C	-3.15327200	5.10217300	-2.04440500
C	1.24284100	-0.63633400	3.59027200	H	-1.17583400	4.50839400	-1.44736000
C	-4.16378000	2.15697300	2.47998400	C	-4.80294400	3.33305700	-2.21204400
C	-5.30960700	-1.14267400	-2.94663500	H	-4.10152500	1.34695800	-1.74661900
C	1.36725900	-5.32310000	-2.39911400	C	-4.46038700	4.68697300	-2.31987500
C	1.99116900	-2.91667200	3.90818000	H	-2.88064800	6.15544900	-2.14015500

H	-5.82001100	3.00336500	-2.43574600	H	-0.45446300	3.22307900	4.05173600
H	-5.21233800	5.41838900	-2.62587000	H	2.23799200	5.84680100	1.93097700
H	0.12260500	-0.45983200	-0.17879300	H	1.09610800	5.18231400	4.04869300
9's				P	-0.47821400	-2.78172100	0.14793100
N	3.41222600	1.14350500	-1.88173200	P	-3.18952200	-1.41551500	-0.45165200
S	3.96637300	-0.25605200	-1.08837900	C	-3.02966100	-4.14307800	0.33086800
C	2.71383200	2.09805600	-1.00736600	C	-1.51941400	-4.30999400	0.14415800
C	2.50925800	0.94710000	-3.03214500	C	-3.69804500	-3.18061600	-0.65147200
O	4.19133000	-1.25770600	-2.13963900	C	1.15841600	-3.48405600	-0.29904100
O	3.10626300	-0.58965600	0.06400300	C	-0.31214700	-2.23417400	1.88988200
C	5.53082900	0.28886200	-0.44397300	C	-3.74604700	-0.95488400	1.23519000
H	2.97485900	3.11206500	-1.34924000	C	-4.34579100	-0.55236200	-1.59036900
H	3.02693000	2.01393900	0.04124400	C	2.19645100	-3.65251000	0.62626000
C	1.23408600	1.83185100	-1.22247600	C	0.53030800	-1.13640200	2.15460100
H	2.78232000	0.05084300	-3.59965500	C	-4.82708800	-1.55869100	1.89684000
C	1.09594600	0.89848400	-2.41526300	C	-5.66767700	-0.24544700	-1.23403700
H	2.62380200	1.82530400	-3.68581000	C	1.36719000	-3.84981400	-1.64018700
C	6.56238800	0.59136600	-1.33677600	C	-1.07053200	-2.77757300	2.93667400
C	5.71320500	0.37334400	0.93812400	C	-3.01736000	0.04742700	1.89525600
C	0.23258100	2.33614300	-0.46262300	C	-3.87307900	-0.18740600	-2.86041900
C	0.75293100	-0.54076900	-1.96230600	C	3.42666600	-4.17343600	0.21545400
H	0.32849100	1.25929700	-3.11482000	C	0.59856800	-0.59183000	3.43735500
C	7.79471500	0.99523500	-0.82681400	C	-5.17119800	-1.15897100	3.19174400
H	6.40262700	0.51423500	-2.41370200	C	-6.50352000	0.41691800	-2.13774700
C	6.95381400	0.77909900	1.42838400	C	2.59560100	-4.37115900	-2.04718700
H	4.89373100	0.12193600	1.61227400	C	-1.00783500	-2.22132800	4.21861600
C	0.48085200	3.15636900	0.75912100	C	-3.36916400	0.45685300	3.18139500
H	0.64333600	-0.56474100	-0.84445500	C	-4.71037600	0.47139800	-3.76293200
H	-0.13384700	-0.94729600	-2.50458700	C	3.63031300	-4.52929000	-1.11926300
C	8.01135200	1.09634400	0.55891300	C	-0.18044200	-1.12501700	4.47114100
H	8.60768300	1.23565800	-1.51612500	C	-4.44734000	-0.14932700	3.83406400
H	7.10636500	0.84968400	2.50849300	C	-6.02638500	0.77786300	-3.40184000
C	-0.16811700	2.80180400	1.95579200	H	-3.25882900	-3.82885800	1.35967600
C	1.34551600	4.26352900	0.76923200	H	-3.49095700	-5.13673500	0.20808300
C	9.34351800	1.52708500	1.10916400	H	-1.10471900	-4.99863000	0.89721000
C	0.05285500	3.52183600	3.13119900	H	-1.31522900	-4.76213800	-0.84011100
H	-0.84135400	1.94388300	1.96930600	H	-4.79354700	-3.23778200	-0.56225100
C	1.56528600	4.98572400	1.94440000	H	-3.45208200	-3.44089400	-1.69450700
H	1.83219600	4.58170100	-0.15349500	H	2.05296200	-3.36775600	1.66919400
H	9.79419800	0.72363400	1.71556000	H	1.15895100	-0.72357800	1.36375800
H	10.04884400	1.78696000	0.30701600	H	-5.40634500	-2.34611600	1.41126100
H	9.23263500	2.40218100	1.77032100	H	-6.04672300	-0.50824900	-0.24474900
C	0.92252200	4.61660300	3.13013400	H	0.56774300	-3.71150200	-2.37347000
				H	-1.72432800	-3.63232000	2.76560200

H	-2.15569200	0.48739300	1.39490800	C	5.94221600	1.52676900	-0.68067500
H	-2.83628000	-0.40119100	-3.12849500	C	4.64345600	0.28768900	0.97098100
H	4.23271500	-4.29177100	0.94390100	C	-0.47664300	2.49377400	-0.07034400
H	1.25849100	0.25768000	3.62821200	C	0.22636800	1.33640900	-3.02956300
H	-6.01028100	-1.63951300	3.70085900	H	0.05807300	3.47042500	-2.78641900
H	-7.53018500	0.65669600	-1.85012300	C	7.05116600	1.46446000	0.16180700
H	2.75074600	-4.64300500	-3.09409400	H	6.00585000	2.02310400	-1.65070600
H	-1.61533800	-2.64723700	5.02063200	C	5.76470000	0.23455500	1.79722400
H	-2.79317200	1.23979600	3.67963300	H	3.70099900	-0.17100500	1.26961500
H	-4.33113200	0.75693200	-4.74727000	C	-0.49557400	2.53094000	1.41490000
H	4.59771700	-4.92268400	-1.44061000	H	0.61482400	0.45927000	-2.49075800
H	-0.13773100	-0.68872600	5.47206100	H	-0.86677300	1.25973100	-3.06967400
H	-4.71993700	0.15943800	4.84621200	C	6.98302700	0.81815600	1.40881700
H	-6.67913400	1.30215200	-4.10412000	H	7.99198600	1.92095200	-0.15515500
Co	-1.10747400	-0.95545600	-0.86278600	H	5.69352900	-0.27464700	2.76173000
C	-1.18763200	2.04345400	-0.79252100	C	-1.29364300	1.60729800	2.11669500
O	-1.58537900	0.89479600	-1.07874700	C	0.25075300	3.46514100	2.15734400
C	-2.18848900	3.13131500	-0.76760700	C	8.18241400	0.74507400	2.31393700
C	-1.81939600	4.48348000	-0.89943500	C	-1.31617300	1.59012200	3.51160000
C	-3.55239800	2.79903900	-0.65371200	H	-1.88608700	0.87413900	1.57123300
C	-2.79545400	5.47888600	-0.91541600	C	0.22674200	3.44843900	3.55351800
H	-0.76988700	4.75619500	-1.00688500	H	0.83501000	4.22905400	1.64475900
C	-4.52340000	3.79700500	-0.65964800	H	8.43731700	-0.30270200	2.54372900
H	-3.83737100	1.75339600	-0.55710300	H	9.06258200	1.22216300	1.86009900
C	-4.14750100	5.13941400	-0.79055200	H	7.97858400	1.24283000	3.27665500
H	-2.50104800	6.52491800	-1.02680400	C	-0.55053000	2.50768600	4.23700600
H	-5.57760900	3.52788300	-0.56286000	H	-1.93436700	0.85313400	4.02681600
H	-4.90950700	5.92273000	-0.79696900	H	0.81396600	4.18279200	4.11038300
H	1.56683500	-1.25181100	-2.13720200	H	-0.56587600	2.49577200	5.32944700
9'_T				P	0.64022000	-2.34516000	-0.41368800
				P	-2.75221600	-1.94971000	0.13153100
N	2.90590900	2.58439700	-1.42316700	C	-1.15387500	-4.29294000	0.69469000
S	3.34430200	0.93859800	-1.35199100	C	-0.01952900	-4.08171000	-0.31367800
C	2.00808200	2.97989900	-0.32598900	C	-2.53057900	-3.79292900	0.23842200
C	2.17419800	2.96822700	-2.64621300	C	1.97553200	-2.58679900	-1.65478100
O	3.77009700	0.56667400	-2.70642200	C	1.43949400	-2.13162300	1.22375300
O	2.28325400	0.16980400	-0.67591800	C	-3.41119600	-1.46926600	1.77745900
C	4.74630900	0.93880100	-0.26168600	C	-4.24018800	-1.81837800	-0.94169300
H	2.15748700	4.05927800	-0.15808700	C	3.34418600	-2.62859900	-1.35568800
H	2.24714400	2.46185500	0.61087200	C	1.11372800	-0.97007600	1.93934800
C	0.60770800	2.69905600	-0.84500000	C	-3.06723700	-2.15939100	2.95096300
H	2.58191800	2.44679500	-3.51876300	C	-5.50297800	-2.28783100	-0.54373300
C	0.67798100	2.65708100	-2.37468900	C	1.56873400	-2.69286100	-2.99501000
H	2.33200400	4.04882400	-2.78096700	C	2.30511800	-3.07058300	1.80581500

C	-4.21529900	-0.31889100	1.87811000	C	-2.57978500	4.50756800	-0.58563200
C	-4.09255600	-1.24392400	-2.21325300	C	-4.09077300	2.77337000	-1.38828800
C	4.28530200	-2.78119200	-2.37599100	C	-3.57886600	5.46110700	-0.77680300
C	1.65347500	-0.73360800	3.20491100	H	-1.60485600	4.80623600	-0.19751800
C	-3.53291600	-1.71969700	4.19477700	C	-5.08415300	3.72941600	-1.57549200
C	-6.59750000	-2.18047700	-1.40419500	H	-4.27349000	1.72316600	-1.62121400
C	2.51041100	-2.85386200	-4.01465200	C	-4.82978400	5.07375200	-1.26962800
C	2.85587100	-2.83191900	3.06865200	H	-3.38428000	6.50921900	-0.53909100
C	-4.68253100	0.11477900	3.11921800	H	-6.06254200	3.43152800	-1.95919500
C	-5.18869400	-1.13765200	-3.07545900	H	-5.61244100	5.82231500	-1.41534600
C	3.87325300	-2.89910100	-3.70638100	H	0.59626700	1.29273400	-4.06545800
C	2.53321600	-1.66371800	3.76875000				
C	-4.34508400	-0.58614800	4.28286800	10's			
C	-6.44276100	-1.60307700	-2.67031900	C	-2.85568100	-0.57347100	0.66347600
H	-0.87809800	-3.85136500	1.66628000	H	-2.99956600	0.51972800	0.63931500
H	-1.24439700	-5.37683000	0.87554700	O	-1.74718700	-1.05773200	0.36395000
H	0.82721900	-4.74591600	-0.07972700	C	-3.99913900	-1.38459400	1.02843100
H	-0.35339500	-4.34784000	-1.33020500	C	-5.22735300	-0.74500000	1.29098700
H	-3.32470500	-4.19943500	0.88460100	C	-3.90752400	-2.79072400	1.10616900
H	-2.73237800	-4.16229300	-0.78028700	C	-6.34827200	-1.50069300	1.62852300
H	3.68537000	-2.51444700	-0.32692600	H	-5.29020800	0.34397400	1.21984400
H	0.43813500	-0.23864000	1.49275700	C	-5.03009400	-3.53795200	1.44543700
H	-2.43704500	-3.04851900	2.90571200	H	-2.95109900	-3.27446800	0.89790900
H	-5.63406400	-2.72946500	0.44698100	C	-6.24967100	-2.89491200	1.70681600
H	0.50521600	-2.63687800	-3.24743100	H	-7.30117500	-1.00651400	1.83038300
H	2.55628200	-3.99133200	1.27527100	H	-4.96417100	-4.62653200	1.50791100
H	-4.48357000	0.23824800	0.97779500	H	-7.12895900	-3.48714200	1.97184100
H	-3.11629800	-0.86627600	-2.52313400	P	-0.17601700	1.35077600	-0.89342500
H	5.34989400	-2.79584100	-2.12915700	P	2.05305200	-0.78731300	-0.62984600
H	1.38563600	0.17691400	3.74548700	C	2.25296700	1.30657700	-2.45748400
H	-3.26046500	-2.27142800	5.09798700	C	0.76565000	1.67772100	-2.45270900
H	-7.57705800	-2.54566900	-1.08539400	C	2.53490400	-0.19312300	-2.30114000
H	2.17825400	-2.93396400	-5.05289700	C	-1.88580100	1.80526500	-1.38391500
H	3.53672200	-3.56403800	3.50994800	C	0.32308700	2.64320200	0.30519700
H	-5.31148700	1.00643900	3.17848800	C	3.34675800	-0.10352700	0.47551800
H	-5.06301300	-0.68450400	-4.06196500	C	2.31688500	-2.59131200	-0.59222100
H	4.61260900	-3.01323200	-4.50298600	C	-2.51116000	2.98996500	-0.97087400
H	2.96396900	-1.48223700	4.75661100	C	-0.12981700	2.49021700	1.62836100
H	-4.71037200	-0.24552600	5.25465600	C	4.71154500	-0.34181300	0.24562400
H	-7.30196100	-1.51576200	-3.34003800	C	1.62741100	-3.27602100	0.42495600
Co	-0.95979900	-0.74678200	-0.67242600	C	-2.60694300	0.87849200	-2.15754200
C	-1.79519700	2.13066500	-0.68769200	C	1.16774500	3.71713400	-0.00784700
O	-2.02711500	0.94769800	-0.98509300	C	2.95512900	0.66746500	1.57886100
C	-2.82830000	3.15556400	-0.88964400	C	3.11329600	-3.30839600	-1.49579700

C	-3.84107900	3.24242100	-1.32520100	C	-3.91848100	1.61491100	-1.25706500
C	0.24785100	3.39846600	2.61707400	C	-5.07514000	0.84976200	-1.49705800
C	5.66973500	0.19561400	1.10696600	C	-4.02717800	2.99315400	-0.98307600
C	1.73972800	-4.66223900	0.54231500	C	-6.32975500	1.45633800	-1.46460200
C	-3.93122300	1.13517400	-2.51398700	H	-4.97877600	-0.22042000	-1.69693000
C	1.55994900	4.61739700	0.98893400	C	-5.28147800	3.59269600	-0.95192300
C	3.91618500	1.20737200	2.43875800	H	-3.12094100	3.57090700	-0.79145600
C	3.22276700	-4.69739200	-1.37562700	C	-6.43154700	2.82513400	-1.19220900
C	-4.55282900	2.31702300	-2.09350900	H	-7.22985300	0.86564000	-1.64775600
C	1.10235600	4.46122900	2.29959000	H	-5.37375800	4.66002500	-0.73849200
C	5.27340100	0.97316500	2.20255600	H	-7.41491900	3.30084400	-1.16437900
C	2.54015700	-5.37357200	-0.35901100	P	-0.50677000	-0.97849600	0.92872600
H	2.79005400	1.86839800	-1.67597400	P	2.32181800	0.77140100	0.44067100
H	2.67712000	1.63876300	-3.41865900	C	1.87579900	-1.16241500	2.50047300
H	0.62738600	2.74016800	-2.70739700	C	0.34204400	-1.17299300	2.55984000
H	0.23058700	1.10076400	-3.22461400	C	2.53190700	0.18970800	2.18755200
H	3.60075600	-0.40665700	-2.47377800	C	-2.28480200	-0.95078600	1.39684600
H	1.95194100	-0.77920700	-3.03000500	C	-0.30523800	-2.57563900	0.05677000
H	-1.96572600	3.71652000	-0.36586400	C	3.23478200	-0.50367900	-0.51751700
H	-0.77254000	1.64325100	1.88226200	C	3.39972100	2.25666300	0.32719200
H	5.02691600	-0.95461100	-0.60268000	C	-3.14230300	-2.05365700	1.26382900
H	0.99513100	-2.71308000	1.12324700	C	-0.65855800	-2.60060900	-1.30453000
H	-2.13361900	-0.06073500	-2.45586400	C	4.57476900	-0.83512800	-0.26418300
H	1.53306500	3.85956000	-1.02577200	C	3.15991000	3.12832400	-0.74904100
H	1.89493600	0.85084900	1.75400500	C	-2.81259600	0.27498800	1.84149500
H	3.64816200	-2.78959500	-2.29409300	C	0.21432100	-3.73754300	0.64515300
H	-4.32196400	4.16702400	-0.99634500	C	2.53224100	-1.18904400	-1.51832500
H	-0.11357300	3.27108200	3.64033100	C	4.42909200	2.56062300	1.23203800
H	6.73072000	0.00674300	0.92532500	C	-4.50024100	-1.93138100	1.57480200
H	1.20149300	-5.18912400	1.33393600	C	-0.50980800	-3.76493300	-2.05846700
H	-4.48462100	0.40637300	-3.11109200	C	5.19520500	-1.84826700	-0.99832300
H	2.22722300	5.44504200	0.73661800	C	3.94285000	4.27000800	-0.92966400
H	3.60109100	1.81335500	3.29167000	C	-4.16552000	0.39163200	2.16453800
H	3.84463900	-5.25483600	-2.08045200	C	0.37855700	-4.90045100	-0.11527100
H	-5.59318000	2.51412800	-2.36340700	C	3.15113200	-2.20556000	-2.25086200
H	1.41223400	5.16534500	3.07553500	C	5.20666700	3.70960700	1.05616900
H	6.02666200	1.39378800	2.87340400	C	-5.01439700	-0.71133100	2.02573300
H	2.62918200	-6.45908900	-0.27063900	C	0.01669300	-4.91810000	-1.46485000
Co	-0.02490500	-0.59067800	-0.07761300	C	4.48350600	-2.53679400	-1.98892600
				C	4.96852800	4.56369800	-0.02448600
				H	2.23488100	-1.92135700	1.78605800
				H	2.24447100	-1.48330900	3.48840600
				H	-0.02135000	-2.09157200	3.04653100
				H	-0.02040600	-0.33174900	3.17376800
10'_T							
C	-2.62878900	0.94413800	-1.24596600				
H	-2.64404900	-0.14503300	-1.44694200				
O	-1.55559600	1.51401500	-1.01546300				

H	3.60969800	0.11605100	2.39832500	C	0.51372700	-1.70433400	-2.55651300
H	2.12636400	0.98132300	2.83975800	C	-3.56471900	-1.14342100	0.16146500
H	-2.75197500	-3.01050600	0.91167400	C	-2.15178200	1.24095600	-0.65815000
H	-1.04881200	-1.69445200	-1.77654700	C	1.39122600	0.85515000	-1.47243300
H	5.13670800	-0.29965400	0.50502800	C	2.85427600	-1.59683000	-0.86249600
H	2.34892900	2.90614900	-1.44948500	C	-4.79335800	-0.62416400	-0.27740700
H	-2.16204100	1.15126300	1.91150200	C	-2.12849000	1.94677400	0.55857800
H	0.49574500	-3.74765100	1.69927100	C	1.85389500	1.21402700	-2.75066200
H	1.48881700	-0.92712900	-1.71113500	C	4.01095500	-0.81838300	-1.01309400
H	4.63505400	1.90623200	2.08026300	C	-3.54133500	-2.13667800	1.15152500
H	-5.16028100	-2.79542400	1.46376700	C	-2.26561400	1.94590000	-1.86375100
H	-0.79358600	-3.77050400	-3.11369300	C	1.09121800	1.86080700	-0.54260100
H	6.23876200	-2.10363100	-0.79784700	C	2.97409100	-2.95912400	-0.53854300
H	3.74788700	4.93620200	-1.77374500	C	-5.98656700	-1.10549000	0.26395200
H	-4.56276100	1.35165900	2.50261100	C	-2.21680100	3.33818800	0.56414900
H	0.79074800	-5.79779200	0.35273700	C	2.01083900	2.55965700	-3.08722300
H	2.59095700	-2.74054800	-3.02135100	C	5.27228800	-1.39975400	-0.84777000
H	6.00402900	3.93668900	1.76828800	C	-4.73859900	-2.61626500	1.69054700
H	-6.07722000	-0.61771000	2.26129400	C	-2.34301400	3.34246200	-1.85314900
H	0.14657500	-5.82826900	-2.05531700	C	1.25575000	3.20581400	-0.87980000
H	4.97150200	-3.33199000	-2.55797900	C	4.23476100	-3.53703700	-0.38441200
H	5.57846000	5.46037700	-0.15904400	C	-5.96026100	-2.10247100	1.24655900
Co	0.18069700	0.83597000	-0.26077600	C	-2.31747300	4.03966100	-0.64329700
TS7's				C	1.71260700	3.55732900	-2.15226700
				C	5.38692500	-2.75701600	-0.53686900
				H	-0.58929000	-0.01139600	-3.33155800
Co	-0.16467400	-1.25518500	0.64994600	H	-0.95802100	-1.54967400	-4.09911100
C	0.27613500	-0.44351100	2.14565700	H	-2.90582700	-0.83389000	-2.80051800
O	-0.81656500	-0.78075300	2.61501900	H	-2.23904100	-2.32635800	-2.12945100
C	1.29293900	0.40966300	2.75656100	H	1.31538500	-1.67715000	-3.31004500
C	2.61047600	0.41021600	2.27074000	H	0.35527500	-2.76535500	-2.30254300
C	0.92143800	1.27683200	3.80041800	H	-4.81718500	0.16154600	-1.03626900
C	3.55369100	1.27078100	2.82733800	H	-2.03809500	1.40513600	1.50349800
H	2.88645700	-0.26890100	1.46454200	H	2.09736200	0.44526300	-3.48627300
C	1.86739000	2.14452700	4.34349300	H	3.93345200	0.24359800	-1.25021400
H	-0.10678100	1.26737400	4.16693400	H	-2.58561300	-2.52450900	1.51150300
C	3.18122600	2.14170000	3.85844600	H	-2.28971200	1.41861200	-2.81805500
H	4.58019300	1.26665100	2.45456200	H	0.71816400	1.59350200	0.44280100
H	1.58320300	2.82438800	5.14979700	H	2.07857500	-3.56944000	-0.39665000
H	3.91970400	2.82294600	4.28809700	H	-6.94125300	-0.69913800	-0.07871700
H	1.02580200	-1.75614900	1.40186300	H	-2.19917600	3.87911000	1.51329500
P	-1.98770300	-0.57321500	-0.56334800	H	2.36796700	2.83043200	-4.08365300
P	1.16898800	-0.90041600	-1.02201000	H	6.16844600	-0.78517300	-0.96193400
C	-0.76432400	-1.07721200	-3.12252800	H	-4.71559600	-3.38797100	2.46375200
C	-2.03207500	-1.25321400	-2.27766800				

