

Supporting Information

Mechanistic insights into the catalyst-dependent divergent cycloaddition reactions via discrimination between diazo compounds

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Table of Contents

1. The other possible transition state for the [3 + 3]-cycloaddition	S2
2. The calculated condensed Fukui function.....	S2
3. A comparison of the [3 + 2]-cycloaddition transition states.....	S3
4. The other pathways for the formation of 2a'	S5
5. Additional results for the Rh-catalyzed C–C bond formation	S8
6. Calculated energies and imaginary frequencies.....	S11
7. Cartesian coordinates of all optimized structures	S13

1. The other possible transition state for the [3 + 3]-cycloaddition

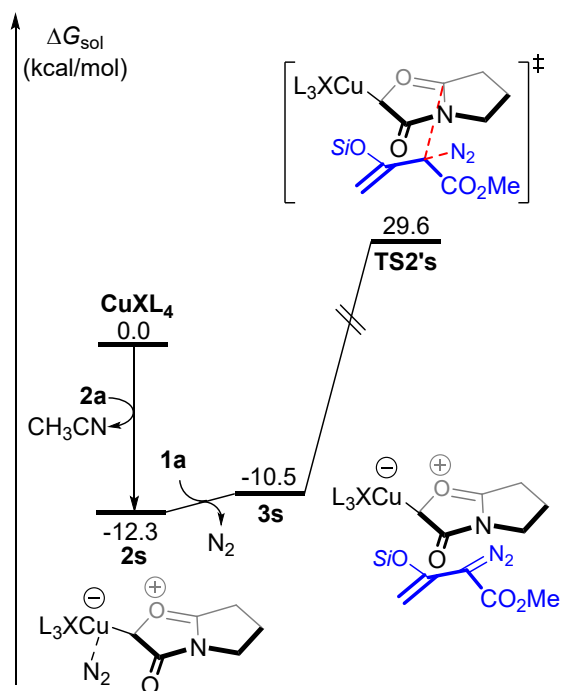


Fig. S1. Free energy profiles for the other possible transition state for the [3 + 3]-cycloaddition.

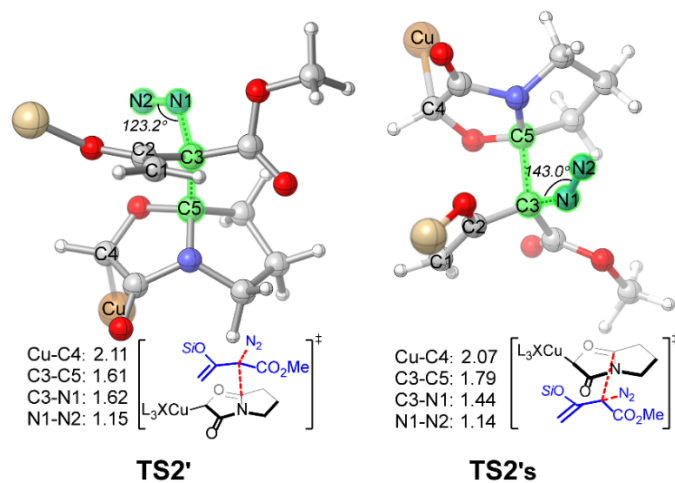


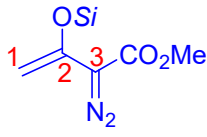
Fig. S2. Optimized structures of transition states TS2' and TS2's with selected bond distances in Å.

2. The calculated condensed Fukui function

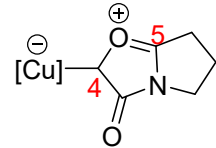
To further study the local reactivity and regioselectivity for the Cu-catalyzed [3+3]-cycloaddition, the condensed Fukui function (f^- and f^+ in Table S1) were calculated by Multiwfn 3.8 for enoldiazoacetate and carbonyl ylide to predict the active site. The f^+ and f^- functions are used to identify the favorable reactive sites for nucleophilic and electrophilic attack respectively. For the enoldiazoacetate, the more electrophilic center corresponds with the carbon atom C1, with $f^- = 0.207$,

while the more nucleophilic center corresponds with the C3, with f^+ =0.077. For the carbonyl ylide, the C4 and C5 atoms are the electrophilic and nucleophilic centers respectively. As a consequence, the more favorable polar interaction should take place between C1 and C5 atoms, which is apparently in contrast to the experimental results. This inconsistency may arise from the steric effects caused by the TIPS group.