H	-2.42304100	3.88530300	-2.79785400	C	4.91236500	1.81321400	-1.08744600
H	1.01437400	3.97851800	-0.14732000	C	-3.26484400	-4.25026300	-1.07880900
H	4.31885200	-4.59781700	-0.13636500	C	-3.99684100	2.73828400	1.27422000
H	-6.89590300	-2.47467100	1.67098000	C	-0.16433600	3.10456200	2.31572700
H	-2.37552100	5.13072200	-0.63891400	C	4.51651500	-0.10271900	-2.51361100
H	1.83393700	4.60990400	-2.41935500	C	-4.65824700	-4.16717900	-1.00051300
H	6.37369800	-3.20817100	-0.40794400	C	-3.92044900	2.31424800	2.60298800
11's				C	-0.13957500	4.43476800	1.88658200
Co	0.05006900	-0.75622200	-0.04325500	C	5.40099800	0.81397300	-1.93324700
C	1.28906900	-1.73325600	0.88535900	H	-1.63063100	2.47828600	-1.89371400
O	0.21816200	-2.28087100	1.20546100	H	-1.68793400	2.06793200	-3.60224400
C	2.61123300	-2.14382700	1.32452600	H	-3.34287500	0.68861100	-2.46822700
C	3.72562000	-1.34066100	1.02265700	H	-2.04245200	-0.35243100	-3.06211700
C	2.77849900	-3.33662200	2.06040500	H	0.63522000	2.31248100	-3.00746100
C	4.99561600	-1.72603000	1.44897500	H	0.35474300	0.59400700	-3.31995000
H	3.58441300	-0.41989700	0.46054000	H	-4.99115700	-0.79909600	-0.56210200
C	4.04997900	-3.71887900	2.47567100	H	-2.32771000	-0.66352500	2.13441100
H	1.90601100	-3.95125400	2.29081700	H	0.84016300	3.96647000	-1.34677100
C	5.15712700	-2.91391900	2.17005100	H	3.17225900	2.67938700	-0.14890100
H	5.86083600	-1.10169200	1.21651500	H	-1.39866600	-3.15335900	-1.01623500
H	4.18646500	-4.64402300	3.04013000	H	-3.55804800	2.28683900	-0.78324700
H	6.15397900	-3.21792000	2.49916100	H	0.13371800	1.04167400	1.77194400
H	0.32933800	-1.39676300	-1.28457300	H	2.46984300	-0.76168800	-2.67535900
P	-2.05934000	-0.35198800	-0.69335400	H	-6.36596400	-2.86008000	-0.75111500
P	0.86863200	0.98314700	-1.01509900	H	-3.27071800	0.74312200	3.94492600
C	-1.40347800	1.67648900	-2.61226300	H	0.24400800	5.78130900	0.23582000
C	-2.27637600	0.44626100	-2.33918500	H	5.59913500	2.53039400	-0.63160700
C	0.10564600	1.42147400	-2.63605200	H	-2.77926100	-5.21960200	-1.21514700
C	-3.10594100	-1.84609300	-0.79425700	H	-4.46319000	3.69574800	1.03011100
C	-2.87126600	0.71419000	0.54895800	H	-0.45685700	2.86160200	3.33924600
C	0.53775900	2.38205200	0.10505400	H	4.89457300	-0.88879000	-3.17152100
C	2.65493400	0.98004900	-1.39270900	H	-5.26479300	-5.07300900	-1.07646800
C	-4.50543100	-1.76605900	-0.71433400	H	-4.32265100	2.94161200	3.40201200
C	-2.80140900	0.29077900	1.88860500	H	-0.40946100	5.23628300	2.57831400
C	0.56175000	3.72028200	-0.31990400	H	6.47184200	0.74609100	-2.13939600
C	3.54269500	1.90049200	-0.81730000	12's			
C	-2.48820500	-3.09324000	-0.97223600	Co	0.52312200	-0.80540000	0.78946700
C	-3.48061900	1.94042800	0.24777100	C	1.55398000	0.17069300	-0.37882000
C	0.17360200	2.08051600	1.42861700	O	0.64116400	0.19185900	-1.20257700
C	3.15053900	-0.02455500	-2.24204100	C	2.85468900	0.82084900	-0.54754600
C	-5.27716100	-2.92512600	-0.81740900	C	3.75938800	0.86067100	0.52224000
C	-3.32862000	1.08290400	2.90810200	C	3.19378100	1.40478200	-1.78296900
C	0.22539800	4.74160700	0.57091600	C	5.00535000	1.46430600	0.35690100

H	3.47697200	0.41152400	1.47466700	H	-1.35520600	-1.76899900	-1.37417400
C	4.44097300	1.99910000	-1.94557500	H	0.93974200	-5.49937200	-0.56285900
H	2.46829100	1.38065100	-2.59843500	H	3.43722200	-2.55451700	-2.07544500
C	5.34787600	2.02449400	-0.87703800	H	-3.86521000	-0.74849300	0.69839100
H	5.71244800	1.49705700	1.18777400	H	-3.36808600	-4.18859800	1.57599400
H	4.71152700	2.45207500	-2.90202200	H	1.06661800	-1.60630000	-2.45491000
H	6.32476200	2.49512400	-1.00647900	H	3.65248700	-2.29993100	2.23771600
H	1.42860300	-1.16956200	1.85356000	H	-3.57209900	-0.30274100	5.64807100
P	-1.34818700	-2.01011800	1.51791400	H	-2.53017800	-2.99902000	-3.18841600
P	1.54343100	-2.67293900	0.23339000	H	0.25909100	-6.50759700	-2.69745700
C	0.03550300	-4.43276400	1.98202500	H	5.87133400	-2.16841900	-2.21144100
C	-0.80299900	-3.35314900	2.66764000	H	-5.68433400	0.37858100	1.94610200
C	1.42561400	-3.98446400	1.52862500	H	-4.54137700	-5.41709600	-0.22872200
C	-2.69434200	-1.19162000	2.46448600	H	0.43841700	-2.63877100	-4.60247500
C	-2.26370600	-2.90807700	0.21135200	H	6.09191900	-1.98163500	2.09446300
C	1.05774300	-3.47306600	-1.34617600	H	-5.54066100	0.62710300	4.42647000
C	3.36763600	-2.47342600	0.08992000	H	-4.12640200	-4.83038000	-2.61786500
C	-2.62302500	-1.05458100	3.86136000	H	0.00683400	-5.09533700	-4.73925800
C	-2.04115600	-2.57682500	-1.13010700	H	7.22149000	-1.89107100	-0.13092500
C	0.82631300	-4.85498500	-1.43387600	N	-1.20802500	2.43990600	-0.25848900
C	4.00860100	-2.42789900	-1.15579900	S	-2.19072700	1.71002200	-1.39516200
C	-3.80450600	-0.66433800	1.78324500	O	-2.46255000	0.35779600	-0.89252200
C	-3.17389600	-3.93061300	0.53213400	O	-1.58622100	1.91747500	-2.71363700
C	0.91144700	-2.68324500	-2.50097600	C	-3.72573400	2.62529400	-1.36142200
C	4.13181700	-2.30310800	1.25657400	C	-4.51655600	2.58831800	-0.20583800
C	-3.64057400	-0.39947100	4.56176700	C	-5.70600800	3.30975500	-0.17783700
C	-2.71255200	-3.26457200	-2.14512700	C	-6.12679800	4.06684800	-1.28851800
C	0.44529200	-5.43212100	-2.64832000	C	-5.31406700	4.08214500	-2.43143100
C	5.38800400	-2.21268800	-1.23267800	C	-4.11426700	3.36710000	-2.47641800
C	-4.82226400	-0.01725700	2.48823500	H	-4.21203800	1.99940100	0.66004100
C	-3.83859700	-4.61975200	-0.48282700	H	-6.32718000	3.28374400	0.72148800
C	0.54680900	-3.26657500	-3.71495300	H	-5.62418800	4.66146500	-3.30458800
C	5.51106700	-2.10908100	1.17780900	H	-3.48553800	3.37872200	-3.36758000
C	-4.74281700	0.12072100	3.87788500	C	-7.42021000	4.83342800	-1.23712700
C	-3.60604500	-4.28857500	-1.82402100	H	-7.61103600	5.36979900	-2.17763600
C	0.30542100	-4.64148000	-3.79126500	H	-8.27016300	4.15695800	-1.04764600
C	6.14350500	-2.05766600	-0.06850300	H	-7.40900400	5.56963900	-0.41620500
H	-0.52843200	-4.86102200	1.13998200	C	-0.84343700	3.83461200	-0.51697300
H	0.18124300	-5.25524200	2.70085200	H	-1.48474500	4.51058900	0.08064100
H	-1.69325900	-3.80283300	3.13126200	H	-1.04380400	4.05260800	-1.57626300
H	-0.22291400	-2.86997700	3.46965400	C	0.56201200	4.12148400	-0.23050700
H	2.00955300	-4.84193100	1.16225800	C	1.71911800	4.37233300	0.04369200
H	1.97475100	-3.57964200	2.39056800	C	3.07618100	4.65365000	0.40007500
H	-1.77592700	-1.46122800	4.41689800	C	3.97377400	5.19274300	-0.54293000

C	3.53296200	4.38853400	1.70775600	C	-0.29159300	-3.18761200	-1.11919800
C	5.29318300	5.46346200	-0.18161200	C	5.16351200	-1.99654800	-1.46008400
H	3.62669900	5.39127800	-1.55854100	C	4.72225800	1.32597000	-1.06640300
C	4.85511000	4.65804200	2.05918000	C	-1.65424300	-3.64723700	2.15182700
H	2.84082800	3.96909600	2.44064600	C	1.06031700	-4.93156300	-0.11733500
C	5.73825900	5.19652100	1.11737800	C	2.83306300	-2.14503100	-2.11116000
H	5.98109300	5.88091900	-0.92076500	C	4.74182600	1.45094400	1.35331400
H	5.19887800	4.44719600	3.07475500	C	-1.61644200	-2.37562300	4.64268700
H	6.77357500	5.40783000	1.39562600	C	-0.56464600	-4.02142700	-2.20477400
C	-1.21758000	1.96034500	1.12045600	C	5.51998100	-2.77094300	-2.56413500
H	-1.51456200	2.79750200	1.78040500	C	5.43993500	2.52230100	-1.13182800
H	-1.98092400	1.18255100	1.23274600	C	-2.71883200	-3.81533100	3.04212800
C	0.12231500	1.45207500	1.58910700	C	0.80143300	-5.75649500	-1.21596100
C	0.29712500	0.61098700	2.64432900	C	3.19357500	-2.92175900	-3.21677300
H	0.99007300	1.98343900	1.19475000	C	5.46511400	2.64388300	1.28390400
H	1.27606900	0.51515000	3.11498500	C	-2.70616600	-3.17753400	4.28581300
H	-0.55583300	0.22323700	3.20422300	C	-0.01261300	-5.30557900	-2.25927800
TS8's				C	4.53452600	-3.23770900	-3.44340300
Co	1.16009600	-0.31930300	0.53152400	C	5.81469400	3.18261300	0.04152500
C	1.27971500	0.98544800	-0.76161600	H	3.65231300	-3.63725500	0.76039400
O	0.83118300	0.17722900	-1.57198200	H	4.28034100	-3.69191500	2.40473700
C	1.58383800	2.38918400	-1.02164900	H	1.92664300	-4.27546600	2.53668600
C	2.08717200	3.19993100	0.00874400	H	2.16283100	-2.70019000	3.28874700
C	1.39504500	2.92134500	-2.31170700	H	5.20734700	-1.69701300	1.43380900
C	2.40578000	4.53081300	-0.24756500	H	3.95691000	-1.15794400	2.57062200
H	2.24733700	2.77168900	0.99722400	H	0.28379300	-1.56346700	4.04128100
C	1.71782700	4.25183100	-2.56330100	H	-0.71200600	-2.18073000	-1.10756200
H	1.00078400	2.27855700	-3.10117400	H	5.94047400	-1.63194100	-0.78441500
C	2.22406300	5.05431300	-1.53219000	H	4.42850600	0.82224400	-1.98881600
H	2.79871600	5.16213600	0.55130400	H	-1.68127100	-4.14324000	1.18060400
H	1.57585200	4.66976700	-3.56247700	H	1.68872800	-5.30684700	0.69153800
H	2.47439100	6.09891200	-1.73187200	H	1.78930400	-1.89668000	-1.94229500
H	1.71293700	0.18648700	1.77584000	H	4.45832800	1.05372400	2.33019100
P	0.81693400	-2.49152300	1.33379100	H	-1.59483400	-1.87990300	5.61625300
P	3.33955600	-0.73114800	0.26985500	H	-1.20397500	-3.65854400	-3.01296400
C	3.60201400	-3.13426300	1.73912300	H	6.57115200	-3.01176500	-2.74055400
C	2.19571400	-3.23025700	2.32390400	H	5.70119300	2.94223100	-2.10593200
C	4.12457900	-1.70188800	1.62832200	H	-3.56267900	-4.44976100	2.75993000
C	-0.56804700	-2.83001400	2.49570200	H	1.23649200	-6.75814800	-1.25358700
C	0.51830600	-3.63876400	-0.06185500	H	2.41845200	-3.28037400	-3.89779100
C	3.81263600	-1.68144100	-1.22446700	H	5.75227900	3.15712400	2.20485300
C	4.37086300	0.77959100	0.17755700	H	-3.54061300	-3.30856600	4.97894700
C	-0.55495500	-2.20104800	3.75267500	H	-0.21563400	-5.95426400	-3.11493700
				H	4.81671500	-3.84598900	-4.30636300

H	6.37475700	4.11922600	-0.01133500	13's			
N	-3.24763700	0.13258900	0.58465200	Co	0.69561900	-0.61738300	0.69305300
S	-3.42987500	0.19391200	-1.09350500	C	1.34091800	0.61505000	-0.47082600
O	-2.72740700	-0.99185300	-1.60855800	O	0.56069900	0.04561200	-1.23385300
O	-3.07936400	1.51673200	-1.63412800	C	2.20946500	1.74211700	-0.73654000
C	-5.18453600	-0.03506500	-1.27898300	C	2.94101900	2.29870300	0.32550300
C	-5.75536200	-1.24677400	-0.87089100	C	2.35243400	2.24566000	-2.04472600
C	-7.12318500	-1.43250000	-1.03952100	C	3.81739600	3.35294200	0.08262400
C	-7.93064400	-0.43001700	-1.61341000	H	2.82019200	1.88750600	1.32782700
C	-7.32518700	0.76929900	-2.01598700	C	3.23902800	3.29089600	-2.28109000
C	-5.95290300	0.97604100	-1.85334300	H	1.77209900	1.80314700	-2.85658500
H	-5.13555500	-2.02691500	-0.42492400	C	3.96957600	3.84205400	-1.21904500
H	-7.58086500	-2.37350100	-0.72319400	H	4.38781100	3.79211800	0.90238000
H	-7.93526500	1.55702600	-2.46437500	H	3.36246300	3.68610900	-3.29172600
H	-5.48115800	1.90901900	-2.16414500	H	4.66199700	4.66448800	-1.40949200
C	-9.40859100	-0.65404200	-1.78114500	P	-0.58683200	-2.52194300	1.15529700
H	-9.89671100	0.20454400	-2.26391300	P	2.56857400	-1.95087100	0.43796700
H	-9.60346700	-1.55116600	-2.39168500	C	1.65214800	-4.20672000	1.88608300
H	-9.89282000	-0.82130000	-0.80448000	C	0.28319200	-3.67854300	2.32022400
C	-3.84073600	1.23221300	1.35251200	C	2.75704400	-3.15192000	1.82711400
H	-3.94468600	0.87189100	2.38865300	C	-2.24847400	-2.46258000	1.95012100
H	-4.86606700	1.40081400	0.98428400	C	-0.88381400	-3.52029800	-0.35479200
C	-3.09215500	2.49400700	1.33441200	C	2.80633000	-2.94461900	-1.08007300
C	-2.43833400	3.51661900	1.27689100	C	4.09755000	-0.94220100	0.54522100
C	-1.64431400	4.69792700	1.13571400	C	-2.35828300	-2.26929200	3.33882100
C	-1.47662800	5.28054900	-0.13862400	C	-1.08924200	-2.86032700	-1.57639200
C	-1.01074000	5.28804600	2.24889600	C	3.70824300	-4.02262000	-1.11323700
C	-0.70178100	6.42948800	-0.28816900	C	4.78860000	-0.56616300	-0.61688500
H	-1.95494800	4.81564400	-1.00279900	C	-3.41930400	-2.54944700	1.18158300
C	-0.23701300	6.43786100	2.08853700	C	-0.93616600	-4.92376900	-0.31527900
H	-1.13489800	4.83802000	3.23607100	C	2.09062500	-2.61059900	-2.23861700
C	-0.08278700	7.01304900	0.82260100	C	4.52724600	-0.44774600	1.78817400
H	-0.57566400	6.86993900	-1.27969500	C	-3.61271400	-2.15835200	3.94289600
H	0.24810300	6.88916900	2.95754300	C	-1.34570000	-3.59393100	-2.73754500
H	0.52397700	7.91358000	0.70088400	C	3.88213300	-4.75625000	-2.28757600
C	-2.00401400	-0.46814500	1.07640300	C	5.89477800	0.28305400	-0.53575400
H	-2.17462900	-0.72962600	2.12764800	C	-4.67289000	-2.43946600	1.78905300
H	-1.87802900	-1.40310700	0.52451100	C	-1.17489200	-5.65366800	-1.48191100
C	-0.81436100	0.46070000	0.92461300	C	2.27253700	-3.34387100	-3.41488900
C	0.03490100	0.85972100	1.94524400	C	5.63943300	0.39378600	1.86607800
H	-0.92746900	1.14050700	0.07759700	C	-4.77472300	-2.23978700	3.16918400
H	0.47307900	1.85813000	1.93135700	C	-1.38060000	-4.99009900	-2.69595400
H	-0.05353400	0.40447900	2.93505100	C	3.16375700	-4.41868100	-3.44063500
				C	6.32497300	0.76289300	0.70443400

H	1.57660500	-4.72948100	0.92011200	C	-2.63955000	3.15279000	1.07846900
H	1.95769300	-4.96951500	2.62038600	H	-2.98320000	3.30875600	2.11408500
H	-0.39726000	-4.51640300	2.53136600	H	-3.44231500	3.54501700	0.43271600
H	0.39251000	-3.12157500	3.26400900	C	-1.41538700	3.93160000	0.85221200
H	3.74719400	-3.62410400	1.74757600	C	-0.42371100	4.61389900	0.68072500
H	2.76248000	-2.55622900	2.75341900	C	0.73661500	5.42504800	0.46831400
H	-1.46487400	-2.18909300	3.96111400	C	1.04666500	5.90246300	-0.82159800
H	-1.06946700	-1.77233100	-1.61102700	C	1.58038700	5.76748000	1.54569600
H	4.28203400	-4.29370100	-0.22506500	C	2.16491600	6.71078700	-1.02183800
H	4.45924000	-0.93161800	-1.59126000	H	0.40372700	5.62898500	-1.66024600
H	-3.35440000	-2.68545400	0.10290900	C	2.69701300	6.57611900	1.33597700
H	-0.79668000	-5.45867500	0.62550200	H	1.34777800	5.39545700	2.54559000
H	1.39218000	-1.77631600	-2.22347700	C	2.99090100	7.05273400	0.05395500
H	3.99285000	-0.71041300	2.70375700	H	2.39627900	7.07281500	-2.02640300
H	-3.68126500	-2.00629100	5.02292800	H	3.34209300	6.83698800	2.17855300
H	-1.50919100	-3.06867400	-3.68180200	H	3.86606700	7.68672100	-0.10757700
H	4.58179200	-5.59549100	-2.30331500	C	-1.80279200	0.88404200	1.82902100
H	6.42068300	0.57251800	-1.44867300	H	-2.01747700	1.32791800	2.81722500
H	-5.57524400	-2.50916800	1.17676100	H	-2.24354600	-0.11620000	1.83720300
H	-1.20389000	-6.74531900	-1.44086700	C	-0.30561800	0.85169800	1.59403600
H	1.70663900	-3.07654200	-4.31022600	C	0.59243900	0.31329400	2.63380300
H	5.96835700	0.76679500	2.83916100	H	0.02493900	1.81674700	1.19679500
H	-5.75622700	-2.15096100	3.64119800	H	1.34377100	1.01885800	3.01812500
H	-1.56927400	-5.56243300	-3.60765500	H	0.09583300	-0.22189500	3.45502800
H	3.30097800	-4.99548600	-4.35857900	H	1.33340100	-0.51641300	2.21553100
H	7.19025400	1.42715300	0.76551800				
N	-2.54450300	1.70783100	0.87304100	TS9's			
S	-2.71737200	1.16331700	-0.69815800	Co	0.37462800	0.39808100	-0.44005600
O	-2.49947600	-0.28932700	-0.64511100	C	0.63519400	-1.10178100	0.80437100
O	-1.94134000	1.98804400	-1.63476600	O	-0.44251400	-0.44028200	1.04763900
C	-4.44627200	1.46243300	-1.02069500	C	1.61262400	-1.25584000	1.91957900
C	-5.40268300	0.79502000	-0.24574900	C	2.98134100	-1.42440700	1.66188100
C	-6.75082000	1.00539100	-0.51456400	C	1.16641000	-1.15626700	3.24793200
C	-7.16240300	1.86966000	-1.54890400	C	3.89349300	-1.48732700	2.71398700
C	-6.17916300	2.51973300	-2.30847300	H	3.32686800	-1.48106600	0.63141200
C	-4.81926000	2.32149300	-2.05239100	C	2.08029100	-1.22092000	4.30065300
H	-5.09318700	0.12562800	0.55870800	H	0.09930800	-1.02661100	3.43888600
H	-7.50522200	0.49120600	0.08688100	C	3.44539600	-1.38741900	4.03566100
H	-6.47985500	3.19322600	-3.11469900	H	4.95849100	-1.60701100	2.50201900
H	-4.05301200	2.82702900	-2.64145500	H	1.72863000	-1.14206400	5.33241300
C	-8.62691200	2.08077700	-1.82021900	H	4.16013200	-1.43599400	4.86101300
H	-8.78807800	2.79467600	-2.64053500	P	-0.44423900	2.51784800	-0.64707900
H	-9.11719300	1.13029800	-2.08936100	P	2.29838000	0.85033500	-1.47961000
H	-9.14246000	2.46264200	-0.92339900	C	1.76953500	3.52614500	-2.21073000

C	0.25170600	3.56542900	-2.00364000	H	-4.96516200	3.28301600	1.29004200
C	2.32451300	2.20304100	-2.74613400	H	1.53549600	6.10814600	2.23738800
C	-2.24337600	2.91452900	-0.74235000	H	3.53168300	2.37501700	3.07139400
C	0.08238300	3.31145700	0.92255800	H	2.87404800	-2.58732100	-5.00566500
C	3.46287800	1.54570200	-0.24080700	H	-6.09292200	3.58448500	-0.91866300
C	3.20986300	-0.51409400	-2.30625900	H	1.26009700	4.78982200	4.33593800
C	-2.88520600	3.09549300	-1.98157900	H	5.80335600	3.19029100	2.41362200
C	-0.07645100	2.57455700	2.11096000	H	5.05876200	-3.43017100	-4.13720200
C	4.73702100	2.01540000	-0.60834700	N	-2.42858200	-1.53021200	-0.39066100
C	4.42924200	-1.00713900	-1.81483800	S	-3.26123200	-1.18311200	1.03887600
C	-3.01208900	2.99320900	0.42977500	O	-3.13729000	0.24939600	1.29970800
C	0.65808800	4.58975100	0.98057400	O	-2.84587300	-2.19303700	2.01675300
C	3.04532200	1.68511500	1.08861700	C	-4.96145700	-1.49370300	0.60095000
C	2.65547100	-1.10238700	-3.45692900	C	-5.67193600	-0.49856500	-0.08273300
C	-4.26026200	3.33349800	-2.04401900	C	-6.98636700	-0.75298400	-0.46280500
C	0.33671000	3.10858500	3.33297400	C	-7.60785100	-1.98156200	-0.16779700
C	5.57416500	2.59835000	0.34394600	C	-6.87127800	-2.95369300	0.52616600
C	5.08992900	-2.04768500	-2.47277800	C	-5.55028600	-2.71947700	0.91543700
C	-4.38564700	3.23461700	0.36524300	H	-5.20579200	0.46359000	-0.30109700
C	1.08109600	5.11493200	2.20484800	H	-7.54853300	0.02011600	-0.99332300
C	3.87942800	2.27590500	2.04128000	H	-7.34042900	-3.90926000	0.77297900
C	3.31807700	-2.14335900	-4.11140900	H	-4.98718000	-3.47257300	1.46854000
C	-5.01693900	3.40009700	-0.87022000	C	-9.03429800	-2.22640800	-0.57775400
C	0.92406100	4.37668400	3.38178700	H	-9.34671400	-3.25857800	-0.36414700
C	5.14645800	2.73032700	1.67122700	H	-9.71683100	-1.54540300	-0.04164500
C	4.54093200	-2.61607500	-3.62463300	H	-9.17448100	-2.03629200	-1.65433100
H	2.29441600	3.80079800	-1.28247600	C	-2.12516900	-2.92066200	-0.67715600
H	2.01681500	4.31336900	-2.94102700	H	-2.22733900	-3.11774000	-1.75711800
H	-0.08372600	4.59806500	-1.82375100	H	-2.79831400	-3.60479600	-0.14089300
H	-0.24548400	3.23534800	-2.92660800	C	-0.74297900	-3.04653000	-0.23566900
H	3.37007900	2.33077800	-3.06399800	C	0.42756900	-2.77969000	0.14612000
H	1.76461500	1.86930900	-3.63120100	C	1.60804600	-3.66963500	0.25955200
H	-2.32124400	3.05631900	-2.91321400	C	1.81911000	-4.38263400	1.44974300
H	-0.51042500	1.57341200	2.07551700	C	2.50067700	-3.81180200	-0.80905000
H	5.08226000	1.92319200	-1.64011900	C	2.92564900	-5.22308600	1.57114400
H	4.87157500	-0.58125200	-0.91455800	H	1.12130200	-4.26301600	2.28008400
H	-2.54504100	2.85124600	1.40243100	C	3.60738300	-4.65612100	-0.67964600
H	0.78513500	5.18640900	0.07642100	H	2.33752900	-3.25616800	-1.73233800
H	2.06166800	1.33702700	1.39358700	C	3.82555300	-5.35886400	0.50814900
H	1.69956100	-0.75561300	-3.84973200	H	3.08730600	-5.77163700	2.50222200
H	-4.73905200	3.47143100	-3.01658000	H	4.30219200	-4.75799300	-1.51522800
H	0.21017100	2.52414600	4.24743100	H	4.69397900	-6.01487200	0.60546600
H	6.56415500	2.95478200	0.04901700	C	-2.18291500	-0.51648300	-1.40170900
H	6.03724200	-2.41872300	-2.07480600	H	-2.79954100	-0.77115000	-2.28668000

H	-2.56416300	0.43390100	-1.01300500	H	3.68261800	3.63281100	-1.81195300
C	-0.72495600	-0.35359000	-1.86653800	H	4.04914500	1.81957700	2.09314100
C	-0.74419900	0.32736000	-3.22450300	H	3.09520500	-1.46659000	1.66063000
H	-0.24421400	-1.33955500	-1.96485300	H	-0.52997000	-2.88294900	-2.66685100
H	-1.18929600	-0.34627300	-3.98033800	H	1.42112600	2.64317600	1.73993000
H	-1.35552200	1.23959000	-3.22276300	H	5.16204800	-0.10317400	-1.62064300
H	0.25094700	0.59929000	-3.58929000	H	3.48662000	-3.46902700	-2.14307300
14's				H	1.33153500	-4.01436300	1.07155900
P	2.70282900	1.17002400	-0.42193400	H	3.59754200	6.02276800	-1.19365100
P	1.49737800	-1.79023600	-0.79346400	H	6.29964000	1.37610300	2.98763700
C	2.81762500	-0.35389400	-2.88842500	H	5.26519100	-2.41010500	2.38904400
C	2.79424300	1.05153100	-2.26951300	H	-1.96430000	-4.89449700	-2.55707100
C	1.65127500	-1.29058600	-2.56647900	H	1.37330100	5.03743300	2.37108900
C	2.55515000	2.96847300	-0.07658100	H	7.40991000	-0.51168700	-0.73118100
C	4.41829700	0.86253800	0.17818700	H	5.67755900	-4.37031000	-1.43584800
C	3.14213400	-2.39635100	-0.28159000	H	-0.12881100	-6.01746700	1.18606300
C	0.49903400	-3.31390200	-0.80406600	H	2.46454000	6.73904800	0.90972600
C	3.16413800	3.93068900	-0.89917500	H	8.00345500	0.20029000	1.58786300
C	4.76864700	1.28255600	1.47334500	H	6.57473200	-3.85951200	0.83463000
C	3.65104200	-2.11238200	0.99032600	H	-1.78901300	-6.45900900	-0.62295700
C	-0.42804900	-3.56891600	-1.82543200	Co	0.64961600	0.00318900	0.10270200
C	1.90737600	3.37888500	1.09793200	C	-0.96710900	1.26162800	-1.88019400
C	5.38953900	0.22642400	-0.60949200	C	-0.99637200	2.54828000	-1.12677400
C	3.87604400	-3.21964200	-1.15377000	C	-0.41635600	3.69182600	-1.70766200
C	0.60723600	-4.20441200	0.27685800	C	-1.65344200	2.65842600	0.11283400
C	3.12399400	5.28067300	-0.54628300	C	-0.49955800	4.92205900	-1.06461200
C	6.04745800	1.04280600	1.97805500	H	0.08108300	3.59678400	-2.67398400
C	4.87767000	-2.64347100	1.39523600	C	-1.72998700	3.89380200	0.75735200
C	-1.24368100	-4.70136100	-1.75908600	H	-2.12099200	1.78109900	0.55653300
C	1.88120700	4.72965300	1.45450700	C	-1.15668800	5.02440400	0.16865800
C	6.67059000	-0.00826300	-0.10396200	H	-0.04838900	5.80691300	-1.51746500
C	5.10848600	-3.73632100	-0.75183200	H	-2.24322500	3.97551600	1.71811400
C	-0.21383600	-5.33147100	0.34015200	H	-1.21763400	5.99172300	0.67258700
C	2.48967200	5.68203000	0.63432000	N	-1.86941100	-1.08309000	1.94201300
C	7.00269000	0.38995500	1.19268000	S	-3.25807300	-1.36879900	2.83631000
C	5.61016100	-3.45131200	0.52374000	O	-3.00486300	-0.82971200	4.18090800
C	-1.14395300	-5.57881400	-0.67504000	O	-3.70818400	-2.76313000	2.69586600
H	3.75966700	-0.86610600	-2.65232700	C	-4.42430400	-0.32314500	1.98319200
H	2.81956100	-0.21468600	-3.98146300	C	-4.29163600	1.06498100	2.09900800
H	3.67956000	1.60855200	-2.60985500	C	-5.15658500	1.88622500	1.38349800
H	1.90429600	1.59190100	-2.62591400	C	-6.15439000	1.34253800	0.55159300
H	1.75925500	-2.21721100	-3.14993900	C	-6.27217900	-0.05209700	0.47038200
H	0.69361900	-0.82945700	-2.84848100	C	-5.41292900	-0.89213500	1.18211100
				H	-3.51482000	1.48992900	2.73698000

H	-5.05425800	2.97171900	1.45937800	C	4.33086900	-2.43285600	-1.04901100
H	-7.03805500	-0.49122700	-0.17206400	C	3.09063700	0.29683400	-2.56749900
H	-5.49718300	-1.97689500	1.10882800	C	1.60849800	3.33006700	-1.52318600
C	-7.06258100	2.24998000	-0.23124200	C	-0.98828000	2.52461100	3.01012800
H	-7.72317700	1.68241400	-0.90164700	C	3.61498000	-2.69732100	1.24727200
H	-7.69453200	2.85023700	0.44500600	C	4.77298000	1.54994100	-1.35803400
H	-6.47902600	2.96076200	-0.83824600	C	1.99420900	4.82307100	0.34500300
C	-1.88096900	-1.59734600	0.56940000	C	-1.28388600	4.03158800	1.13432700
H	-2.92314400	-1.68483500	0.24329900	C	4.71831100	-3.77612100	-1.07563100
H	-1.44804400	-2.60711800	0.54471100	C	3.49173900	0.90104100	-3.75981200
C	-1.12957100	-0.60417300	-0.26588100	C	2.09868200	4.29938100	-2.40281600
C	-1.70584100	0.08021400	-1.28427500	C	-2.17276400	3.00142700	3.57422200
C	-3.03722400	-0.17704700	-1.89635400	C	4.00083400	-4.03774000	1.21722000
C	-3.86152500	0.89663400	-2.28910200	C	5.16469300	2.16324700	-2.55146600
C	-3.50399800	-1.48685800	-2.12092700	C	2.48898000	5.78794700	-0.53309500
C	-5.11253400	0.66779700	-2.86377800	C	-2.46957900	4.50095200	1.70090000
H	-3.53084100	1.92448200	-2.12900900	C	4.54681900	-4.58463800	0.05146500
C	-4.75895700	-1.71396100	-2.68822400	C	4.52508900	1.84392700	-3.75228800
H	-2.86888400	-2.33530500	-1.86850800	C	2.54309400	5.52738400	-1.90794900
C	-5.57077400	-0.63817200	-3.06085200	C	-2.92041900	3.98220300	2.91688200
H	-5.73582100	1.51705800	-3.15292000	H	3.88931100	2.70639900	1.12910000
H	-5.09877200	-2.74014000	-2.84948600	H	4.26169700	2.31250800	2.79904800
H	-6.55187000	-0.81640800	-3.50761900	H	5.07007900	0.48651800	1.40297800
C	-0.57761900	-1.11184400	2.60105600	H	3.76308700	-0.07693700	2.44751300
H	-0.73432900	-0.85792700	3.66107400	H	2.08313000	3.22459100	2.89547700
H	-0.14119200	-2.12997900	2.57537700	H	1.83489900	1.48118900	3.07236500
C	0.40133700	-0.12119000	2.00263700	H	4.46942200	-1.82052500	-1.94032400
C	1.63525600	-0.02232000	2.87488400	H	2.28648200	-0.44121700	-2.58583300
H	-0.09563200	0.87514100	1.90902200	H	1.26999500	2.37240300	-1.91283500
H	2.47042800	0.49044800	2.38795800	H	-0.42601100	1.74361600	3.52514800
H	1.39466900	0.54845200	3.79066300	H	3.18338500	-2.29166900	2.16146200
O	-0.40645600	1.17089600	-2.96504700	H	5.29264100	1.80777300	-0.43489200
H	1.97800000	-1.01501700	3.20242000	H	1.94877300	5.03987200	1.41444800
				H	-0.94611300	4.43654700	0.17902700
				H	5.15675300	-4.19092400	-1.98661300
15's				H	2.99152900	0.63949600	-4.69529100
P	3.08932600	-0.17425700	0.16859700	H	2.13863000	4.08791700	-3.47326300
P	0.93221900	2.28970100	0.98784200	H	-2.52179800	2.59167900	4.52501000
C	3.62253600	2.02318100	1.94931600	H	3.86537300	-4.65706000	2.10701400
C	3.98922500	0.57886500	1.59203100	H	5.97547100	2.89548200	-2.54026800
C	2.16860000	2.26136100	2.37067100	H	2.83252200	6.74947500	-0.14406200
C	3.76342500	-1.88238400	0.11150200	H	-3.05246400	5.26359600	1.18018500
C	3.72498500	0.61756000	-1.35299400	H	4.84237100	-5.63608400	0.02347400
C	1.55227600	3.58183700	-0.14626600	H	4.83209000	2.32826600	-4.68226200
C	-0.53904600	3.03131800	1.77787100				

H	2.93198900	6.28528200	-2.59232200	H	-2.62194700	-2.55025100	-1.22510200
H	-3.85964500	4.33479100	3.34869800	C	-0.51372500	-4.68503200	-2.84592300
Co	0.75452500	0.16368600	0.20989600	H	1.62749700	-4.78690000	-2.53328700
C	0.07455200	-1.71520300	1.41833800	H	-2.65124200	-4.35130300	-2.92705000
C	0.27562000	-2.95606200	2.17836100	H	-0.52720300	-5.48326400	-3.59205900
C	0.99810300	-2.89047800	3.38708000	C	-2.25469100	1.57497000	-1.07545600
C	-0.27412600	-4.18752200	1.77335100	H	-3.00871500	1.93170800	-1.78742200
C	1.18973800	-4.03345400	4.15823600	H	-1.46597000	2.34176300	-1.01944500
H	1.40614300	-1.93130900	3.70703100	C	-1.66834400	0.21015800	-1.44573200
C	-0.07559600	-5.33026500	2.54658900	C	-0.64953400	0.24262800	-2.57675500
H	-0.86186400	-4.25336900	0.86022000	H	-2.51763700	-0.42929100	-1.74499800
C	0.66138500	-5.25882300	3.73362700	H	-0.43893000	-0.76229500	-2.96636200
H	1.75461800	-3.97383900	5.09116300	H	-1.00028000	0.86795900	-3.41228900
H	-0.50108600	-6.28238500	2.22225600	O	0.44800700	-0.59456800	1.94560400
H	0.81855900	-6.15864100	4.33331400	H	0.30697700	0.66895100	-2.22942600
N	-2.83137000	1.36614400	0.26219700				
S	-4.47643400	1.56061600	0.45090300	16's			
O	-4.83103000	2.83287600	-0.18784200	Co	-1.61877000	0.43632700	-0.23296200
O	-4.76421100	1.31348600	1.86825500	C	-2.95129300	-0.35166000	0.76424800
C	-5.21402300	0.23540900	-0.49768500	O	-3.03066100	0.78902200	1.23251700
C	-5.46093700	0.41856200	-1.86172600	C	-3.77230000	-1.48270300	1.17728500
C	-5.87933700	-0.66860700	-2.63015600	C	-3.52398500	-2.76664300	0.66450500
C	-6.05895300	-1.93873500	-2.05791800	C	-4.78316300	-1.29319100	2.14098000
C	-5.83111600	-2.08784100	-0.67818000	C	-4.27935300	-3.85105400	1.10608600
C	-5.41505800	-1.01254900	0.10555600	H	-2.74007100	-2.90882500	-0.07561900
H	-5.33416500	1.40344000	-2.31297500	C	-5.53536500	-2.37907400	2.57867100
H	-6.07185700	-0.52807300	-3.69671100	H	-4.95798400	-0.29294200	2.54102200
H	-5.98585200	-3.06356900	-0.21002000	C	-5.28374500	-3.65717800	2.06121500
H	-5.25596000	-1.13230600	1.17790000	H	-4.08698500	-4.84860700	0.70560400
C	-6.51122300	-3.10982700	-2.88727200	H	-6.31786000	-2.23646800	3.32736400
H	-5.90209500	-4.00391500	-2.67880600	H	-5.87583300	-4.50810000	2.40721700
H	-7.55714600	-3.37272600	-2.65319300	H	-2.61109100	0.72312200	-1.23375800
H	-6.45255000	-2.89015200	-3.96302900	P	-0.87679800	2.43581900	-0.99555200
C	-2.21251400	0.19548300	0.91054500	P	-1.13032500	-0.89061500	-1.87602400
H	-2.94810100	-0.61624700	1.04601600	C	0.26023700	1.18935300	-3.32509500
H	-1.82102200	0.45314100	1.89903300	C	-0.36792800	2.47251300	-2.77331500
C	-1.15489800	-0.25684300	-0.08641600	C	-0.72561600	0.01984500	-3.43067700
C	-0.46871600	-1.54506800	0.09247800	C	-2.19621900	3.72035200	-0.95801600
C	-0.47846400	-2.62216800	-0.92785000	C	0.23977100	-2.07515300	-1.60795600
C	0.70969700	-3.27224300	-1.30457800	C	0.44258400	3.23307000	-0.01159900
C	-1.68663700	-3.02659800	-1.52329500	C	-2.51246000	-1.96357100	-2.44742800
C	0.69280200	-4.29468000	-2.25383500	C	-1.85320100	5.08017300	-1.05249100
H	1.65058300	-2.97039900	-0.84555100	C	1.28997100	-2.24765900	-2.52192000
C	-1.70304400	-4.04823800	-2.47579900	C	0.23100300	3.29090500	1.37761900