Table S1. The calculated condensed Fukui function for enoldiazoacetate and carbonyl ylide.



enoldiazoacetate



carbonyl ylide

	C1	C2	C3	C4	C5
f^-	0.207	0.085	0.078	0.069	0.032
f^+	0.068	0.022	0.077	0.051	0.156

3. A comparison of the [3 + 2]-cycloaddition transition states

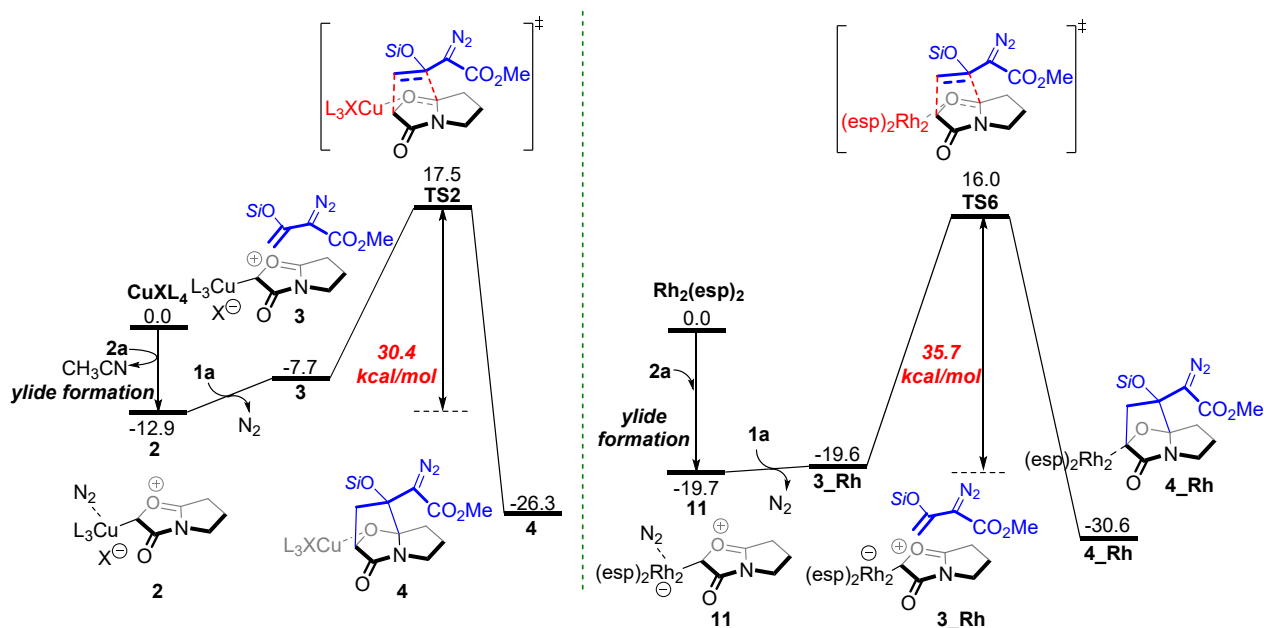


Fig. S3. Free energy profiles for the [3+2]-cycloaddition for both Cu(CH₃CN)₄BF₄ and Rh₂(esp)₂ catalysts.

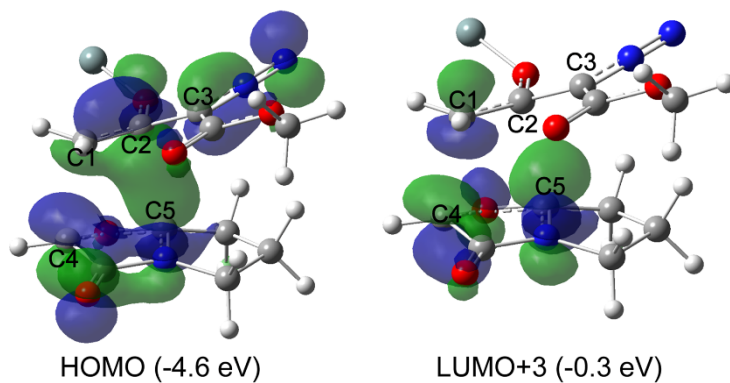


Fig. S4. Molecular orbitals showing the dominant orbital interactions in **TS2** at the B3LYP-D3(BJ)/6-31G(d,p)/ECP10MDF_AVDZ(Cu) level (isovalue = 0.03; the coordinated Cu-catalyst is omitted for clarity).