C	-2.28656400	-3.29028800	-2.84606100	S	4.15790800	1.35784300	-0.14911800
C	-3.54945200	3.35990800	-0.87888300	O	4.87584700	2.38118400	0.61660800
C	0.23226400	-2.82789700	-0.42118100	O	3.63268700	1.64543000	-1.49169000
C	1.60574000	3.79148200	-0.55307500	C	5.23407400	-0.05939100	-0.27702900
C	-3.81799100	-1.44848200	-2.49344900	C	4.92951200	-1.06885300	-1.19637100
C	-2.84887900	6.05844100	-1.07946700	C	5.71835300	-2.21596300	-1.22582200
C	2.31690200	-3.15606800	-2.24757900	C	6.81303300	-2.37087700	-0.35575900
C	1.16501800	3.90837900	2.20801300	C	7.10288100	-1.33289400	0.54450200
C	-3.35270300	-4.09076100	-3.26754100	C	6.32223400	-0.17697400	0.59038500
C	-4.54457100	4.34175400	-0.90584600	H	4.08785300	-0.95545400	-1.87910400
C	1.25981400	-3.73030700	-0.14808400	H	5.48324800	-3.00957900	-1.93921500
C	2.54198200	4.40692600	0.28277100	H	7.95476600	-1.43069000	1.22186100
C	-4.87850800	-2.24654500	-2.92430800	H	6.55043700	0.62572000	1.29249500
C	-4.19725000	5.69137900	-1.00707400	C	7.65729900	-3.61477100	-0.41164000
C	2.30820300	-3.89304800	-1.06064500	H	8.22815200	-3.65605800	-1.35496800
C	2.32527600	4.46724400	1.65973200	H	8.37517700	-3.65470400	0.42005500
C	-4.65004100	-3.57305300	-3.30486100	H	7.03146800	-4.52107100	-0.37651100
H	1.15892100	0.91049300	-2.75408500	C	1.79801400	0.13278900	0.06911300
H	0.61841200	1.41207300	-4.34294200	H	2.10609600	-0.91068700	-0.11590600
H	0.29442000	3.33569400	-2.93324600	H	1.65097100	0.60923700	-0.90167700
H	-1.29689200	2.68734800	-3.32444400	C	0.54069900	0.06425100	0.83151800
H	-0.38242700	-0.72719300	-4.16131300	C	-0.19457400	-0.19913800	1.77801900
H	-1.69696300	0.38374900	-3.80142300	C	-0.93342800	-0.55769300	2.94715800
H	-0.80358600	5.37797000	-1.10068100	C	-1.16896900	-1.91761700	3.23514000
H	1.32201900	-1.67762600	-3.45087300	C	-1.43547200	0.43228700	3.81395500
H	-0.67321100	2.85253400	1.80605300	C	-1.89656600	-2.27621200	4.36794800
H	-1.27995600	-3.70961700	-2.81991500	H	-0.78021200	-2.68288600	2.56278000
H	-3.82719500	2.30951800	-0.78694100	C	-2.16139400	0.06402900	4.94546100
H	-0.57026600	-2.68797200	0.30228200	H	-1.25474800	1.48367700	3.58787700
H	1.80675500	3.73384800	-1.62214800	C	-2.39700800	-1.28762800	5.22210300
H	-4.01324100	-0.42344700	-2.17183500	H	-2.08096700	-3.33127400	4.58170200
H	-2.57030600	7.11252800	-1.15419000	H	-2.54974000	0.83575000	5.61389500
H	3.13016900	-3.28240500	-2.96562500	H	-2.97267600	-1.57086700	6.10648800
H	0.99066500	3.94842700	3.28611900	C	3.11204600	0.49896400	2.17987700
H	-3.16532900	-5.12496700	-3.56646900	H	4.00300400	1.06280600	2.49291200
H	-5.59526400	4.04846300	-0.84081800	H	2.27717100	0.86494500	2.79616200
H	1.24887300	-4.29972000	0.78407100	C	3.30907200	-0.98073300	2.38625600
H	3.45780000	4.81692900	-0.14574700	C	2.58008300	-1.71983500	3.22598900
H	-5.89012100	-1.83454000	-2.94947700	H	4.10301200	-1.45347900	1.79881500
H	-4.97544700	6.45845400	-1.02450600	H	2.76857100	-2.78995700	3.35556500
H	3.11951600	-4.59168800	-0.84388600	H	1.77452700	-1.28110900	3.82317800
H	3.06645800	4.93876100	2.30933100				
H	-5.48304800	-4.20175300	-3.62856900	TS11's			
N	2.83981200	0.87648400	0.78296600	Co	-0.88003100	0.24978200	0.45888200

C	-1.49202900	-0.74517200	2.07976800	H	0.09386300	1.40046300	-3.81907900
O	-1.43168400	0.09376200	2.95690700	H	1.18661700	2.52760500	-1.78833000
C	-2.45154900	-1.87395300	2.08976900	H	-0.25216500	3.33133300	-2.43436200
C	-2.35491800	-2.97031200	1.22265000	H	-1.78710600	-0.01643600	-3.61014500
C	-3.52411900	-1.79741300	2.99870100	H	-2.33565300	1.46218100	-2.81541800
C	-3.32205700	-3.97453400	1.25597500	H	-2.26642000	3.72874100	-2.42269200
H	-1.51974100	-3.04744800	0.53271400	H	0.40987300	-1.74260000	-1.91101500
C	-4.49528500	-2.79526400	3.02022300	H	0.13753700	2.15924300	2.55885100
H	-3.58824300	-0.93988800	3.67032300	H	-4.08593200	-0.52633400	-3.37634500
C	-4.39505900	-3.88661900	2.14795600	H	-2.58079600	2.80077500	1.79215000
H	-3.23792100	-4.82532000	0.57740600	H	-3.79316400	-2.77220600	-1.78830700
H	-5.33346900	-2.72545800	3.71740900	H	0.65412900	4.93958500	-0.71055400
H	-5.15517800	-4.67150600	2.16637800	H	-4.06106100	0.09730400	0.90312900
H	-2.22750200	0.72725000	0.63273000	H	-4.50541700	4.75188300	-2.36029700
P	-0.63257500	2.32441800	-0.25170100	H	0.94219300	-4.02137800	-2.68485200
P	-2.07081900	-0.37647900	-1.25107100	H	1.37831200	3.70799700	4.06367800
C	-0.16761100	1.16436700	-2.77581900	H	-6.54148900	-0.26955500	-3.39369500
C	0.10373000	2.41998500	-1.93285100	H	-4.82250500	3.84893100	1.84879500
C	-1.60717100	0.64252500	-2.74898100	H	-3.24903500	-5.05376200	-2.56364100
C	-2.26058200	3.18750500	-0.31788800	H	1.90598400	6.46832600	0.78568000
C	-1.73366000	-2.08808500	-1.81672600	H	-6.51872000	0.33186500	0.88186000
C	0.32812900	3.44123700	0.82751400	H	-5.80752000	4.81501700	-0.23404500
C	-3.89531300	-0.23172800	-1.22963500	H	-0.88022400	-5.69936700	-3.01131700
C	-2.81065800	3.74764800	-1.47783600	H	2.27298400	5.86011500	3.17624900
C	-0.40055000	-2.45466000	-2.06462400	H	-7.77695800	0.15831300	-1.26791700
C	0.52688900	3.10428200	2.17390300	N	2.84419100	1.17355500	-0.11632300
C	-4.60974700	-0.33305000	-2.43817600	S	3.24783500	0.29090900	-1.48252200
C	-2.99718900	3.23522200	0.87988000	O	3.29860300	1.23800600	-2.60272300
C	-2.75606000	-3.03196100	-1.99890700	O	2.31231500	-0.84616300	-1.51312800
C	0.81718400	4.66076700	0.33264500	C	4.88089300	-0.37299700	-1.24118900
C	-4.59658800	0.00786600	-0.04106200	C	5.04367900	-1.52068200	-0.45712600
C	-4.08399400	4.32871600	-1.44533100	C	6.33301300	-1.98706100	-0.20584800
C	-0.09871900	-3.74726600	-2.49730900	C	7.46052600	-1.33319200	-0.73224800
C	1.22253800	3.97639700	3.01616900	C	7.26180900	-0.19112200	-1.52760000
C	-5.99787000	-0.19276800	-2.44909900	C	5.98125200	0.29445700	-1.78699300
C	-4.26113000	3.82207200	0.91182400	H	4.17800800	-2.04617600	-0.05260300
C	-2.44632600	-4.32455300	-2.42993200	H	6.46728200	-2.88106800	0.40807300
C	1.51842900	5.52458300	1.17659300	H	8.12632700	0.32538900	-1.95208400
C	-5.98740200	0.14396200	-0.05391900	H	5.83231000	1.18006900	-2.40601000
C	-4.81212100	4.36507800	-0.25510500	C	8.84560600	-1.86309700	-0.48217000
C	-1.11917000	-4.68618200	-2.67913600	H	9.15511400	-2.53299400	-1.30361500
C	1.72297800	5.18314000	2.51825200	H	9.58435600	-1.04915400	-0.43093900
C	-6.69006000	0.04668000	-1.25671000	H	8.89315100	-2.44358100	0.45098800
H	0.52341200	0.37195800	-2.46507100	C	2.33908000	0.41935000	1.03105400

H	2.41379200	1.09327400	1.89833200	C	-1.51269500	0.51841800	-3.01598100
H	2.98533900	-0.44334700	1.27581200	C	-2.68835800	2.82557600	-0.19564100
C	0.92638600	-0.02144200	0.94638800	C	-1.66998100	-2.24400700	-2.09771600
C	0.28828900	-1.09388000	1.36424800	C	-0.12176300	3.38152900	0.95308300
C	0.72582100	-2.44947800	1.72658300	C	-3.83659900	-0.42022500	-1.45694100
C	1.52944300	-3.15180300	0.80745600	C	-3.36198600	3.16853800	-1.37422700
C	0.41703600	-3.04684600	2.96133700	C	-0.32583700	-2.60986000	-2.28998900
C	1.99072300	-4.43389400	1.11157400	C	0.15727300	3.01544400	2.27831800
H	1.78101400	-2.68256600	-0.14285100	C	-4.63137600	-0.23617800	-2.60066600
C	0.89111100	-4.32414600	3.26319900	C	-3.36750700	2.91670100	1.03289200
H	-0.18884900	-2.50893500	3.69199000	C	-2.68001100	-3.20180500	-2.26892000
C	1.67070000	-5.02578500	2.33751100	C	0.20903200	4.67047900	0.50277500
H	2.60390500	-4.97192600	0.38428500	C	-4.45203100	-0.54702200	-0.20226200
H	0.64651700	-4.77534900	4.22777000	C	-4.69959800	3.57868800	-1.32864500
H	2.03078300	-6.03001500	2.57366600	C	-0.00275000	-3.91702900	-2.65910900
C	3.65003300	2.37994100	0.16322300	C	0.77101000	3.92907600	3.14059000
H	4.01336000	2.75355200	-0.80522200	C	-6.02143200	-0.17088100	-2.48528200
H	2.96963000	3.14262600	0.56318300	C	-4.69483300	3.33782500	1.07686300
C	4.79371700	2.15154700	1.11372300	C	-2.34829100	-4.51006900	-2.63577800
C	4.90801600	2.77659300	2.28882500	C	0.82822800	5.57567300	1.36695700
H	5.55680700	1.43021400	0.80290200	C	-5.84318400	-0.48787500	-0.09139300
H	5.76018800	2.59718300	2.95146300	C	-5.36868300	3.66230400	-0.10733800
H	4.15503200	3.49784200	2.62416900	C	-1.01216400	-4.87121200	-2.83061100
TS11'_T				C	1.11061900	5.20653400	2.68683300
Co	-0.86778500	0.08174100	0.46163900	C	-6.62918000	-0.29517100	-1.23102900
C	-1.15953000	-0.67116300	2.46572500	H	0.55055900	0.53365800	-2.37794300
O	-1.04192600	0.01726100	3.45519900	H	0.21302700	1.58904600	-3.73382500
C	-2.05649000	-1.85339000	2.35374200	H	0.77998000	2.81496900	-1.66448200
C	-1.93866700	-2.79997500	1.32511300	H	-0.78651900	3.30028500	-2.31818200
C	-3.11210900	-1.95521200	3.27669500	H	-1.42798800	-0.14454700	-3.88855300
C	-2.86571700	-3.83619900	1.21776700	H	-2.32397200	1.23006500	-3.22274700
H	-1.12320400	-2.72936900	0.60564100	H	-2.86298700	3.11150600	-2.34119800
C	-4.04354300	-2.98564400	3.15923000	H	0.47635600	-1.88360200	-2.14183100
H	-3.19825400	-1.21022900	4.06960600	H	-0.10304600	2.01975100	2.64319600
C	-3.92186600	-3.92746500	2.12999000	H	-4.16926000	-0.14664700	-3.58587900
H	-2.76440600	-4.56754100	0.41435400	H	-2.85571200	2.65115500	1.96093900
H	-4.86901400	-3.05609400	3.87147400	H	-3.72574000	-2.93392400	-2.11088100
H	-4.65267900	-4.73471700	2.03962300	H	-0.01429800	4.97492100	-0.52181100
H	-2.08659900	0.56207700	1.22394600	H	-3.83991900	-0.68616300	0.68900500
P	-0.96074600	2.19652400	-0.15813800	H	-5.21719100	3.82852500	-2.25774600
P	-2.01776900	-0.52730100	-1.56073600	H	1.04499000	-4.19084000	-2.80637500
C	-0.18778100	1.24543600	-2.76751200	H	0.98671200	3.63651200	4.17092300
C	-0.24533600	2.46887900	-1.84343900	H	-6.63269100	-0.02319900	-3.37888700
				H	-5.20962000	3.40596200	2.03811500

H	-3.14148400	-5.25040300	-2.76651900	C	4.45511200	2.82076400	0.24300300
H	1.09019000	6.57382500	1.00815400	C	4.46873100	3.66323900	1.27963400
H	-6.31092800	-0.58621500	0.89095900	H	5.34715000	2.23166500	0.00395500
H	-6.41377400	3.97899900	-0.07439500	H	5.36193800	3.79596800	1.89771300
H	-0.75689100	-5.89535900	-3.11350300	H	3.58621900	4.25641700	1.54228900
H	1.59601000	5.91624700	3.36092700				
H	-7.71704400	-0.24105700	-1.14332600				
N	2.69096700	1.24896500	-0.58385100	17-1's			
S	3.20662600	0.14204500	-1.73147500	P	-1.10596900	-1.11516200	-1.61774000
O	3.18565400	0.82995100	-3.02628400	P	-2.43349500	1.74499400	-0.90078400
O	2.38295600	-1.05915900	-1.51082000	C	-2.54573100	0.52968500	-3.46883900
C	4.89432900	-0.29040600	-1.36102700	C	-1.27880800	-0.30289200	-3.27178300
C	5.16420700	-1.24546300	-0.37601700	C	-2.51634700	1.87065100	-2.73606300
C	6.49238600	-1.52077700	-0.04832400	C	0.32319100	-2.22826300	-1.86557700
C	7.55281200	-0.86481800	-0.69379200	C	-2.56316900	-2.21533700	-1.52792600
C	7.24825000	0.07934900	-1.69177000	C	-4.11714300	1.34903800	-0.31839200
C	5.92972100	0.37173500	-2.03073800	C	-2.12403100	3.47942300	-0.39961200
H	4.35312300	-1.77551400	0.12344500	C	1.42028300	-1.81050400	-2.63832400
H	6.70850700	-2.26587400	0.72110900	C	-3.53427500	-2.08937800	-0.52797200
H	8.06143100	0.59028900	-2.21368100	C	-4.27991100	1.06036500	1.04789400
H	5.69972700	1.10083200	-2.80866800	C	-0.84220500	4.00248300	-0.64347900
C	8.98471400	-1.16935400	-0.34874800	C	0.36193700	-3.47983000	-1.23394000
H	9.50171800	-1.63362500	-1.20550300	C	-2.73276100	-3.18022200	-2.53887400
H	9.53680900	-0.24744000	-0.10384000	C	-5.22629700	1.27019600	-1.17225500
H	9.05830800	-1.85595300	0.50657800	C	-3.08401300	4.27371100	0.24232400
C	2.34261500	0.71824400	0.73058800	C	2.53669700	-2.63882500	-2.77673100
H	2.36847400	1.57092400	1.42672300	C	-4.66232000	-2.91486600	-0.53234500
H	3.10457500	0.01360800	1.11035400	C	-5.53186400	0.71123700	1.55277000
C	1.00204300	0.09960400	0.86711100	C	-0.52391900	5.30143900	-0.24816100
C	0.53882900	-0.86773300	1.63001500	C	1.48340300	-4.29952600	-1.36752100
C	1.16034800	-2.07325300	2.20521400	C	-3.85771300	-4.00444700	-2.53818800
C	1.96736200	-2.85091500	1.34973300	C	-6.47793300	0.90457700	-0.66588600
C	0.99849800	-2.46891900	3.54367900	C	-2.76060800	5.57720500	0.63518900
C	2.60106100	-3.99704600	1.83096500	C	2.57189300	-3.88239400	-2.13923100
H	2.08270700	-2.54680900	0.30808800	C	-4.82585400	-3.87241100	-1.53491900
C	1.64053000	-3.61445900	4.01825100	C	-6.63424500	0.62707200	0.69433600
H	0.37942600	-1.87544300	4.21729300	C	-1.48339800	6.09179000	0.39478100
C	2.44004200	-4.38267800	3.16614200	H	-3.43559900	-0.05399700	-3.18445700
H	3.22106400	-4.59360300	1.15709400	H	-2.64631800	0.73592100	-4.54627000
H	1.51219200	-3.90916800	5.06252300	H	-1.23281300	-1.11907000	-4.00893300
H	2.93409500	-5.28220400	3.54117400	H	-0.38609500	0.32438000	-3.42270900
C	3.25197600	2.61346900	-0.63644900	H	-3.37672300	2.50153500	-3.00486300
H	3.48716800	2.82033400	-1.69018300	H	-1.61348400	2.43445200	-3.02022800
H	2.44984900	3.30494600	-0.33997300	H	1.41490100	-0.84003600	-3.13613800
				H	-3.41315900	-1.34682600	0.25823100

H	-3.41901000	1.09458700	1.71868800	H	3.70836300	1.04476600	-2.51854300
H	-0.06944400	3.39532200	-1.12043300	C	8.01964400	-0.48870700	-1.44485000
H	-0.48090300	-3.81504800	-0.62982400	H	7.95311800	-1.03382900	-2.39706200
H	-1.98256300	-3.29373600	-3.32466700	H	8.91538800	0.15316700	-1.47480700
H	-5.12870800	1.48270100	-2.23738200	H	8.18072600	-1.22334400	-0.63805600
H	-4.08205600	3.87948900	0.44166500	C	1.37688400	0.55144700	-0.07590000
H	3.38375800	-2.30679600	-3.38135900	H	2.01042000	0.10409300	-0.85567700
H	-5.41059300	-2.80460000	0.25541500	H	0.61471500	1.13003800	-0.72454800
H	-5.64398300	0.49009600	2.61619200	C	0.64230900	-0.50615000	0.68147900
H	0.48437200	5.68285900	-0.42564800	C	1.10450700	-1.51063400	1.45126500
H	1.50757700	-5.26408100	-0.85638100	C	2.54843400	-1.77031900	1.71014000
H	-3.97896000	-4.75453100	-3.32322700	C	2.97985700	-2.09312300	3.01053400
H	-7.33367800	0.83679700	-1.34177000	C	3.50831500	-1.68492800	0.68886500
H	-3.51327000	6.19138000	1.13567400	C	4.33308500	-2.29698900	3.28426100
H	3.44995900	-4.52451100	-2.23951200	H	2.24601300	-2.17284700	3.81624200
H	-5.70624100	-4.51966700	-1.53688300	C	4.86105400	-1.90036100	0.95950000
H	-7.61327300	0.34151700	1.08649400	H	3.19443900	-1.47942900	-0.33273900
H	-1.23342800	7.10673400	0.71313000	C	5.28059900	-2.19775900	2.25921000
Co	-0.86018000	0.32157400	-0.03858400	H	4.64996200	-2.53597200	4.30257000
C	0.16139200	-2.55935600	1.97590300	H	5.58804700	-1.83616200	0.14809300
C	-1.15248300	-2.16669300	2.56922400	H	6.34025700	-2.35906200	2.47214400
C	-1.33337400	-0.93303800	3.21520900	C	2.22385200	1.56158400	2.13326600
C	-2.20669100	-3.09356000	2.54643200	H	2.55228900	0.57054200	2.47968700
C	-2.55262500	-0.62879200	3.82271400	H	3.03850600	2.25251700	2.39625500
H	-0.51740000	-0.21358000	3.24379800	C	0.98909300	1.97496700	2.87812700
C	-3.43316100	-2.77866300	3.13097900	C	-0.14960200	2.39163800	2.32106900
H	-2.05294300	-4.05580300	2.05470500	H	1.07831400	1.90763600	3.96894000
C	-3.60728200	-1.54689100	3.77342400	H	-1.01781700	2.68069100	2.91822200
H	-2.68198100	0.32849800	4.33325700	H	-0.23720200	2.48424700	1.23663000
H	-4.25643500	-3.49577900	3.09084900	O	0.47858000	-3.73903100	1.91134900
H	-4.56477400	-1.30614900	4.24133900	H	-1.82329500	-0.50779800	0.59665500
N	2.09372300	1.56414800	0.68079800				
S	2.96068900	2.66008800	-0.24116900	17-1'T			
O	3.27089400	3.80926700	0.61262100	P	-0.51986600	-1.78068000	-1.52972300
O	2.20033700	2.83519800	-1.49083700	P	-2.01124000	1.26156100	-1.04735000
C	4.47229300	1.81065700	-0.64664900	C	-1.75120900	-0.16050200	-3.52171500
C	5.54244200	1.85673200	0.25419500	C	-0.57637300	-1.10684400	-3.24645700
C	6.68669000	1.11446900	-0.02245500	C	-1.65322400	1.22568400	-2.86642400
C	6.78241400	0.32470900	-1.18315100	C	1.04873800	-2.73651700	-1.46211400
C	5.69739300	0.30838700	-2.07244700	C	-1.82227300	-3.06732900	-1.47033500
C	4.54135800	1.04782600	-1.81502800	C	-3.75013800	0.68423000	-0.94244700
H	5.48006900	2.47076500	1.15371700	C	-2.17678600	3.05464600	-0.67812400
H	7.52650900	1.14522500	0.67639700	C	1.97095800	-2.77907000	-2.51950000
H	5.75820100	-0.28975400	-2.98473400	C	-2.65315800	-3.12779100	-0.34326100

C	-4.14043200	-0.08686800	0.15925300	Co	-0.41282500	-0.04903800	0.03810900
C	-1.36472300	4.00676000	-1.31449200	C	-0.30971600	-1.47402500	2.68762200
C	1.36522900	-3.38154900	-0.25256000	C	-1.62717100	-0.83501700	3.01015100
C	-1.99764700	-4.00219800	-2.50450000	C	-1.79107000	0.53747000	3.27584100
C	-4.70475200	1.01063900	-1.92137500	C	-2.74088300	-1.68895600	3.13097500
C	-3.07967000	3.47953800	0.31179000	C	-3.04559500	1.04371200	3.62213200
C	3.18704000	-3.45442300	-2.36875500	H	-0.93864600	1.21445300	3.23694600
C	-3.65219000	-4.10077600	-0.24846200	C	-3.98786000	-1.18374100	3.48966700
C	-5.45914900	-0.53414900	0.28434600	H	-2.59952400	-2.75434200	2.94605400
C	-1.47013900	5.35968400	-0.97890800	C	-4.14541700	0.18721700	3.72736700
C	2.57563800	-4.06160400	-0.10973400	H	-3.16018200	2.11162300	3.82105700
C	-2.99703300	-4.97220500	-2.41098000	H	-4.84256100	-1.85764000	3.58073400
C	-6.01927400	0.55743800	-1.80119800	H	-5.12537200	0.58650900	3.99889900
C	-3.17893900	4.83179100	0.64577700	N	1.64339800	2.46741700	0.31359600
C	3.49273100	-4.09726300	-1.16598900	S	1.96366900	1.91016300	-1.22839800
C	-3.82722500	-5.02171400	-1.28403700	O	1.66219100	2.98417400	-2.17727700
C	-6.39882100	-0.21805800	-0.69885700	O	1.21938600	0.62655500	-1.31901700
C	-2.37756000	5.77757200	-0.00197100	C	3.68232100	1.48283600	-1.33619000
H	-2.70524600	-0.64672200	-3.25970400	C	4.63440300	2.50740800	-1.42568800
H	-1.78777300	0.00079300	-4.61109000	C	5.98291400	2.16551500	-1.45548800
H	-0.59226400	-1.94464600	-3.95986900	C	6.39748900	0.82024000	-1.40524200
H	0.37160400	-0.56950200	-3.39054900	C	5.41711300	-0.18119600	-1.33304400
H	-2.34091400	1.92700200	-3.36209400	C	4.05930300	0.13849600	-1.29602700
H	-0.63851600	1.62831000	-2.99582700	H	4.32661500	3.55289500	-1.48016500
H	1.75641000	-2.28112800	-3.46554800	H	6.73384000	2.95653600	-1.52472900
H	-2.51782600	-2.41172200	0.46628800	H	5.71718300	-1.23130000	-1.30793200
H	-3.41090800	-0.33859900	0.92776400	H	3.30375400	-0.64539300	-1.25799300
H	-0.63320800	3.70231000	-2.06243200	C	7.86077700	0.47754200	-1.43873000
H	0.67841500	-3.34134200	0.59657700	H	8.02388400	-0.60756200	-1.37650700
H	-1.34751500	-3.97912200	-3.38235900	H	8.32743800	0.84493100	-2.36777600
H	-4.42728100	1.62256400	-2.78168200	H	8.39466300	0.95774300	-0.60212000
H	-3.71580000	2.75186500	0.82024800	C	1.89636200	1.48372900	1.37515600
H	3.89825000	-3.47479100	-3.19833200	H	1.97162300	2.05120600	2.31357200
H	-4.29555800	-4.13302100	0.63420000	H	2.87421500	0.99769700	1.24111300
H	-5.74626800	-1.13454500	1.14984800	C	0.79481100	0.46980400	1.54172100
H	-0.83320700	6.08993000	-1.48453700	C	0.88247200	-0.63204700	2.33967800
H	2.80883900	-4.55040600	0.83893800	C	2.18142000	-1.12008600	2.87795500
H	-3.12850300	-5.69580100	-3.21928500	C	2.33914300	-1.35227900	4.25467400
H	-6.75241700	0.81160000	-2.57063100	C	3.26315400	-1.37389800	2.01934800
H	-3.88970800	5.14815400	1.41340300	C	3.55898700	-1.80650900	4.76067900
H	4.44396300	-4.62241300	-1.04991900	H	1.50192300	-1.17071100	4.93309900
H	-4.60924400	-5.78196200	-1.21504300	C	4.48118900	-1.83129400	2.52418400
H	-7.42826100	-0.57335000	-0.60844500	H	3.13830500	-1.22848800	0.94703000
H	-2.45724200	6.83588000	0.25810000	C	4.63396900	-2.04548500	3.89783400

H	3.66986500	-1.97760900	5.83425100	H	-3.44972000	-0.31514100	-2.91411300
H	5.30939900	-2.03008700	1.83962700	H	-2.67735200	0.46228200	-4.28527900
H	5.58633800	-2.40508900	4.29498500	H	-1.27527200	-1.39759500	-3.80080100
C	2.00842400	3.85740000	0.61601900	H	-0.40114000	0.02156900	-3.18094100
H	3.05972400	3.91700300	0.95626400	H	-3.36329600	2.23744100	-2.79598600
H	1.94324300	4.43528200	-0.31783800	H	-1.59949500	2.15323500	-2.82001500
C	1.11278500	4.48990100	1.64379700	H	1.24801800	-1.37962100	-3.15149200
C	-0.03690700	4.00034200	2.11188200	H	-3.79159900	-1.17196400	-0.21150600
H	1.48209800	5.45522100	2.00953400	H	-3.63023400	2.64159700	1.79416800
H	-0.62127100	4.55130500	2.85292800	H	0.03979100	2.95372000	0.33389600
H	-0.44856700	3.05243000	1.76103600	H	-0.36098300	-3.83627400	0.02332000
O	-0.18615000	-2.69153900	2.75578400	H	-1.69091400	-4.10859300	-2.57755700
H	-0.25304200	0.80964100	1.15887500	H	-5.00007300	0.60798400	-1.77188000
17's				H	-3.82755000	4.21105100	-1.11729600
P	-1.16820100	-1.42181200	-1.39061800	H	3.28326600	-2.77332200	-3.19100900
P	-2.41876400	1.66029600	-0.64912800	H	-5.86417700	-2.52635800	-0.35740400
C	-2.55727000	0.25697600	-3.20955000	H	-5.92668700	2.54981100	2.71821600
C	-1.29965300	-0.60023500	-3.04232900	H	0.78067800	5.29830300	0.43589300
C	-2.50575500	1.61257900	-2.50190300	H	1.69568300	-5.20646200	0.00204800
C	0.29451100	-2.50696800	-1.55475400	H	-3.74937300	-5.48679900	-2.68533500
C	-2.61067000	-2.53918800	-1.39247700	H	-7.27923700	0.51471500	-0.84117200
C	-4.14700500	1.62136300	-0.04847300	H	-3.10489400	6.57529500	-0.96914100
C	-1.93285300	3.41490500	-0.41265500	H	3.53069600	-4.68879500	-1.61208300
C	1.33089400	-2.21760000	-2.45805000	H	-5.84636200	-4.69881600	-1.58949600
C	-3.78792400	-2.10726800	-0.76834200	H	-7.76247500	1.47405000	1.41161000
C	-4.42712100	2.16780400	1.21596000	H	-0.80023500	7.13959400	-0.19871500
C	-0.64594400	3.74076500	0.03111700	Co	-0.96897800	0.16915200	0.29926700
C	0.43906100	-3.59409300	-0.67603100	C	0.22158100	-2.45586700	2.37629900
C	-2.60193100	-3.76128600	-2.08640300	C	-1.24646000	-2.13755000	2.37285000
C	-5.18565200	1.03289800	-0.78544400	C	-1.71786200	-0.83239900	2.63158700
C	-2.81705100	4.44635500	-0.77572200	C	-2.16881600	-3.18037800	2.21743000
C	2.48622900	-3.00634200	-2.48112600	C	-3.09729800	-0.57898800	2.67719800
C	-4.95215300	-2.87567200	-0.84671200	H	-1.01816300	-0.05387900	2.93231000
C	-5.72096800	2.11774000	1.73600700	C	-3.53902300	-2.92159900	2.27519500
C	-0.23468300	5.07430300	0.10301300	H	-1.79994300	-4.19404400	2.05218300
C	1.59461000	-4.37415900	-0.69777400	C	-4.00719100	-1.61981700	2.49127300
C	-3.76189400	-4.53519900	-2.14851100	H	-3.45124400	0.42754900	2.89654300
C	-6.47990200	0.97805900	-0.25798100	H	-4.24949500	-3.73896200	2.13691000
C	-2.41009200	5.77881400	-0.69170100	H	-5.08026500	-1.41927900	2.52160400
C	2.62277800	-4.08147700	-1.60019400	H	-0.89547500	1.27692900	1.25656000
C	-4.93959900	-4.09160900	-1.53373300	N	2.03516700	1.49666500	0.47570400
C	-6.75014400	1.51602900	1.00281100	S	2.74536000	2.47193400	-0.70326000
C	-1.11670000	6.09524800	-0.25700900	O	3.00225600	3.77725100	-0.09209300
				O	1.88683600	2.33757100	-1.88912400

C	4.30059800	1.68107400	-1.04282500	C	-2.00410400	-1.37489900	-3.10467300
C	5.42048700	2.01470700	-0.27295500	C	-1.93357500	1.22928500	-3.16212900
C	6.61005700	1.32241400	-0.48299700	C	-1.46086400	-3.54371600	-1.25058800
C	6.70067400	0.30392200	-1.44902000	C	-3.58702000	-1.69136700	-0.70845100
C	5.56314700	0.00468900	-2.21579600	C	-3.18833100	2.24818000	-0.68022900
C	4.36107400	0.68619300	-2.02199900	C	-0.62153400	3.21302800	-1.58023900
H	5.36096300	2.81121200	0.46996800	C	-0.97138700	-4.24291400	-2.36319600
H	7.48967900	1.57674900	0.11378800	C	-3.89692700	-0.83039800	0.35113200
H	5.62059100	-0.77372000	-2.98031100	C	-3.20228700	2.54072800	0.69506800
H	3.48456100	0.45626700	-2.62849200	C	0.71148300	3.09150400	-2.00480600
C	7.98726200	-0.45155800	-1.63413600	C	-1.60701200	-4.21366100	-0.02287400
H	7.93094400	-1.14759600	-2.48304700	C	-4.60810000	-2.45040800	-1.30319000
H	8.83038800	0.23755900	-1.80334000	C	-4.36614700	2.39969700	-1.42517800
H	8.22818700	-1.03398100	-0.72857700	C	-1.15487900	4.48837100	-1.33602700
C	1.24223000	0.41223900	-0.00819300	C	-0.64209200	-5.59842200	-2.25180200
H	1.71462300	-0.12001800	-0.84903100	C	-5.21062700	-0.71346600	0.81238000
H	0.33506500	0.89999100	-0.62696400	C	-4.37222200	2.98270500	1.31214400
C	0.64436200	-0.53349000	0.93917900	C	1.49632900	4.22957700	-2.19690300
C	1.15500000	-1.48190900	1.75077100	C	-1.28395700	-5.56582000	0.08041600
C	2.61630400	-1.69564200	1.93742800	C	-5.92106000	-2.33421900	-0.84403100
C	3.13566000	-1.93946900	3.22268900	C	-5.54274300	2.82493200	-0.79991900
C	3.51210300	-1.60936200	0.85912200	C	-0.36228000	5.62500900	-1.52241800
C	4.51047600	-2.07612500	3.42134800	C	-0.80015900	-6.26253700	-1.03337100
H	2.45585700	-2.01243800	4.07306700	C	-6.22405400	-1.46427300	0.21184300
C	4.88691000	-1.75217200	1.05693200	C	-5.54842000	3.11837700	0.56586800
H	3.13714300	-1.44810600	-0.15021200	C	0.96086600	5.49820200	-1.95557300
C	5.39267600	-1.98066200	2.33949300	H	-3.69481000	-0.03101500	-2.92568900
H	4.89568200	-2.25642800	4.42815500	H	-2.94126800	-0.07193600	-4.51227700
H	5.56152900	-1.68227100	0.20183200	H	-2.54988500	-2.20748200	-3.57414700
H	6.46897000	-2.08678000	2.49632800	H	-0.98485000	-1.37571600	-3.52477800
C	2.36420600	1.72390700	1.89383500	H	-2.43325900	2.09065800	-3.63219900
H	2.48377700	0.73965500	2.36359500	H	-0.93169300	1.16570200	-3.61810400
H	3.34628100	2.21301500	1.93441200	H	-0.83864200	-3.74179900	-3.32326500
C	1.34857900	2.54274900	2.64104300	H	-3.10359400	-0.24102300	0.81131200
C	1.59507000	3.75254700	3.14764700	H	-2.29250000	2.42408700	1.28955800
H	0.35858900	2.09002300	2.76072800	H	1.15355500	2.10796000	-2.17537200
H	0.82914700	4.30864000	3.69659300	H	-1.94649100	-3.66622000	0.85858600
H	2.57170500	4.23353700	3.02740300	H	-4.37581400	-3.13453600	-2.12316200
O	0.60581200	-3.52577800	2.82692700	H	-4.38034100	2.18889300	-2.49498000
				H	-2.18809700	4.59966800	-1.00393100
				H	-0.26199100	-6.13518500	-3.12461900
17'_T				H	-5.43966100	-0.03204100	1.63419500
P	-1.85396000	-1.75575100	-1.29808600	H	-4.36763300	3.21163600	2.37960900
P	-1.60800800	1.67665100	-1.39803500	H	2.53751400	4.11405700	-2.49967300
C	-2.71832500	-0.05880900	-3.43319800				

H	-1.39705600	-6.07579900	1.03998300	C	0.30270100	-1.16398800	1.55629700
H	-6.71377200	-2.92493000	-1.30964500	C	0.92383800	-2.49920900	1.31175900
H	-6.45799300	2.92977600	-1.38723200	C	1.13098400	-3.37770000	2.38919800
H	-0.78481400	6.61435700	-1.32993400	C	1.37588200	-2.88885600	0.04064800
H	-0.54157100	-7.32082800	-0.94818400	C	1.78326000	-4.59812700	2.20118000
H	-7.25376700	-1.37536300	0.56666600	H	0.78203700	-3.10354700	3.38619000
H	-6.46864900	3.45244900	1.05096400	C	2.03513100	-4.10255500	-0.14892700
H	1.57894000	6.38831000	-2.09592100	H	1.18336400	-2.24435300	-0.81740400
Co	-0.67850400	-0.07568600	-0.12608500	C	2.24147100	-4.96437600	0.93231900
C	-0.87914500	-1.13134700	2.48398000	H	1.93300500	-5.26653800	3.05258900
C	-1.19274600	0.10616700	3.27519700	H	2.36526000	-4.38754000	-1.15029200
C	-0.20303900	0.94201000	3.82283700	H	2.74622100	-5.92198800	0.78400900
C	-2.54457500	0.38178600	3.54715300	C	3.06712700	2.25407500	1.37915000
C	-0.56265400	2.05344600	4.58829100	H	2.91782100	1.65603900	2.29302200
H	0.85251000	0.71048400	3.67827900	H	4.11902000	2.57654500	1.38732500
C	-2.90210600	1.49584200	4.30491500	C	2.15491200	3.44811500	1.38715000
H	-3.30775100	-0.29214600	3.15737000	C	2.57176700	4.71518100	1.37957400
C	-1.91186700	2.34084300	4.81888100	H	1.08088900	3.22737700	1.39326300
H	0.21519200	2.69278700	5.01215400	H	1.86439700	5.54911200	1.39545500
H	-3.95631500	1.70511500	4.49921400	H	3.63796600	4.96390200	1.34691700
H	-2.19116900	3.21543400	5.41136100	O	-1.61268400	-2.10724500	2.58958700
H	0.59713600	0.95982700	1.52322100				
N	2.80501200	1.35682100	0.23669200	TS12's			
S	3.83664400	1.47138900	-1.08409800	P	-1.53686300	1.27909800	1.26571000
O	4.23909400	2.87740500	-1.18629700	P	-2.74355300	-1.53242100	0.18937500
O	3.15201900	0.80322700	-2.20324700	C	-2.97527700	-0.68803400	2.87067900
C	5.27890600	0.50525900	-0.67857200	C	-1.91562600	0.41605400	2.86514800
C	6.36779400	1.13228600	-0.06124800	C	-2.66177800	-1.90281700	1.99446000
C	7.46336500	0.36110800	0.32040400	C	-0.25569900	2.45640200	1.86085300
C	7.49154200	-1.02749500	0.09701500	C	-2.98404700	2.33895900	0.89848300
C	6.38758200	-1.62604000	-0.53128200	C	-4.45441900	-0.93593500	-0.08084900
C	5.28182200	-0.87110900	-0.92372300	C	-2.75937000	-3.18015500	-0.61091100
H	6.35857300	2.21085900	0.10114100	C	0.86611400	1.94798300	2.53685600
H	8.31898200	0.84585100	0.79771300	C	-3.02323400	3.01639100	-0.33283400
H	6.39501100	-2.70206900	-0.72134500	C	-4.71371500	0.17960300	-0.88766400
H	4.43772900	-1.34562100	-1.42526800	C	-1.96464800	-4.22390400	-0.10952000
C	8.68801500	-1.83971900	0.51089900	C	-0.37024500	3.84066500	1.67733800
H	8.52130200	-2.91490300	0.35376300	C	-4.04443600	2.49683700	1.80300900
H	9.57967700	-1.54383400	-0.06728400	C	-5.53059700	-1.61580200	0.51800900
H	8.92798100	-1.67624500	1.57409300	C	-3.49018700	-3.37920800	-1.79497500
C	2.32553600	0.00805700	0.51905900	C	1.83896800	2.80924500	3.04482600
H	3.01329200	-0.52189600	1.20795600	C	-4.10940400	3.83211500	-0.65235000
H	2.34316800	-0.54924000	-0.42187500	C	-6.02602800	0.61861800	-1.08670600
C	0.94112100	0.00263900	1.12031900	C	-1.89538800	-5.44235800	-0.78853800