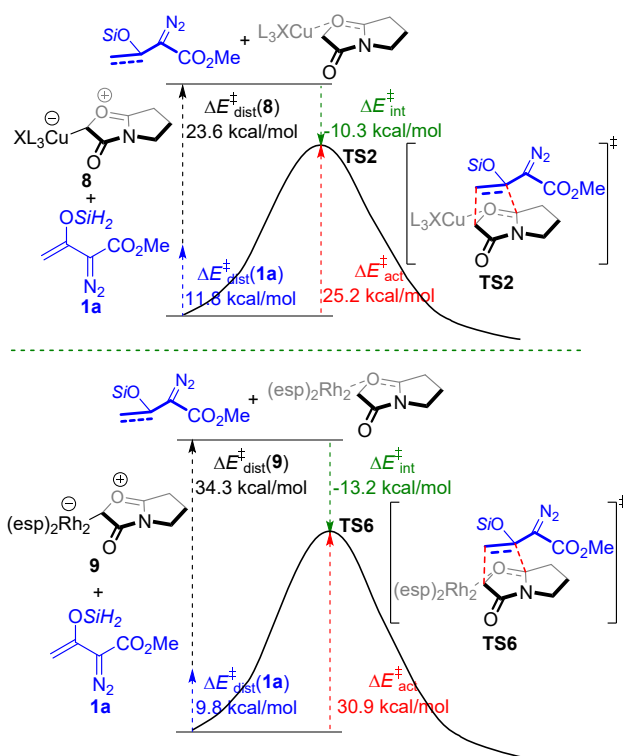


Fig. S5. Distortion-interaction analysis.

4. The other pathways for the formation of 2a'

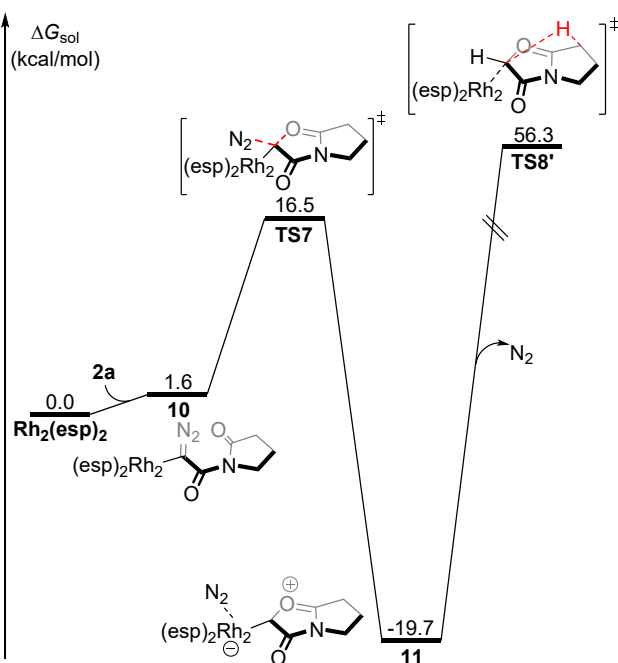


Fig. S6. Free energy profiles for the formation of **2a'** via the direct 1,4-hydrogen transfer.