C	0.61407300	4.70156600	2.17381200	H	4.91598100	3.92189800	-3.78731800
C	-5.13896200	3.30049800	1.46995500	H	2.30062900	6.99966600	-2.26131300
C	-6.83874400	-1.17147000	0.32435000	H	4.33807600	6.33500800	-3.53843500
C	-3.41852400	-4.60094400	-2.46856800	N	1.30592200	-2.02987800	-0.71663400
C	1.71509300	4.19073000	2.86533900	S	1.66959600	-3.51189800	0.04388900
C	-5.17542700	3.96797600	0.24352800	O	1.52171500	-4.54190500	-0.98969300
C	-7.08874300	-0.05115800	-0.47725000	O	0.89482700	-3.61059800	1.29616300
C	-2.61896200	-5.63399300	-1.96908300	C	3.38405000	-3.35584300	0.47762500
H	-3.96108400	-0.28224600	2.59857000	C	4.34910700	-3.65273600	-0.49020700
H	-3.06890700	-1.04063900	3.91041300	C	5.69434800	-3.56024000	-0.14457200
H	-2.16341600	1.19332800	3.60362000	C	6.09016700	-3.16665800	1.14722200
H	-0.94935400	-0.00747500	3.18080700	C	5.09546500	-2.87873400	2.09477700
H	-3.35922000	-2.72424100	2.21398100	C	3.74161100	-2.97762700	1.77303400
H	-1.64470100	-2.27594800	2.19435400	H	4.04802800	-3.96320000	-1.49188800
H	0.99388500	0.87107100	2.66651700	H	6.45658100	-3.79640500	-0.89113900
H	-2.18861500	2.91353000	-1.02703100	H	5.38489400	-2.57941700	3.10487600
H	-3.89611000	0.72428300	-1.35496700	H	2.97200400	-2.77792100	2.51934700
H	-1.35770600	-4.08509400	0.78456000	C	7.54694300	-3.02104500	1.48729600
H	-1.22674000	4.25684700	1.14729100	H	7.71985300	-3.10002500	2.57046400
H	-4.03612400	1.99747500	2.77154000	H	8.15795900	-3.77881700	0.97394900
H	-5.34969600	-2.49876100	1.13505500	H	7.91633500	-2.03144000	1.16470800
H	-4.12611500	-2.58334700	-2.18834700	C	0.98663500	-0.96181900	0.24466700
H	2.70577600	2.39794700	3.56658500	H	1.70759800	-0.94493600	1.07531100
H	-4.12624400	4.35951800	-1.60922100	H	0.01154400	-1.24498200	0.77862300
H	-6.21217800	1.49371200	-1.71260800	C	0.79824100	0.39536900	-0.36404700
H	-1.25721500	-6.23782200	-0.39758100	C	1.69287200	1.37464700	-0.63334800
H	0.51246000	5.77880000	2.02136800	C	3.13372400	1.26134800	-0.27858700
H	-5.96565600	3.40392700	2.17679200	C	3.78466700	2.31653400	0.38904300
H	-7.66727500	-1.70268100	0.79890500	C	3.87737100	0.10874800	-0.58785100
H	-3.99182900	-4.74572400	-3.38744600	C	5.13314600	2.22356500	0.73378200
H	2.48056800	4.86570600	3.25560300	H	3.22605800	3.21771400	0.63894900
H	-6.03253700	4.59495700	-0.01387400	C	5.23075000	0.02009500	-0.25014000
H	-8.11384800	0.29671000	-0.62606000	H	3.39546000	-0.71732800	-1.11230700
H	-2.55984000	-6.58684400	-2.50046100	C	5.86450300	1.07448700	0.41273200
Co	-0.97691300	-0.14885700	-0.37532200	H	5.61607900	3.05473000	1.25410100
C	1.15456600	2.59712900	-1.29559500	H	5.79037700	-0.87909600	-0.51109900
C	2.08970900	3.60706700	-1.89457900	H	6.92307300	1.00325600	0.67502100
C	3.23698700	3.23966600	-2.61568700	C	0.35539700	-2.15933700	-1.85953200
C	1.74921900	4.96566300	-1.79048600	H	0.90948800	-2.59176200	-2.70576600
C	4.03246900	4.21740600	-3.21626900	H	-0.47937300	-2.82961000	-1.62093300
H	3.50407100	2.18754000	-2.71954700	C	-0.13077200	-0.78712400	-2.21300500
C	2.56143800	5.94353600	-2.36553800	C	-1.45307800	-0.34715100	-2.43346300
H	0.84592400	5.24322800	-1.24408400	H	0.64875200	-0.13140800	-2.60069500
C	3.70463600	5.57052800	-3.08152000	H	-1.57557800	0.51053500	-3.10531100

H	-2.27130800	-1.06774300	-2.48797800	H	-0.35689400	-3.80857100	-0.06029300
O	-0.05293000	2.79878900	-1.39739900	H	-1.78929800	-4.15227200	-2.18207700
H	-1.79155400	0.61971700	-1.33573900	H	-4.90711200	1.72933600	-1.98759100
18's				H	-3.78357200	4.03765100	0.88597300
P	-1.19359500	-1.31637100	-1.37454600	H	2.95439900	-2.88580700	-3.65253600
P	-2.31382300	1.75881700	-0.44678400	H	-6.04048100	-2.01670800	-0.71304200
C	-2.50789900	0.53734700	-3.09273000	H	-5.97557000	1.30902600	2.85605200
C	-1.33454700	-0.43386500	-2.99428500	H	0.58571500	5.74780400	-0.78162800
C	-2.30779800	1.82768700	-2.30158700	H	1.56229600	-5.32339900	-0.37376800
C	0.19660300	-2.47279100	-1.67480900	H	-3.89478000	-5.43556000	-2.24745400
C	-2.70429200	-2.35586400	-1.37362600	H	-7.24708600	1.51476600	-1.26415900
C	-4.08367800	1.61729100	0.02284400	H	-3.17983600	6.40782500	1.23161900
C	-1.94148400	3.54020100	-0.14656800	H	3.23130400	-4.88199000	-2.17998000
C	1.14473200	-2.22506200	-2.68179600	H	-6.03839700	-4.38316000	-1.52259100
C	-3.91469100	-1.77272200	-0.96661200	H	-7.80788300	1.29533000	1.15760200
C	-4.41009500	1.50317300	1.38541800	H	-0.99354500	7.28609000	0.41038000
C	-0.72076500	4.04611200	-0.62184800	Co	-0.76617300	0.17061800	0.41087700
C	0.36494300	-3.59748600	-0.84795100	C	0.69431800	-2.48633600	2.28711400
C	-2.71128200	-3.67956000	-1.84328500	C	-0.81599800	-2.51146500	2.20687500
C	-5.12092200	1.63185200	-0.92357500	C	-1.67146500	-1.42040400	1.94207100
C	-2.82557100	4.40412800	0.51592200	C	-1.40401700	-3.76361300	2.45054800
C	2.22792100	-3.09189200	-2.86297100	C	-3.05980100	-1.58487800	1.96148800
C	-5.10953800	-2.49152100	-1.03120900	H	-1.29817800	-0.36896800	2.01541400
C	-5.74124000	1.39456400	1.79247400	C	-2.78848300	-3.93438900	2.42372200
C	-0.38006700	5.38511800	-0.42360200	H	-0.74646100	-4.60784900	2.66089500
C	1.44681700	-4.45805100	-1.03026300	C	-3.62326200	-2.83997900	2.18826100
C	-3.90540400	-4.40412200	-1.88711800	H	-3.70077600	-0.72278100	1.79508800
C	-6.45208400	1.51116000	-0.51472200	H	-3.21595900	-4.92483500	2.59608900
C	-2.48293900	5.74568400	0.71203300	H	-4.70794400	-2.96105600	2.17704900
C	2.38181400	-4.20953400	-2.04072800	N	1.88372400	1.60943900	0.51843800
C	-5.10682900	-3.81349500	-1.48350200	S	2.73582500	2.65109600	-0.52651600
C	-6.76625500	1.38934600	0.84167800	O	2.83545100	3.93477300	0.17496100
C	-1.25978400	6.23875500	0.24896500	O	2.12231000	2.59621600	-1.86881000
H	-3.44980100	0.04064500	-2.81753800	C	4.33765700	1.89481900	-0.62029000
H	-2.61586800	0.81935000	-4.15229000	C	5.12573500	1.84806200	0.53595500
H	-1.40682300	-1.21176600	-3.76941000	C	6.39654500	1.29283200	0.45386600
H	-0.39239000	0.11316000	-3.15490200	C	6.89575500	0.78907700	-0.76279500
H	-3.05248100	2.58415000	-2.58910500	C	6.08347300	0.86038200	-1.90326400
H	-1.32667100	2.25634700	-2.55669300	C	4.80205200	1.41314300	-1.84326300
H	1.05260300	-1.35820100	-3.33573500	H	4.74630200	2.23400800	1.48356600
H	-3.93378500	-0.75128300	-0.59556500	H	7.01695000	1.24009800	1.35146100
H	-3.62114900	1.50996200	2.13627800	H	6.45669200	0.47649700	-2.85562000
H	-0.01731500	3.40096000	-1.14937800	H	4.17150200	1.47392300	-2.73102000
				C	8.25849500	0.15781800	-0.81425600

H	8.56164900	-0.07152700	-1.84568500	C	-0.15302900	-3.97248300	-1.28319000
H	9.01898700	0.81517100	-0.36321900	C	-3.13124700	-2.87839800	-2.44521100
H	8.26773200	-0.78327900	-0.23802000	C	-5.05398400	1.39224400	-1.27162400
C	1.28008500	0.48400300	-0.14514600	C	-3.08180600	4.35090300	0.40245700
H	1.80883900	0.18446800	-1.06060500	C	2.35235700	-3.33003700	-2.34583200
H	0.26795700	0.90050000	-0.66397100	C	-4.88585000	-2.38461900	-0.32004600
C	0.86628100	-0.62122900	0.70663400	C	-5.75600100	0.86825100	1.38583900
C	1.48325700	-1.53449500	1.46943500	C	-0.69498800	5.57370700	-0.39691100
C	2.96829500	-1.66195400	1.48718100	C	0.79224600	-4.97758200	-1.50840900
C	3.68358700	-1.67625900	2.69685400	C	-4.42166500	-3.40650000	-2.46741100
C	3.67967600	-1.77118900	0.28181500	C	-6.37353300	1.06667200	-0.94477900
C	5.07474100	-1.80266700	2.69505400	C	-2.85389600	5.70127500	0.68563500
H	3.14661700	-1.59146400	3.64240600	C	2.04198200	-4.66110100	-2.04542200
C	5.06866900	-1.90846000	0.28085800	C	-5.30193800	-3.15642400	-1.40604400
H	3.13312300	-1.77454700	-0.66068000	C	-6.72700500	0.80270700	0.38095300
C	5.77124600	-1.92625600	1.48865300	C	-1.66072600	6.31401000	0.29238000
H	5.61807600	-1.80853600	3.64344900	H	-3.14383100	-0.00652700	-3.04987700
H	5.60225700	-2.00177500	-0.66713000	H	-2.18666100	0.76444100	-4.30710000
H	6.85872300	-2.03236400	1.49058100	H	-0.98281000	-1.21310200	-3.74846200
C	1.03371000	2.25820600	1.53941200	H	-0.06118400	0.11915600	-3.03037700
H	1.66520900	2.53768700	2.39858800	H	-2.90167900	2.53251900	-2.84713900
H	0.61138700	3.18740300	1.13770500	H	-1.16647400	2.32370900	-2.64813100
C	-0.08502500	1.34386200	2.01878600	H	1.67749800	-1.28851600	-2.34442400
C	-1.10342200	2.11174900	2.84255400	H	-3.27156800	-1.25456600	0.55381400
H	0.35295000	0.57908100	2.67292000	H	-3.68748500	1.22482300	1.85303400
H	-1.84025600	1.43705500	3.30386100	H	-0.13696900	3.66899800	-1.20800400
H	-0.59231500	2.62999400	3.67605500	H	-1.13058700	-4.23335500	-0.87730000
O	1.24858300	-3.32591600	2.98526900	H	-2.45053900	-3.07353000	-3.27681700
H	-1.63732600	2.88083300	2.27075100	H	-4.80005400	1.59792500	-2.31183200
18'_T				H	-4.01563800	3.88439900	0.71995000
P	-1.06825700	-1.29846900	-1.34057200	H	3.33309700	-3.07249300	-2.75209000
P	-2.31902200	1.80926800	-0.62986300	H	-5.56532700	-2.18804400	0.51104200
C	-2.19175000	0.51431000	-3.23400400	H	-6.02448900	0.66711700	2.42557500
C	-1.01615700	-0.42814200	-2.97771900	H	0.24795800	6.03505800	-0.69970700
C	-2.13732400	1.83528800	-2.47151000	H	0.54601300	-6.01331800	-1.26323200
C	0.14897500	-2.63895300	-1.59133200	H	-4.74525300	-4.01342700	-3.31635400
C	-2.70952000	-2.09549100	-1.35485900	H	-7.12789400	1.01874500	-1.73352300
C	-4.07216200	1.44419900	-0.27137900	H	-3.61557500	6.27520000	1.21900800
C	-2.11259700	3.60246900	-0.28130000	H	2.77833100	-5.44849600	-2.22232200
C	1.41599500	-2.32288700	-2.11412600	H	-6.31440800	-3.56669700	-1.42944800
C	-3.59203700	-1.85684100	-0.29501100	H	-7.75876000	0.54556700	0.63195700
C	-4.43586100	1.18146000	1.06098600	H	-1.48313800	7.36708300	0.52333900
C	-0.91841200	4.22645500	-0.68593100	Co	-0.79207700	0.23695000	0.55693200
				C	0.63079600	-2.74382800	1.88017500

C	-0.80950600	-2.54430700	2.25936500	H	6.84347600	-2.34980100	1.62829300
C	-1.24494300	-1.44570900	3.01653400	C	0.98383000	2.38029100	1.45374500
C	-1.71338900	-3.58489800	1.98403500	H	1.41246400	3.00608100	2.25311800
C	-2.57011500	-1.37786800	3.46419800	H	0.43614900	3.05899100	0.78498300
H	-0.53109900	-0.68593400	3.32338300	C	0.02369200	1.38207800	2.05111900
C	-3.03353400	-3.51201800	2.42258900	C	-1.15590600	2.05112800	2.74380400
H	-1.35912300	-4.45480100	1.43077500	H	0.56078900	0.76229900	2.77843500
C	-3.46797700	-2.40355300	3.15897200	H	-1.88163400	1.31902400	3.12566600
H	-2.89267500	-0.53090400	4.07419000	H	-0.78948200	2.61422800	3.62310000
H	-3.72952400	-4.32031700	2.18855900	O	1.08475400	-3.87823400	1.95495700
H	-4.50261500	-2.34694600	3.50529500	H	-1.68161900	2.76921800	2.10246800
N	2.11652000	1.73092700	0.74852500				
S	2.89103100	2.85595900	-0.26814300	19's			
O	3.08925600	4.06929000	0.53316600	P	0.00471900	-0.99608800	-1.43549800
O	2.15632100	2.96975400	-1.54759400	P	-1.55270500	1.87647300	-1.06680500
C	4.45051700	2.07166600	-0.59115300	C	-0.60527300	0.86040400	-3.54512300
C	5.42462300	2.07328400	0.41206300	C	0.47661600	-0.03880200	-2.95755500
C	6.63740300	1.43591200	0.16786700	C	-0.81560900	2.13377000	-2.73196500
C	6.88925700	0.79335800	-1.05848100	C	1.48330900	-2.08852700	-1.33376500
C	5.89486200	0.82289400	-2.04901300	C	-1.34506300	-2.03233300	-2.13838300
C	4.67448600	1.46144100	-1.82609600	C	-3.35174500	1.66346500	-1.34430800
H	5.23087700	2.56342500	1.36750800	C	-1.40818400	3.56496600	-0.34384100
H	7.40582100	1.42891500	0.94469700	C	2.75725300	-1.49981200	-1.43673900
H	6.07929100	0.33911000	-3.01125700	C	-2.68003300	-1.74150000	-1.82327800
H	3.90326300	1.48921700	-2.59679100	C	-4.15425300	1.34214700	-0.23684400
C	8.18778100	0.07044400	-1.28483500	C	-0.16148700	4.21283900	-0.39576900
H	8.34790600	-0.15153200	-2.34969000	C	1.39469400	-3.48059000	-1.19821900
H	9.04274500	0.65736500	-0.91463500	C	-1.07956100	-3.00772700	-3.11671900
H	8.19233500	-0.88774200	-0.73680500	C	-3.95010800	1.78695500	-2.60768700
C	1.83863500	0.47262300	0.03345100	C	-2.48476500	4.20815100	0.28644600
H	2.79896100	0.01701900	-0.24381500	C	3.91078300	-2.28344600	-1.37348500
H	1.29672600	0.68781200	-0.91129500	C	-3.72976200	-2.42871200	-2.43910900
C	0.99337400	-0.48781200	0.83002100	C	-5.53174100	1.17104600	-0.38380600
C	1.48803100	-1.61756100	1.39753200	C	0.00396600	5.47680000	0.17389600
C	2.96578500	-1.84948400	1.45005100	C	2.54887700	-4.26399700	-1.14534500
C	3.78406400	-0.91246300	2.10536800	C	-2.12732200	-3.70039600	-3.72573700
C	3.57267300	-2.97193300	0.85934700	C	-5.32631900	1.59440000	-2.75619900
C	5.16822200	-1.09052300	2.17188700	C	-2.31351500	5.47221800	0.85763300
H	3.32817000	-0.03150500	2.56111000	C	3.81059000	-3.66953900	-1.22523400
C	4.95732300	-3.14431600	0.91795100	C	-3.45496800	-3.41807200	-3.38502400
H	2.95537700	-3.70501700	0.34725300	C	-6.12063900	1.29215000	-1.64619400
C	5.76086500	-2.20816500	1.57780000	C	-1.07055600	6.10993900	0.80463300
H	5.78424300	-0.35115700	2.68834500	H	-1.54967500	0.30771300	-3.67427200
H	5.41159300	-4.01868400	0.44428800	H	-0.28366700	1.15628000	-4.55669500

H	0.77183700	-0.81025100	-3.68421900	C	7.18107200	0.34451500	-0.23327600
H	1.36547900	0.55464500	-2.70935100	C	6.43008100	0.61157400	-1.38880900
H	-1.44238300	2.86479400	-3.26361700	C	5.15478900	1.17324500	-1.30812000
H	0.15506500	2.61615600	-2.55355400	H	4.93030900	1.48231400	2.09212900
H	2.85692500	-0.42245100	-1.56032700	H	7.19506300	0.46865300	1.92824100
H	-2.91141500	-0.95253600	-1.11344400	H	6.84729300	0.37045600	-2.36937600
H	-3.70398600	1.21623900	0.74966800	H	4.57383800	1.36828400	-2.21032000
H	0.69843000	3.73076700	-0.86006800	C	8.54485400	-0.28395400	-0.31569700
H	0.42457400	-3.96399400	-1.12875000	H	8.88029100	-0.39008400	-1.35706600
H	-0.05374400	-3.22835100	-3.41424000	H	9.29008500	0.31656500	0.23074600
H	-3.35271300	2.03166900	-3.48599700	H	8.54040700	-1.28559100	0.14657800
H	-3.46456400	3.73223100	0.33195600	C	2.06520000	0.15334500	1.44198500
H	4.88805100	-1.80168900	-1.44317400	H	2.65958600	-0.32011300	2.24141100
H	-4.76184100	-2.17919700	-2.18272600	H	2.33296500	-0.34620000	0.50883300
H	-6.14205900	0.92853600	0.48845900	C	0.59290400	0.09908200	1.77858000
H	0.98523100	5.95460200	0.13398900	C	-0.23068900	-1.05768200	1.87127600
H	2.45543500	-5.34608300	-1.03193700	C	0.22610500	-2.48212500	1.70243400
H	-1.90446100	-4.46130300	-4.47749400	C	1.46324700	-2.90555200	2.21967600
H	-5.77908900	1.68601500	-3.74630200	C	-0.65812900	-3.46793600	1.22615700
H	-3.16115300	5.96165000	1.34342400	C	1.80946400	-4.25786700	2.24216600
H	4.71274500	-4.28410500	-1.17651600	H	2.15486200	-2.17788100	2.64035900
H	-4.27185900	-3.96107100	-3.86622700	C	-0.32274000	-4.82196600	1.26864500
H	-7.19710400	1.14790400	-1.76517900	H	-1.62118900	-3.17655000	0.81182800
H	-0.94037500	7.09749800	1.25371400	C	0.91464800	-5.22515600	1.77639800
Co	-0.76821600	0.16784600	0.32730700	H	2.78070000	-4.55750300	2.64360100
C	-1.21788300	-1.09769500	3.05397500	H	-1.03161900	-5.56343800	0.89188400
C	-2.67865400	-1.29627400	2.83186000	H	1.18063000	-6.28442600	1.80852900
C	-3.52755000	-1.41613200	3.94697000	C	1.34720200	2.37569400	2.10971700
C	-3.22538600	-1.37328600	1.54569900	H	1.78336600	3.00836700	2.89587500
C	-4.89379100	-1.61916900	3.76802300	H	0.81808000	3.03066300	1.40735400
H	-3.09240500	-1.35163500	4.94569200	C	0.38751200	1.32636200	2.68196300
C	-4.59000900	-1.59406900	1.36161700	C	-1.01442200	1.90016100	2.89454500
H	-2.56375800	-1.28993300	0.68234800	H	0.76801900	1.00687500	3.66880300
C	-5.42644400	-1.71561400	2.47441100	H	-1.63046100	1.28698700	3.56110500
H	-5.55071300	-1.71069300	4.63615900	H	-0.93852500	2.89972600	3.35007000
H	-4.99874800	-1.66489200	0.35295800	O	-0.76224000	-1.02647600	4.18251400
H	-6.49689300	-1.88652400	2.33620700	H	-1.55777900	2.04006900	1.94605400
N	2.39152700	1.59080400	1.42210600				
S	3.02995600	2.25518100	0.04233400	19'T			
O	3.16135600	3.69592900	0.30314500	P	-0.02044900	-1.25659000	-1.49617800
O	2.27771000	1.86866700	-1.17812800	P	-1.60781600	1.81878300	-1.06689200
C	4.62596900	1.47237100	-0.05114200	C	-0.73619000	0.63896700	-3.53439700
C	5.35706800	1.23612400	1.11872100	C	0.37727400	-0.28523500	-3.03811000
C	6.62372100	0.66782400	1.01790700	C	-0.87115900	1.95051700	-2.75548100

C	1.48759500	-2.30312100	-1.39332000	H	-5.82664200	1.45580600	-3.74319400
C	-1.37064400	-2.31323700	-2.15504500	H	-3.39231400	5.91230300	1.18783900
C	-3.39615300	1.51257400	-1.34296100	H	4.81448900	-4.32996900	-1.06124500
C	-1.55810600	3.57148500	-0.49644900	H	-4.38501500	-4.19850600	-3.77341700
C	2.73416800	-1.64849300	-1.41427200	H	-7.21589300	0.82260000	-1.76971300
C	-2.68984100	-1.98926800	-1.80335300	H	-1.27585100	7.20740300	0.90916500
C	-4.18468100	1.14789000	-0.23968900	Co	-0.57574600	0.18335800	0.33851800
C	-0.37266900	4.31066100	-0.65632200	C	-1.10978700	-0.96998800	3.30713100
C	1.46235600	-3.69672900	-1.24547500	C	-2.54047800	-1.24809800	2.99770100
C	-1.15244900	-3.31255600	-3.11991200	C	-3.45005700	-1.31106600	4.06986900
C	-4.00313000	1.62572700	-2.60411500	C	-3.00911800	-1.45776800	1.69340400
C	-2.64195300	4.16472500	0.17083300	C	-4.79518000	-1.58520500	3.83756100
C	3.92189900	-2.37053300	-1.29273000	H	-3.07613500	-1.14511200	5.08138400
C	-3.77124600	-2.65982000	-2.38231200	C	-4.35299600	-1.75239200	1.46032600
C	-5.55290100	0.91146700	-0.38782500	H	-2.32067600	-1.43701800	0.84731200
C	-0.27357000	5.61014200	-0.15382700	C	-5.24819000	-1.81326300	2.53109300
C	2.65374300	-4.41918700	-1.13218500	H	-5.49569600	-1.63052100	4.67463200
C	-2.23176600	-3.99139100	-3.68914700	H	-4.69982600	-1.93045600	0.44190600
C	-5.36886500	1.37147200	-2.75465300	H	-6.30144600	-2.04014800	2.34893200
C	-2.53888700	5.46530000	0.67192400	N	2.29438500	1.83094500	1.36504900
C	3.88582300	-3.76188100	-1.15489300	S	2.83501500	2.37154200	-0.11097700
C	-3.54327500	-3.66903100	-3.32052000	O	2.91401000	3.83516200	-0.01378100
C	-6.14754300	1.01712500	-1.64857000	O	2.02634200	1.81644400	-1.22638800
C	-1.35489200	6.19192100	0.51352700	C	4.45517900	1.64372800	-0.20832200
H	-1.69774700	0.10241800	-3.57636400	C	5.26314900	1.58480200	0.93312000
H	-0.49975200	0.90746900	-4.57693500	C	6.54265800	1.04791100	0.82412300
H	0.62454300	-1.02956900	-3.81042600	C	7.03623700	0.58270400	-0.40906900
H	1.28297400	0.30001400	-2.83076000	C	6.20881600	0.67659800	-1.53924500
H	-1.46356300	2.68611600	-3.31963500	C	4.91919400	1.20275500	-1.44894600
H	0.12514200	2.38844100	-2.60615600	H	4.88633400	1.94112900	1.89286000
H	2.78079600	-0.56435900	-1.51840300	H	7.17474400	0.98639800	1.71370800
H	-2.88023700	-1.18568200	-1.09350500	H	6.57606100	0.32499700	-2.50618800
H	-3.72899300	1.04354500	0.74627900	H	4.27770000	1.26033100	-2.32895700
H	0.49554900	3.87204200	-1.14651500	C	8.41357000	-0.01444700	-0.49778400
H	0.51332200	-4.22909400	-1.21177800	H	8.70323100	-0.21241500	-1.53947600
H	-0.13821100	-3.55814600	-3.43940400	H	9.16462000	0.65397200	-0.04690400
H	-3.41943800	1.91315400	-3.47886800	H	8.45941500	-0.96732700	0.05659800
H	-3.57521500	3.61609400	0.30310900	C	2.07926800	0.38309500	1.52528200
H	4.87541500	-1.83824400	-1.30520600	H	2.80585800	0.00149700	2.26021200
H	-4.79100700	-2.38435800	-2.10360400	H	2.24005800	-0.17219400	0.59326000
H	-6.15022600	0.63257200	0.48276300	C	0.66501200	0.26349500	2.05342900
H	0.66215600	6.16018100	-0.27687700	C	-0.03360200	-0.92762600	2.21964700
H	2.61289800	-5.50440100	-1.01439800	C	0.52061200	-2.30934600	2.01764000
H	-2.04837400	-4.77041300	-4.43326900	C	1.82408300	-2.62146200	2.44565000

C	-0.29532500	-3.37008300	1.57796500	C	-6.57954700	1.22607000	0.25387300
C	2.29490100	-3.93623500	2.42555800	C	-2.87253200	5.66281400	1.63192500
H	2.47017800	-1.84009600	2.84160200	C	0.82597400	-4.33629400	-3.19447300
C	0.16893100	-4.68489600	1.57495800	C	-5.86499800	-2.87337100	-0.68605600
H	-1.30883400	-3.17598100	1.23481000	C	-6.63593200	0.74374000	1.56341100
C	1.46694700	-4.97693700	1.99954300	C	-1.67621900	6.28387700	1.26389800
H	3.31313400	-4.14624200	2.76161500	H	-4.05041200	0.67982200	-2.65661900
H	-0.48956400	-5.48479400	1.22792000	H	-3.24655000	1.54672400	-3.95916100
H	1.83246300	-6.00636700	1.99361100	H	-2.18903000	-0.61157100	-3.82919200
C	1.20025300	2.60931500	1.98152000	H	-1.02663500	0.57364900	-3.22726900
H	1.59985200	3.40645000	2.62317200	H	-3.57294100	3.10693400	-2.10793400
H	0.56959600	3.07906500	1.21533800	H	-1.84892900	2.81636400	-2.34076400
C	0.37589000	1.58260600	2.77293300	H	0.68903600	-0.93676600	-3.09863900
C	-1.07346900	2.04425900	2.91886300	H	-3.18210000	-1.62798600	1.00384100
H	0.81578900	1.47112800	3.78048600	H	-3.32750600	0.92270900	2.35297100
H	-1.63219800	1.46241400	3.66082100	H	-0.30155600	3.78524800	-0.59323900
H	-1.09785800	3.09571000	3.24403200	H	-1.87746100	-3.83576600	-1.17792700
O	-0.73426700	-0.81751300	4.45654700	H	-3.84746500	-1.91298900	-3.25421700
H	-1.60272800	1.98885600	1.95513600	H	-5.33932600	2.00086800	-1.32083400
TS14's				H	-4.09461500	3.88866600	1.49255000
P	-1.73879700	-0.88387700	-1.44946300	H	2.03276100	-2.76657500	-4.06865600
P	-2.54570100	1.97965400	-0.23342700	H	-5.39236000	-2.66993200	1.41545700
C	-3.09760600	1.15007900	-2.94163500	H	-5.49974100	0.27512100	3.34590600
C	-1.99450500	0.09460200	-3.00941500	H	0.18772900	6.06981100	0.17458800
C	-2.79105400	2.33587900	-2.02983400	H	-0.53081100	-5.66797400	-2.16246700
C	-0.70533000	-2.25901100	-2.08642400	H	-6.04488600	-2.95282200	-2.84254600
C	-3.36749600	-1.67053900	-1.14628100	H	-7.49112400	1.30110200	-0.34359400
C	-4.17530400	1.50918000	0.44705300	H	-3.59176800	6.18897800	2.26446100
C	-2.24269000	3.67987900	0.38555800	H	1.42073600	-5.14473700	-3.62578300
C	0.40827700	-1.97176000	-2.89352800	H	-6.83937900	-3.33454700	-0.50684200
C	-3.81401800	-1.90364800	0.16136900	H	-7.59243300	0.43805300	1.99406500
C	-4.23981200	1.02134100	1.76346200	H	-1.45510000	7.29623600	1.61072500
C	-1.04017100	4.30843900	0.01836700	Co	-0.95779400	0.47611300	0.17587600
C	-1.02660000	-3.59708400	-1.81653600	C	0.34303000	-2.63059900	1.42246500
C	-4.17958400	-2.06319300	-2.22551600	C	1.01778900	-3.33637900	2.55287600
C	-5.35688700	1.61671900	-0.30096100	C	2.29212900	-2.96003700	3.01062500
C	-3.15793500	4.36368400	1.19668400	C	0.32148000	-4.36226100	3.21517600
C	1.16667800	-3.00426900	-3.44663900	C	2.86006400	-3.60250100	4.11176100
C	-5.05606700	-2.50120700	0.39008900	H	2.83792900	-2.15780400	2.51308800
C	-5.46339000	0.65091800	2.32070900	C	0.89743100	-5.01453700	4.30356400
C	-0.75908200	5.60280900	0.45515800	H	-0.67275500	-4.63623900	2.85756400
C	-0.26652300	-4.62891800	-2.37384200	C	2.16801600	-4.63459000	4.75398200
C	-5.42137600	-2.65741800	-1.99520300	H	3.84738500	-3.29960100	4.46800900
				H	0.35709000	-5.81993300	4.80673900

H	2.61880200	-5.14387800	5.60938500	H	-1.90154200	-0.22069600	0.95932100
N	2.16129600	1.34221500	0.37919400				
S	2.63194800	2.89394500	-0.03794800	20's			
O	2.43500800	3.77387100	1.12068400	P	1.85333200	1.04882300	-1.70658400
O	1.96320400	3.18139800	-1.31813200	P	1.72502800	-2.19789800	-1.14370000
C	4.37698300	2.73745100	-0.34002000	C	2.89761900	-0.91983100	-3.46443300
C	5.28229800	3.07758600	0.66528800	C	2.08962600	0.37653100	-3.42230000
C	6.64565100	2.87595500	0.43925900	C	2.14621900	-2.14260500	-2.94016500
C	7.11112700	2.34068600	-0.77144700	C	1.14133200	2.70578000	-2.05947300
C	6.17029700	2.01536900	-1.76759600	C	3.58201200	1.41004300	-1.21102400
C	4.80725300	2.21036100	-1.56360400	C	3.27130500	-2.51733300	-0.22611000
H	4.92619400	3.49702900	1.60721700	C	0.78273300	-3.76869800	-1.07083000
H	7.36160500	3.14249500	1.22038800	C	0.22185000	2.87573300	-3.10873900
H	6.51678900	1.60715600	-2.72057000	C	4.13113900	0.83126600	-0.06037600
H	4.08515400	1.96510200	-2.34406700	C	3.24049300	-2.48167500	1.17987000
C	8.57915700	2.12412300	-1.01686700	C	-0.51561400	-3.78973300	-1.60906100
H	8.78364300	1.07347900	-1.28077900	C	1.51460700	3.82148000	-1.29177400
H	8.92919800	2.73986300	-1.86227000	C	4.38792400	2.23454800	-2.01568500
H	9.18030500	2.38216400	-0.13347800	C	4.48178500	-2.79034300	-0.87951300
C	1.34402700	0.56361300	-0.54231200	C	1.30431200	-4.92925900	-0.48286100
H	1.89588400	0.17589600	-1.40778100	C	-0.28520600	4.14382300	-3.40626000
H	0.53689200	1.21505300	-0.98953400	C	5.46670300	1.06345300	0.28109900
C	0.72826400	-0.50738100	0.31466100	C	4.40291600	-2.70970500	1.91585000
C	1.17143100	-1.78254700	0.49372600	C	-1.28516600	-4.95107700	-1.54746000
C	2.38169100	-2.37473400	-0.10325500	C	1.00707500	5.08552500	-1.59443700
C	2.42947600	-3.76252900	-0.34003900	C	5.72036400	2.46829000	-1.67304900
C	3.52581000	-1.60816600	-0.41388700	C	5.64702100	-3.00841200	-0.13742200
C	3.56176700	-4.35965400	-0.89201600	C	0.53307000	-6.09521400	-0.43259400
H	1.55958100	-4.37692200	-0.10659500	C	0.11296200	5.25284600	-2.65577700
C	4.65527700	-2.20682500	-0.97164700	C	6.26350600	1.88049400	-0.52396200
H	3.55551000	-0.54374000	-0.18386100	C	5.61151400	-2.96614300	1.25814900
C	4.67812200	-3.58404000	-1.21877800	C	-0.76172800	-6.10711000	-0.95795600
H	3.56816900	-5.43658600	-1.07617300	H	3.85283600	-0.78881400	-2.93294100
H	5.52977400	-1.59266200	-1.20080200	H	3.15961300	-1.12320300	-4.51530000
H	5.56539900	-4.05093700	-1.65314300	H	2.57690000	1.15562600	-4.02730400
C	1.96464200	0.93231800	1.77344400	H	1.08979500	0.20752500	-3.85251900
H	2.65389600	0.11363700	2.02965000	H	2.69363700	-3.07292500	-3.15738500
H	2.14529300	1.78387800	2.44095700	H	1.17321700	-2.23441000	-3.45075600
C	0.50920500	0.45658000	1.88085200	H	-0.09739900	2.02470000	-3.71348600
C	-0.47000500	1.51320300	1.79700400	H	3.51385100	0.19765300	0.57216400
H	0.33456100	-0.31714200	2.63272100	H	2.30649500	-2.26867300	1.70163300
H	-1.27452500	1.52412400	2.53688700	H	-0.94965800	-2.89074600	-2.05209200
H	-0.08572500	2.50860400	1.55595100	H	2.19833100	3.69578900	-0.45369500
O	-0.86909600	-2.70201900	1.27735400	H	3.97278900	2.70233900	-2.91130300

H	4.53382800	-2.83497000	-1.96729500	H	-9.76240300	1.13732900	-0.06359700
H	2.30969400	-4.92809600	-0.05885500	C	-2.72627700	0.62967700	0.84242100
H	-0.99211600	4.26258300	-4.23120300	H	-3.31326800	1.44641100	1.29442100
H	5.88142200	0.60206200	1.18033100	H	-2.78322600	0.75109000	-0.24619400
H	4.36581300	-2.68000300	3.00725500	C	-1.29629000	0.64355100	1.36766600
H	-2.30294500	-4.94452100	-1.94376000	C	-0.52217600	1.75571000	1.47134600
H	1.30683200	5.94451400	-0.98978900	C	-0.98219000	3.11257100	1.06934900
H	6.33793800	3.11191000	-2.30434100	C	-0.68210800	4.20607700	1.90607500
H	6.58630300	-3.21073200	-0.65729700	C	-1.74281400	3.35221300	-0.08670700
H	0.94687800	-6.99585800	0.02744700	C	-1.15457200	5.48494800	1.61184100
H	-0.28335800	6.24399400	-2.88844200	H	-0.08360800	4.05173000	2.80661800
H	7.30757900	2.06325700	-0.25776200	C	-2.21778200	4.63114600	-0.38027800
H	6.52437300	-3.13412300	1.83457000	H	-1.93846000	2.54248200	-0.78735000
H	-1.36604200	-7.01592000	-0.90450200	C	-1.93241500	5.70198800	0.47007000
Co	0.66296800	-0.45267800	-0.40699400	H	-0.91580700	6.31612900	2.27983600
C	0.87710800	1.72040900	2.04792000	H	-2.79943300	4.79329100	-1.29002200
C	1.13223200	1.09204000	3.37586100	H	-2.30184100	6.70365600	0.23764600
C	0.14609800	1.04945300	4.37459800	C	-2.38088900	-1.27632300	2.24006700
C	2.41666100	0.59069800	3.64390800	H	-2.68558500	-0.89265200	3.22807300
C	0.44024600	0.50181500	5.62414900	H	-2.46586200	-2.36835100	2.24208500
H	-0.84942400	1.44908900	4.17122400	C	-0.98200500	-0.76861200	1.84935500
C	2.70049000	0.02068400	4.88439900	C	-0.37685700	-1.60688100	0.72932900
H	3.17826000	0.64727200	2.86469400	H	-0.30990000	-0.76261100	2.71119400
C	1.71282700	-0.02272500	5.87626100	H	0.07914900	-2.51676800	1.14309300
H	-0.32550600	0.47969500	6.40302100	O	1.78958500	2.26203300	1.44364100
H	3.69507900	-0.38521400	5.08388600	H	1.64580300	-0.39546100	0.60246200
H	1.93735400	-0.46336500	6.85072900	H	-1.15078600	-1.92584200	0.01279000
N	-3.26842000	-0.68376900	1.22363100	TS15's			
S	-3.83021700	-1.65104300	-0.03717300	P	2.76922200	0.14500500	-1.21227200
O	-3.87744700	-3.02662900	0.47461400	P	1.31276000	-2.58013600	-0.60025900
O	-3.09833900	-1.38547500	-1.29561700	C	2.82200600	-2.13096800	-2.98098700
C	-5.48700000	-1.03883900	-0.26028000	C	2.90266500	-0.60538200	-2.89506300
C	-6.38365000	-1.10284600	0.81341400	C	1.53053500	-2.74245000	-2.43376800
C	-7.68614000	-0.65251600	0.62830900	C	2.75552900	1.93013400	-1.63332200
C	-8.11253700	-0.14173000	-0.61388500	C	4.37592000	-0.09945500	-0.37480300
C	-7.19128300	-0.09717200	-1.67009400	C	2.80843000	-3.37464900	0.10094600
C	-5.87804600	-0.54501600	-1.50366600	C	-0.02874900	-3.78109100	-0.25986600
H	-6.06163700	-1.49304600	1.78060900	C	1.52420100	2.51591300	-1.96436600
H	-8.39223100	-0.69488700	1.46176000	C	4.49447800	0.37744500	0.94363000
H	-7.50420900	0.29394100	-2.64124700	C	3.41751800	-2.82162800	1.23581100
H	-5.16278300	-0.51127100	-2.32615700	C	-1.22953500	-3.67993100	-0.98103200
C	-9.52682700	0.33991800	-0.78768700	C	3.91465100	2.72003300	-1.63326000
H	-9.70092800	0.73096800	-1.80021300	C	5.46068000	-0.75991700	-0.96675200
H	-10.24393700	-0.47798400	-0.60606400				

C	3.35992200	-4.52821400	-0.48229400	C	2.39826800	3.72246800	1.51921600
C	0.08438300	-4.74230700	0.75568700	C	0.91096600	5.26466700	3.32355100
C	1.44509800	3.87360100	-2.27789000	H	-0.74135400	3.95140900	2.85776900
C	5.68411600	0.20411600	1.65012800	C	2.99307800	4.80426500	2.16474000
C	4.56346000	-3.40699900	1.78004900	H	2.96465500	3.11599600	0.81412900
C	-2.29525000	-4.53423400	-0.69882800	C	2.25184100	5.57372000	3.06983300
C	3.83510100	4.07979100	-1.94972200	H	0.33791000	5.85617400	4.04102700
C	6.64575700	-0.94882800	-0.24753100	H	4.03866400	5.04834500	1.96377500
C	4.50841100	-5.10850400	0.05884400	H	2.72234900	6.41657800	3.58194100
C	-0.98500600	-5.59930800	1.03302900	N	-3.66674300	-0.12839400	1.51908500
C	2.60244600	4.65932800	-2.26570500	S	-4.11361700	-1.33916700	0.42711000
C	6.76107900	-0.46664100	1.05807500	O	-4.08549900	-2.59841100	1.18128000
C	5.11325500	-4.54754600	1.18979700	O	-3.36719500	-1.23502300	-0.84422300
C	-2.17424700	-5.49879600	0.30576900	C	-5.80181800	-0.89350100	0.07787500
H	3.68843000	-2.58788600	-2.47973700	C	-6.73709500	-0.91577200	1.11971600
H	2.90392000	-2.40818100	-4.04467300	C	-8.06077800	-0.59359200	0.84051700
H	3.82508900	-0.23218000	-3.36610700	C	-8.46945100	-0.25255600	-0.46428900
H	2.06292500	-0.15417500	-3.44919000	C	-7.50903900	-0.24677300	-1.48598500
H	1.47887200	-3.81228500	-2.68483400	C	-6.17407400	-0.56757000	-1.22515500
H	0.64948000	-2.26348600	-2.89158300	H	-6.42802100	-1.17706600	2.13345200
H	0.61556000	1.91116700	-1.96122000	H	-8.79808400	-0.60557600	1.64756000
H	3.64776200	0.87879000	1.41670900	H	-7.80812300	0.01212400	-2.50461500
H	2.99449700	-1.92249500	1.68363700	H	-5.42806300	-0.56580100	-2.02066600
H	-1.35244400	-2.91167100	-1.74640500	C	-9.90635700	0.09682400	-0.73913800
H	4.87904000	2.27988800	-1.37358700	H	-10.07512600	0.31187800	-1.80394400
H	5.39404800	-1.13764400	-1.98749200	H	-10.57484100	-0.72829500	-0.44273500
H	2.89149500	-4.98039100	-1.35896300	H	-10.21324100	0.98140800	-0.15630900
H	1.00671600	-4.82317600	1.33344700	C	-3.26380500	1.14627100	0.91310400
H	0.47639700	4.31734400	-2.51545000	H	-3.76381600	1.97957400	1.43656700
H	5.76787400	0.58257500	2.67181400	H	-3.56228200	1.20003400	-0.13960800
H	5.03173200	-2.96252600	2.66089500	C	-1.76392600	1.23883900	1.12883200
H	-3.23164700	-4.42793000	-1.24954100	C	-0.98795900	2.24815100	0.67748000
H	4.74156000	4.69009000	-1.94152500	C	-1.48224900	3.27160100	-0.29630200
H	7.48154800	-1.47557900	-0.71415500	C	-1.45564600	4.65858100	-0.07824900
H	4.93315800	-6.00302800	-0.40321400	C	-1.96376100	2.80214400	-1.53447600
H	-0.88711600	-6.34649400	1.82467400	C	-1.90381000	5.54440400	-1.06264100
H	2.54207300	5.72494700	-2.49951400	H	-1.08717600	5.05976000	0.86348700
H	7.68818300	-0.61535500	1.61692200	C	-2.41128800	3.68590700	-2.51675000
H	6.01401900	-5.00207000	1.60965800	H	-1.97381800	1.72765800	-1.72962900
H	-3.01248300	-6.16240300	0.53149000	C	-2.38154100	5.06502200	-2.28459400
Co	1.01569200	-0.52532500	0.13143900	H	-1.87682900	6.61932000	-0.86811700
C	0.43637500	2.24725300	1.09537400	H	-2.77580900	3.29583200	-3.47018800
C	1.04423700	3.42428100	1.75004500	H	-2.72674200	5.76077400	-3.05308600
C	0.30269500	4.19991700	2.65778600	C	-2.65985500	-0.45355500	2.54472200