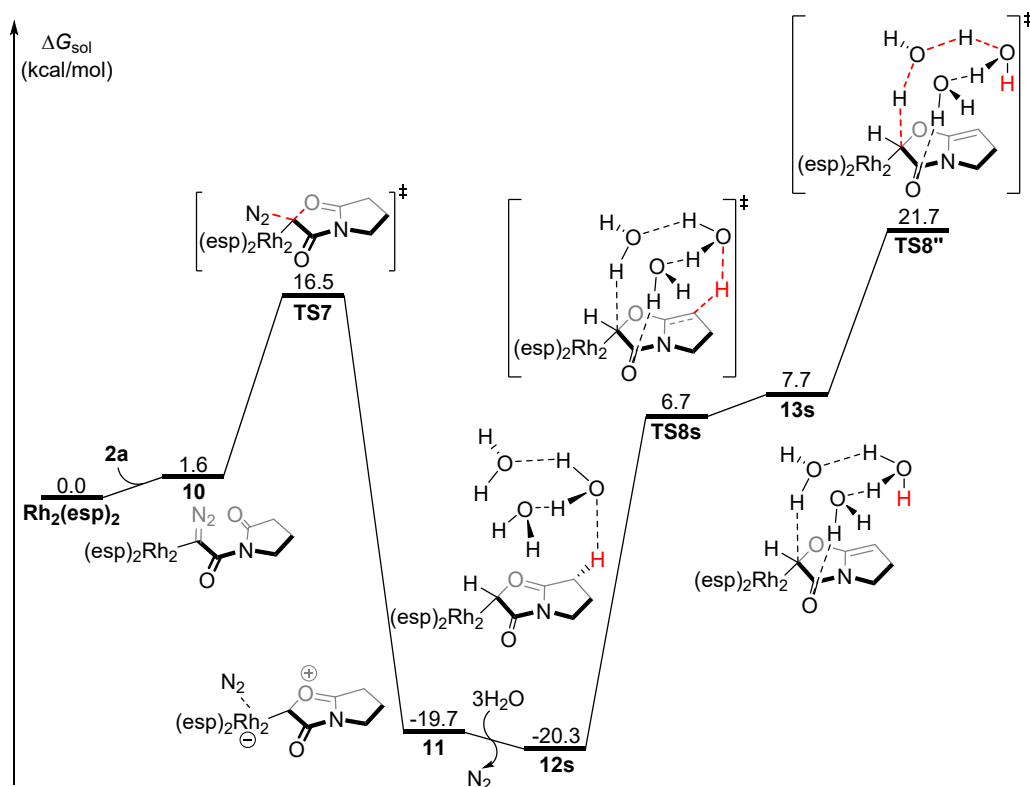


Fig. S7. Free energy profiles for the formation of **2a'** via the water-assisted stepwise H-shift process.

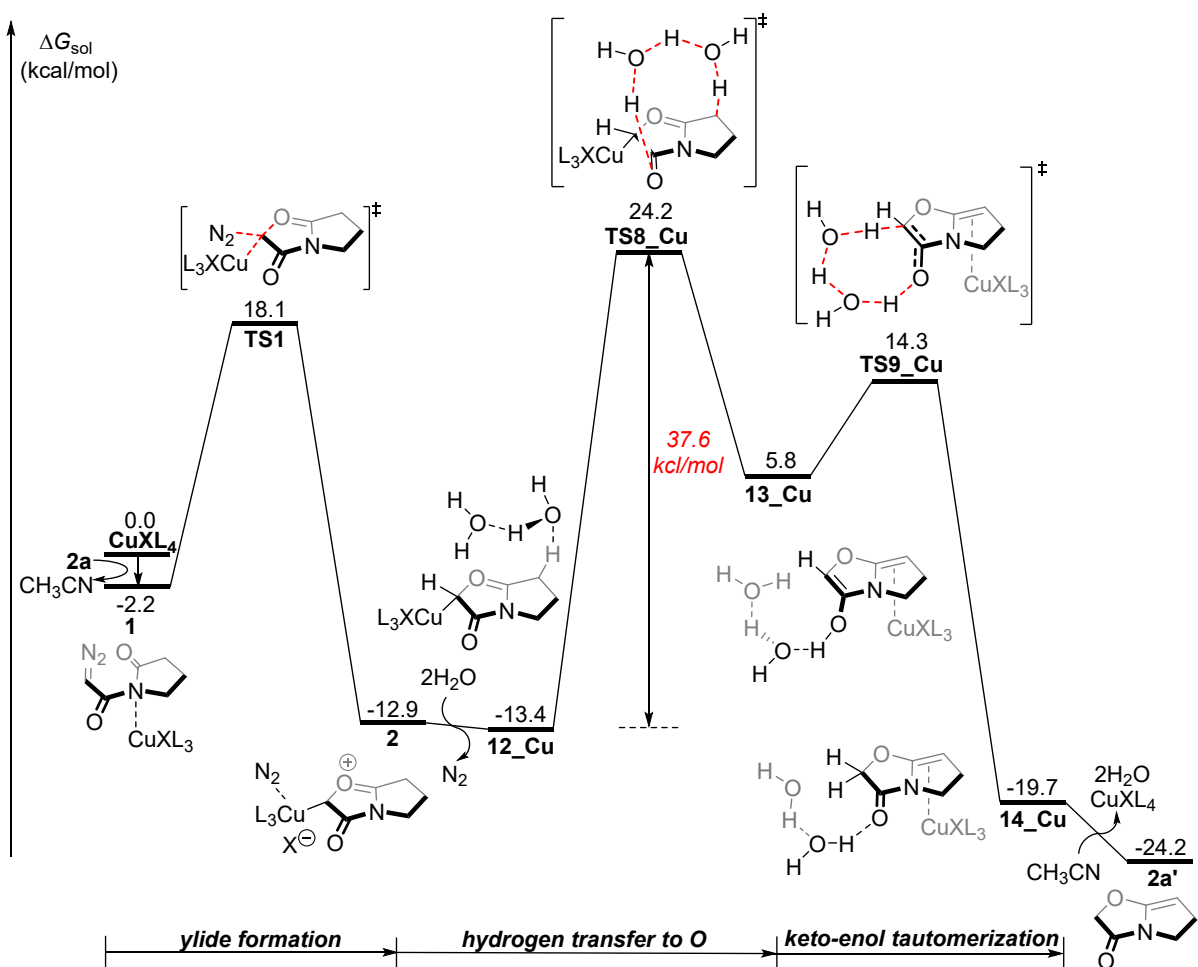


Fig. S8. Free energy profiles for the formation of **2a'** for the Cu(I) catalyst.