H	-2.93035900	0.09752600	3.45986200	H	-2.32799300	-3.97168400	2.08802800
H	-2.66685100	-1.52603400	2.76788900	H	-0.69303400	-3.28031100	2.06552600
C	-1.31830000	0.05885400	1.97175000	H	1.44845200	0.21841500	1.25299900
C	-0.64183600	-1.00650600	1.09294400	H	-2.63805900	2.45275600	0.24684200
H	-0.64485700	0.36744300	2.78587800	H	-3.76945700	-0.11007800	-0.33272800
H	-0.75442100	-1.99032700	1.56857500	H	0.38952600	-3.85620900	0.04143400
O	1.14145200	1.23690200	0.94297100	H	-1.17912100	2.93398600	3.34438700
H	0.96539300	-1.11605600	1.44061600	H	-3.46302000	0.44127800	3.98364200
H	-1.15860600	-1.08123400	0.11698800	H	-4.32139400	-4.21472400	0.87536400
21's				H	-3.49752100	-3.79015900	-1.85573800
P	-1.37603200	0.37131100	1.77935000	H	3.41629900	1.52701000	2.02930700
P	-2.05864900	-2.32494400	0.32741200	H	-4.70091500	3.79691400	0.51895400
C	-2.14677500	-2.06293600	3.12934000	H	-6.24239400	0.22034900	-0.34885500
C	-1.25447000	-0.82332400	3.18918300	H	1.11803200	-5.62882300	-1.50213600
C	-1.76421500	-3.02988500	2.00915000	H	0.78586000	4.24372500	4.10843500
C	0.00709200	1.48907300	2.24771700	H	-5.54125400	1.74446400	4.22288300
C	-2.89280000	1.35858500	2.09788200	H	-6.78062700	-3.89019500	0.86319400
C	-3.88544800	-2.17911800	0.26121100	H	-2.75446100	-5.56584400	-3.41761800
C	-1.62276800	-3.72731900	-0.77003800	H	3.08883800	3.54179600	3.46210400
C	1.30567000	1.10163800	1.87894700	H	-6.17988000	3.43129500	2.50030600
C	-3.26370300	2.30884600	1.12910500	H	-7.75044200	-1.67497000	0.25603500
C	-4.43836900	-0.93746500	-0.08664200	H	-0.44921700	-6.50388500	-3.24758300
C	-0.32137100	-4.25390900	-0.68511600	Co	-1.17837500	-0.41196100	-0.22717800
C	-0.17380200	2.62425000	3.05141700	C	-0.34114500	1.97964000	-1.77246600
C	-3.72190200	1.16847600	3.21330100	C	-0.87028100	2.95102800	-2.73810500
C	-4.73795700	-3.24177400	0.60386500	C	-0.00824300	3.68960800	-3.57148800
C	-2.49068100	-4.20179000	-1.76446400	C	-2.26486600	3.12649400	-2.85195800
C	2.40941000	1.83385100	2.32186000	C	-0.53273500	4.59084700	-4.49639400
C	-4.43078200	3.05837600	1.27791500	H	1.07118700	3.55434400	-3.49434700
C	-5.82374300	-0.75470300	-0.08827800	C	-2.78240700	4.03111100	-3.77414500
C	0.09692500	-5.24780700	-1.57055600	H	-2.92792800	2.54461000	-2.21025200
C	0.93382900	3.35763600	3.48607600	C	-1.91752200	4.76545000	-4.59684000
C	-4.90106000	1.90937200	3.35272500	H	0.13962500	5.16078500	-5.14133900
C	-6.12240300	-3.05961300	0.59647600	H	-3.86300600	4.16752300	-3.85737200
C	-2.06916500	-5.20092000	-2.64838300	H	-2.32597800	5.47524600	-5.32027400
C	2.22578200	2.96267100	3.12557800	N	3.23417000	-1.15738800	-1.82038200
C	-5.25837400	2.85474200	2.38862300	S	3.06729800	-2.18943000	-0.49120600
C	-6.66668400	-1.81573200	0.25345300	O	3.05453700	-3.55145200	-1.04052600
C	-0.77774500	-5.72733200	-2.55238300	O	1.95887200	-1.79603700	0.40762100
H	-3.20637900	-1.77532600	3.03470100	C	4.58867300	-1.86928900	0.36971800
H	-2.05703300	-2.59408200	4.09102000	C	5.80131300	-2.18934000	-0.25221500
H	-1.41811100	-0.25769800	4.11909500	C	6.98824600	-1.94053300	0.42888300
H	-0.19566200	-1.12825600	3.19270300	C	6.98430100	-1.38048400	1.72185200
				C	5.75081300	-1.07941600	2.31850700

C	4.54746100	-1.32243500	1.65202600	H	-0.05191700	0.06813000	1.68461900
H	5.81118700	-2.61925300	-1.25538500	C	-0.69971700	-0.08157100	-0.39679700
H	7.94137900	-2.18342000	-0.04786600	H	1.04893700	0.82480200	0.49596800
H	5.72832800	-0.64758900	3.32188700	H	0.85082200	-3.02700900	-0.70605700
H	3.58979000	-1.08832500	2.11742700	C	-0.69127100	-1.46781300	-1.00889100
C	8.28130400	-1.12293400	2.43818100	H	1.41791000	-1.55389600	-1.55770400
H	8.11855500	-0.62699600	3.40558400	C	4.28267400	-1.09554300	-0.83808100
H	8.81916700	-2.06804600	2.62280200	C	3.90161400	0.78193300	0.66453700
H	8.94824900	-0.48995400	1.83019100	C	-1.54365900	0.89295000	-0.78570300
C	3.15743800	0.28513900	-1.54912300	C	-1.71247000	-2.42805200	-0.32701600
H	3.88496700	0.77331900	-2.21771300	H	-0.91880000	-1.42720200	-2.08374300
H	3.44389800	0.53266400	-0.51787200	C	5.11856100	-0.29046400	-1.61398500
C	1.73142200	0.68155600	-1.88762900	H	4.11402500	-2.14117900	-1.09915700
C	1.12794100	1.83788200	-1.53137400	C	4.73823700	1.57017300	-0.12301500
C	1.75205100	3.00848600	-0.86572900	H	3.43763700	1.18415400	1.56602900
C	0.95165500	3.86237600	-0.08076900	C	-1.73061200	2.24808800	-0.25770400
C	3.11080400	3.34018400	-1.02627000	H	-2.20573100	0.64805000	-1.62189900
C	1.48954800	4.99158500	0.53231300	H	-1.45161300	-2.52382300	0.73210200
H	-0.10266300	3.63214100	0.07546600	H	-1.59780900	-3.41222500	-0.80649100
C	3.65068300	4.46775800	-0.40452700	C	5.35726800	1.05083200	-1.27435400
H	3.75264600	2.74065900	-1.66880800	H	5.60002000	-0.71451600	-2.49874400
C	2.84448800	5.29845500	0.37829000	H	4.92069500	2.60955700	0.16273500
H	0.84774200	5.62826800	1.14473500	C	-2.58168500	3.12158000	-0.96986900
H	4.70808000	4.70444800	-0.54621500	C	-1.13850800	2.73402200	0.92841800
H	3.26850000	6.18142300	0.86236800	O	-2.17831800	-0.95818600	2.20478000
C	2.32825100	-1.38630900	-2.95631300	C	-3.13668700	-1.96790400	-0.49768100
H	2.87479500	-1.09974100	-3.86768400	C	6.26331800	1.91775600	-2.10633800
H	2.05966700	-2.44605300	-3.03531600	C	-2.81710700	4.42464900	-0.53326900
C	1.11753100	-0.44571100	-2.72619800	H	-3.06281700	2.75991200	-1.88248400
C	-0.04551500	-1.21058800	-2.07513700	C	-1.37634900	4.03860900	1.36521400
H	0.77780400	-0.03810200	-3.69082500	H	-0.50361900	2.09080500	1.53363400
H	-0.15505600	-2.20873400	-2.51503100	C	-3.22859100	-0.62430500	1.69207800
O	-1.13446200	1.27475200	-1.11746500	C	-3.79597800	-1.09721400	0.40924100
H	0.18469600	-1.37803200	-0.99318100	C	-3.82693000	-2.34556500	-1.65789500
H	-1.02204500	-0.71569700	-2.24231200	H	7.15101600	2.22542200	-1.52822200
				H	6.60953700	1.39351900	-3.00859300
A				H	5.74918000	2.84167100	-2.41808800
N	1.04263600	-1.32710100	0.53861300	C	-2.21118000	4.89275400	0.63777300
S	2.52941300	-1.54053600	1.24288400	H	-3.47868800	5.07829200	-1.10767900
C	0.36481600	-0.02696400	0.67265600	H	-0.90738800	4.38834200	2.28854600
C	0.74769400	-1.93652700	-0.76442200	H	-3.89126300	0.11059900	2.21343700
O	2.88145600	-2.95186700	1.04898900	C	-5.09237200	-0.63217300	0.11854600
O	2.43800400	-0.96132200	2.58797100	C	-5.11639300	-1.88256600	-1.93399000
C	3.67489900	-0.54964500	0.29596800	H	-3.33456300	-3.01746400	-2.36623100

H	-2.39377800	5.91290200	0.98439700	C	5.60753900	-0.84755900	-0.14945900
C	-5.75608900	-1.01496400	-1.04399000	H	-6.78390700	3.72821600	-0.03812600
H	-5.57770400	0.04242600	0.82943400	H	-7.46215300	2.84562400	1.35637000
H	-5.62126300	-2.19951200	-2.85010000	H	-6.01575200	3.84520100	1.56780900
H	-6.76192800	-0.64492500	-1.25465700	C	2.06491700	3.80112000	-1.23661000
B				H	1.08811000	4.20184100	0.65308900
N	-1.64367100	-1.32332300	0.52512600	H	3.03362200	3.08837700	-3.03555700
S	-3.02499000	-1.66092900	-0.35883700	C	5.54339600	1.20665300	1.74338000
C	-0.70335800	-0.34057800	-0.03681300	H	3.40343700	0.96448800	1.72588100
C	-0.89053300	-2.42847600	1.14984400	C	6.79655200	-0.25134100	0.26904700
O	-3.62705900	-2.85179000	0.25605200	H	5.61722000	-1.66248500	-0.87582900
O	-2.75981900	-1.66507600	-1.81045900	H	2.13431500	4.85492400	-1.51759000
C	-4.03712000	-0.23541300	-0.01011300	C	6.76636700	0.77759100	1.21770100
H	-0.95020400	-0.10677900	-1.08569300	H	5.51730500	2.00000000	2.49429000
C	0.65692600	-1.00950300	0.04437200	H	7.75097600	-0.59056300	-0.14101000
H	-0.74605100	0.60057500	0.52694400	H	7.69771700	1.24308000	1.54997200
H	-1.46383200	-3.36131500	1.10133900	H	1.20162600	-3.24439900	-1.51842200
C	0.42850700	-2.47379900	0.36287500	H	0.08783600	-4.35606900	-0.67208400
H	-0.71602500	-2.18261100	2.21022000	H	-0.56156000	-2.94060200	-1.53632600
C	-4.42555800	0.01222200	1.31218500	10"s			
C	-4.44770800	0.59245000	-1.05317700	C	2.37059700	-1.02685300	-0.71895000
C	1.83295200	-0.36541700	-0.14709500	H	2.86094900	-0.28127800	-0.06914500
C	0.28033700	-3.30114700	-0.92548300	O	1.14337000	-0.95097400	-0.92064500
H	1.24854400	-2.88763800	0.96405400	C	3.20405200	-2.05764900	-1.30208400
C	-5.22991600	1.11438400	1.58169100	C	4.58311200	-2.05910700	-1.01028400
H	-4.09695800	-0.64837000	2.11679700	C	2.66398500	-3.04842500	-2.15006300
C	-5.25640500	1.69494600	-0.76308900	C	5.41079000	-3.03641300	-1.55921900
H	-4.13469500	0.37585300	-2.07516500	H	4.99133000	-1.28904900	-0.35051600
C	1.88918800	1.08424400	-0.50765700	C	3.49620100	-4.02038500	-2.69394100
C	3.13030900	-1.11864800	-0.09372900	H	1.59467600	-3.03827900	-2.36951100
C	-5.65811100	1.97436700	0.55087200	C	4.86836500	-4.01537100	-2.40006000
H	-5.53620900	1.31695300	2.61138600	H	6.47952100	-3.03871600	-1.33420600
H	-5.58026900	2.34985500	-1.57575200	H	3.08284800	-4.78877400	-3.35124900
C	1.39095500	2.08855800	0.33977400	H	5.51757900	-4.78140100	-2.83110400
C	2.48286100	1.46527200	-1.72258000	P	0.40414000	1.62567900	0.56991700
O	3.20525700	-2.29805700	-0.41377300	P	-2.43833100	0.22913800	0.20155700
C	4.37250800	-0.40507200	0.35427300	C	1.57587400	0.99898800	1.84554800
C	-6.52546100	3.16201300	0.86806000	C	1.38187300	2.76325700	-0.48467100
C	1.47606200	3.43450800	-0.02166700	C	-3.80415100	0.19895200	-1.01223100
H	0.95367200	1.81353300	1.30224600	C	-2.50660400	-1.39416400	1.04265300
C	2.56887500	2.81188500	-2.08582000	C	2.81657700	1.58971200	2.12728800
H	2.88217500	0.69593100	-2.38848700	C	1.74229200	2.32651200	-1.77014400
C	4.35085000	0.62572100	1.30765000	C	-5.09671700	-0.22212900	-0.65949800

C	-2.30425700	-2.53005200	0.23442000	H	-3.36065200	2.33773200	0.81751500
C	1.20167100	-0.17226200	2.52900400	H	-0.07504800	3.34835600	2.19703800
C	1.77441300	4.04515500	-0.06247800	H	-1.14958400	3.45539600	0.78549700
C	-3.54313300	0.62120400	-2.32430900				
C	-2.58831700	-1.54996500	2.43476700	TS7"s			
C	3.66661700	1.01990300	3.08088700	C	-3.23821200	-0.70251400	2.00051200
C	2.49859700	3.14600300	-2.61182200	H	-4.28378000	-0.83037600	2.37280200
C	-6.11788700	-0.21022800	-1.61126400	O	-2.74324000	0.40488200	1.92111800
C	-2.18561100	-3.79529200	0.81060700	C	-2.54541400	-1.96546200	1.68550400
C	2.04747500	-0.73248700	3.48795200	C	-3.15729800	-3.16341200	2.09224300
C	2.52689000	4.86458100	-0.90784900	C	-1.27230500	-1.99743100	1.07300900
C	-4.56843900	0.63229500	-3.27503100	C	-2.50292100	-4.38826500	1.95331200
C	-2.46967800	-2.82006900	3.00793400	H	-4.15379500	-3.12080200	2.54144900
C	3.28433100	-0.13920500	3.76296500	C	-0.60382500	-3.23607500	0.98889100
C	2.89383700	4.41568800	-2.18095800	C	-1.21053300	-4.42220700	1.41682100
C	-5.85481800	0.21760000	-2.91847300	H	-2.98859200	-5.31170000	2.27585800
C	-2.26456100	-3.94277100	2.20034700	H	0.41044600	-3.29525400	0.56247900
H	3.13280900	2.48843600	1.59545300	H	-0.67925000	-5.37236600	1.32001500
H	1.41443300	1.34306400	-2.11178200	P	1.93672700	-0.17308600	-0.69492600
H	-5.30196100	-0.56527400	0.35771600	P	-1.13259300	0.61622700	-0.82141300
H	-2.24350100	-2.42162800	-0.85279300	C	-0.90147700	2.27270500	-0.09504300
H	0.25096600	-0.65381200	2.28964400	C	-1.15680000	3.43599500	-0.84232100
H	1.49848400	4.41180100	0.92781400	C	-0.41015500	2.38983400	1.21321700
H	-2.53295800	0.94021300	-2.59534900	C	-0.92316300	4.69416900	-0.28283500
H	-2.74509900	-0.68433100	3.07994700	H	-1.53736700	3.36948600	-1.86337700
H	4.63441600	1.48355000	3.28765300	C	-0.17651000	3.64877800	1.76840100
H	2.77303600	2.79356400	-3.60909800	H	-0.20589200	1.49179500	1.79290200
H	-7.12299900	-0.53826400	-1.33479700	C	-0.43070100	4.80250900	1.02183400
H	-2.03089600	-4.66972400	0.17389000	H	-1.12485600	5.59319900	-0.87007400
H	1.74458500	-1.64194800	4.01266800	H	0.21277700	3.72618200	2.78570900
H	2.82789500	5.85927700	-0.56995000	H	-0.24336200	5.78797000	1.45530400
H	-4.36147500	0.96210500	-4.29603400	C	-2.92454100	0.32653200	-1.03759900
H	-2.53860200	-2.93136400	4.09285800	C	-3.32929800	-0.94251400	-1.48084000
H	3.95293200	-0.58398000	4.50410900	C	-3.88839900	1.31026200	-0.77777200
H	3.48254000	5.05939700	-2.83912600	C	-4.68455500	-1.22322000	-1.66511500
H	-6.65633800	0.22378300	-3.66133500	H	-2.58536100	-1.72111700	-1.66645700
H	-2.16898000	-4.93291100	2.65228600	C	-5.24348400	1.02578200	-0.96338300
Co	-0.39424400	-0.05450200	-0.43262000	H	-3.58692700	2.29182200	-0.41031100
C	-1.80892200	2.04166900	2.30444200	C	-5.64416800	-0.23933900	-1.40431000
C	-2.94464900	1.51440200	1.42050900	H	-4.99233900	-2.21452200	-2.00643400
C	-0.70787000	2.75897200	1.51706100	H	-5.99025100	1.79548300	-0.75404400
H	-1.37683200	1.22822300	2.90934400	H	-6.70542200	-0.46001300	-1.54271200
H	-2.24334500	2.75692900	3.02116200	C	2.60337400	1.17139400	0.34272300
H	-3.77184400	1.11359300	2.02684900	C	2.63386900	0.95662000	1.73216800

C	3.03128000	2.40263600	-0.17220800
C	3.09414800	1.95390700	2.59046700
H	2.29127900	0.00344900	2.14304700
C	3.47557000	3.40752300	0.69358200
H	3.01792000	2.59521700	-1.24550200
C	3.50924100	3.18630000	2.07217300
H	3.11776700	1.77449600	3.66797000
H	3.79686300	4.36821000	0.28442700
H	3.85622800	3.97408000	2.74506200
C	3.20789700	-1.49075800	-0.67404000
C	4.52010800	-1.28010800	-0.22656900
C	2.83171200	-2.76060000	-1.14523000
C	5.44313300	-2.32994300	-0.25205500
C	3.75817500	-3.80454900	-1.17539100
H	1.80816000	-2.93161600	-1.49053700
C	5.06544500	-3.59036400	-0.72508500
H	6.46377600	-2.16066000	0.09954700
H	3.45789600	-4.78804500	-1.54478800
H	5.78979800	-4.40830100	-0.74095000
H	4.82311500	-0.29899500	0.14361500
Co	-0.02763300	-0.98683500	0.09880900
H	-0.52621500	-0.64499200	1.41689000
C	0.81416100	1.35553900	-2.81747000
C	-0.59609200	0.80763800	-2.58856500
C	1.95047300	0.39915600	-2.44622500
H	0.93106500	2.31106100	-2.28458700
H	0.91356700	1.58970600	-3.88977900
H	-1.33974300	1.46161300	-3.06908400
H	-0.71525800	-0.18814700	-3.04720900
H	2.93418700	0.83756500	-2.67446600
H	1.87114700	-0.52915300	-3.03528700