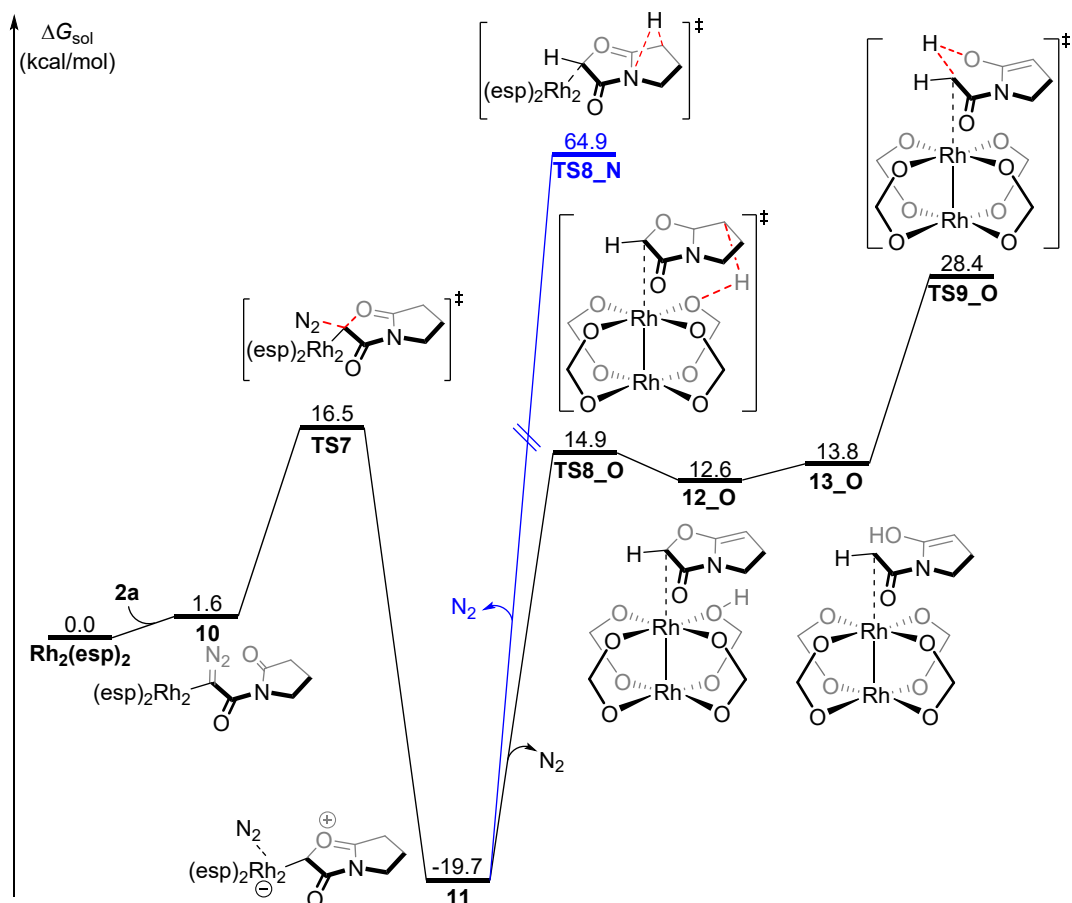


Fig. S9. Free energy profiles for the formation of **2a'** via hydrogen transfer to nitrogen atom or the carbonyl oxygen of the esp ligands.

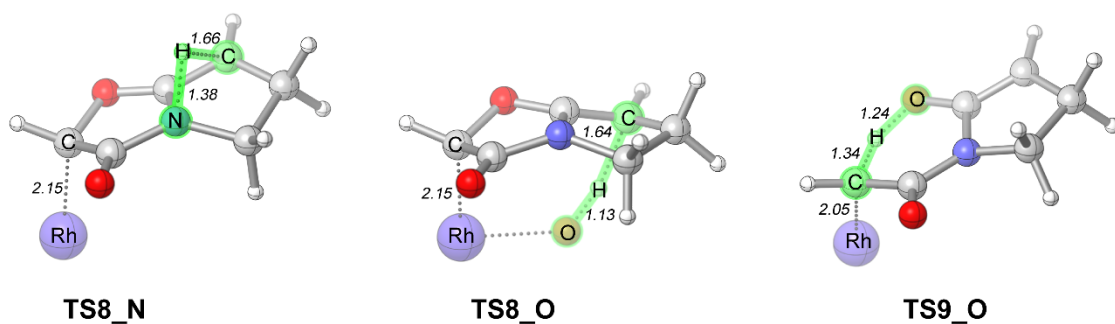


Fig. S10. Optimized structures of transition states **TS8_N**, **TS8_O** and **TS9_O** with selected bond distances in Å.

5. Additional results for the Rh-catalyzed C–C bond formation

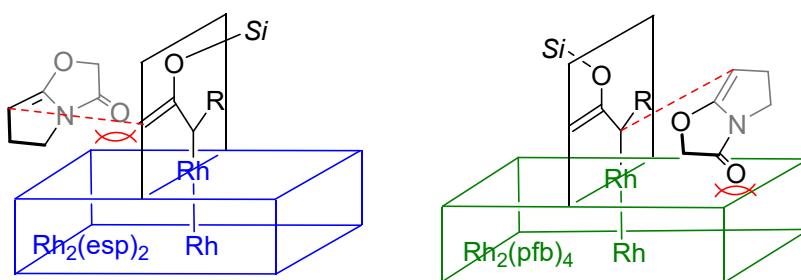


Fig. S11. The unfavorable transition states due to the steric repulsions.

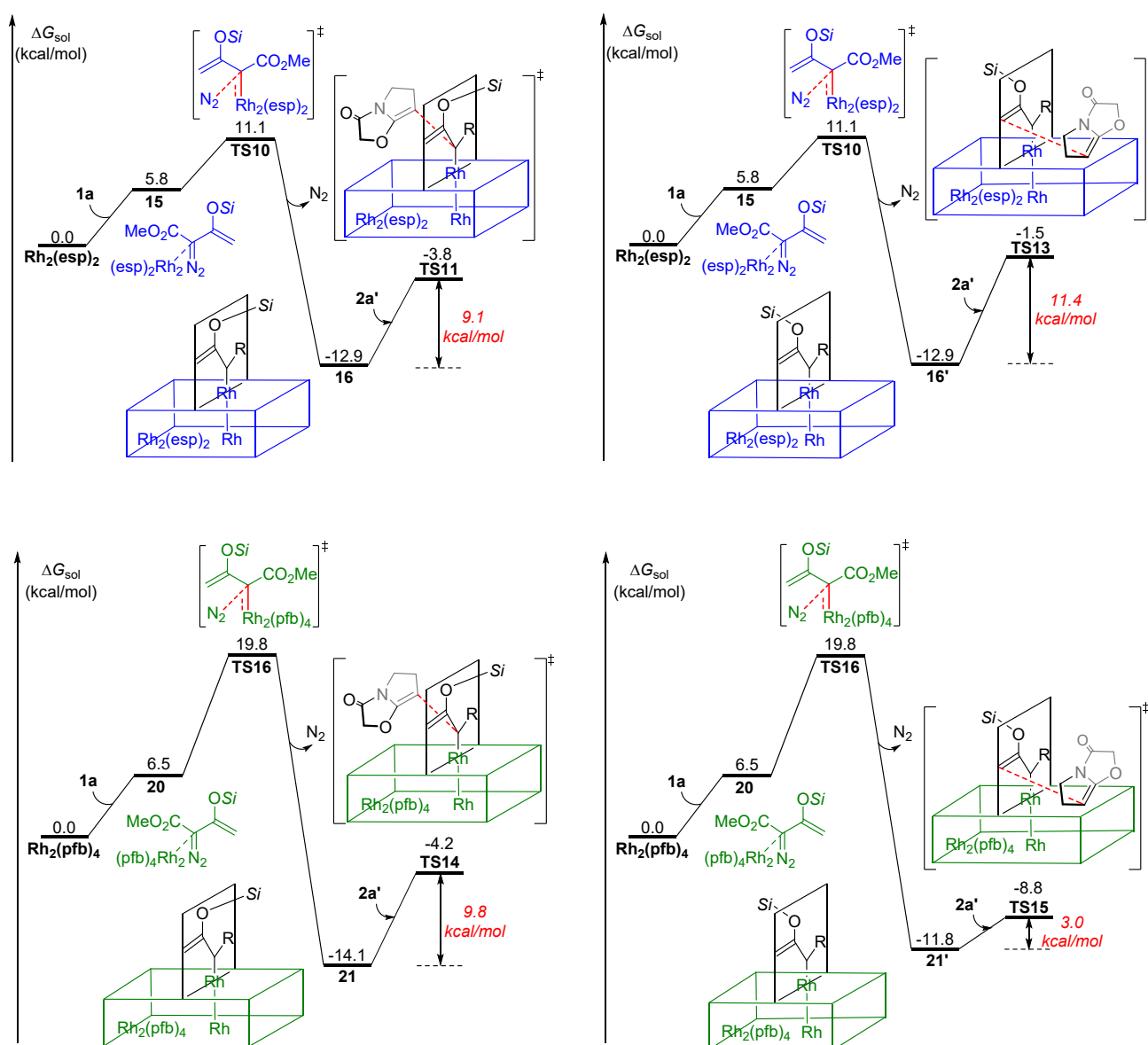


Fig. S12. Free energy profiles for the four C–C bond formation transition states.

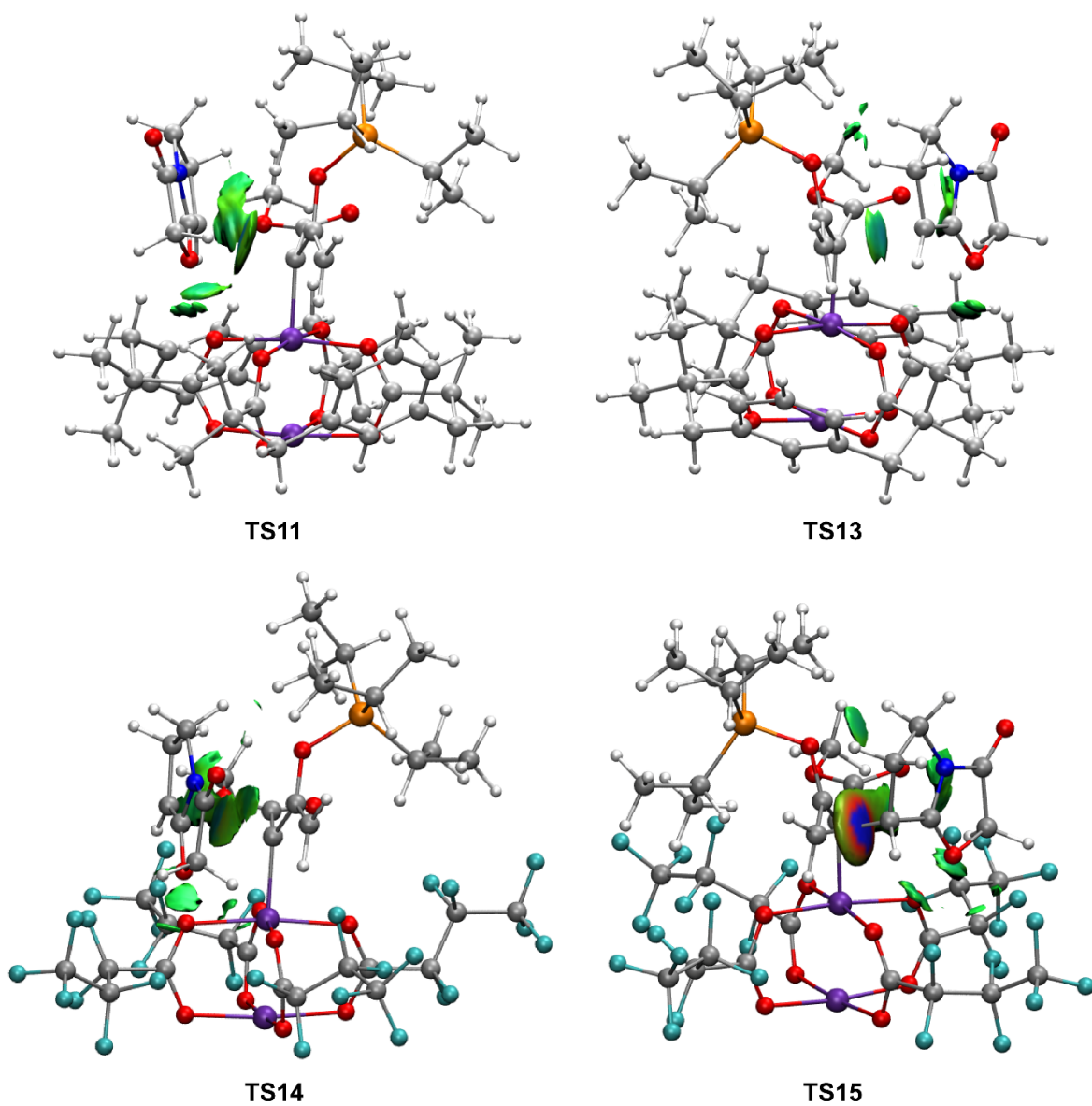


Fig. S13. IGMH maps of the four transition states (isovalue = 0.01 a.u.).

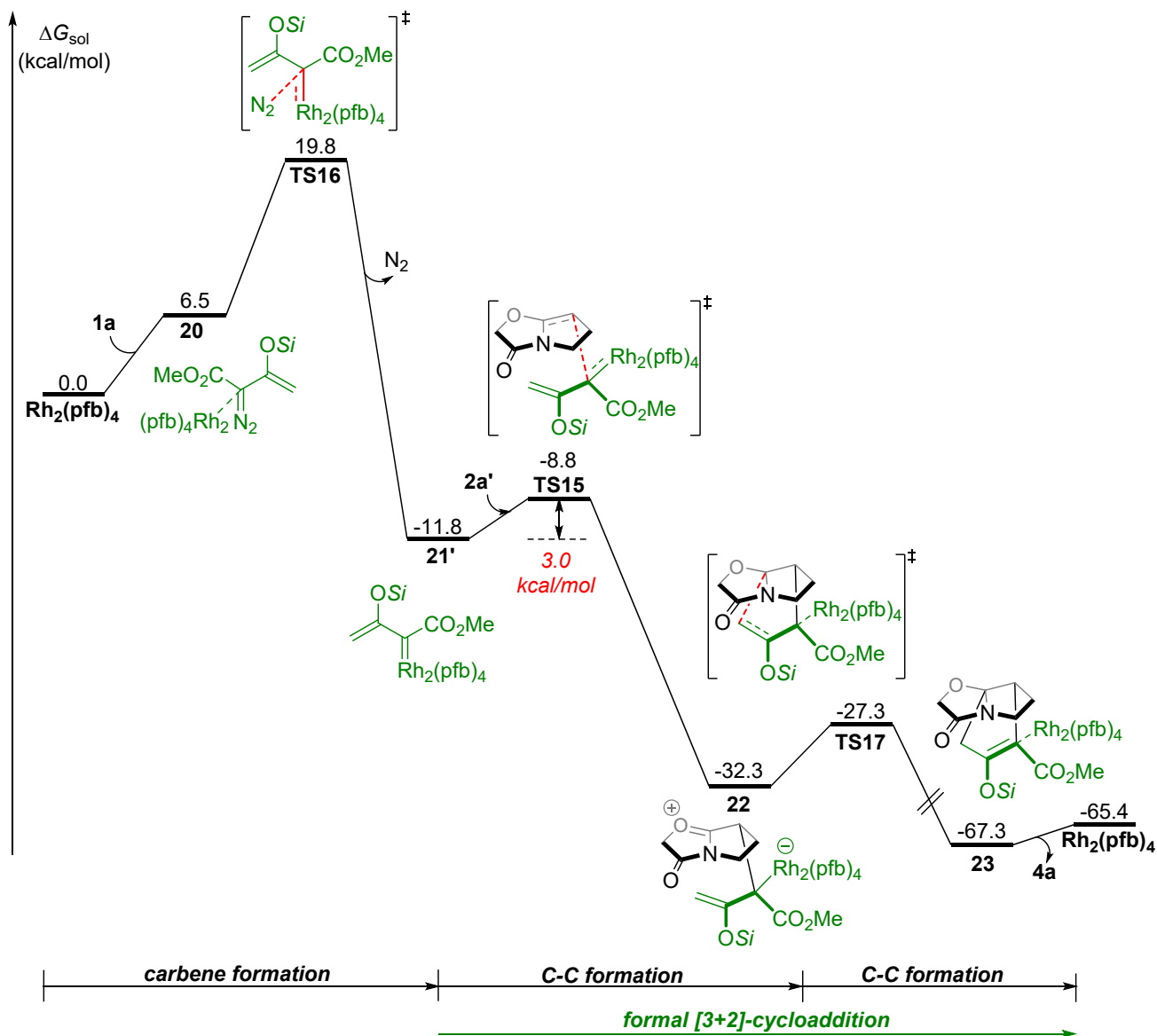


Fig. S14. Free energy profiles for $\text{Rh}_2(\text{pfb})_4$ -catalyzed [3 + 2]-cycloaddition between diazo compounds **1a** and **2a'**.

6. Calculated energies and imaginary frequencies

Table S2. Calculated energies and imaginary frequencies.

Stationary point	Corrected thermal correction to Gibbs free energy at B3LYP-D3(BJ)/6-31G(d,p)/ECP10MDF_AVZDZ(Cu/Rh) (in a.u.)	Single-point energy including solvation energy at B3LYP-D3(BJ)/def2-TZVPP (in a.u.)	Imaginary frequencies (in cm^{-1})
Cu(CH₃CN)₄BF₄	0.143624	-2596.6656181	
CH₃CN	0.022395	-132.8258093	
N₂	-0.012841	-109.5683455	
1a	0.333129	-1174.3179746	
2a	0.099707	-547.7898907	
3a	0.45314	-1503.0985321	
1	0.221404	-3011.6337262	
TS1	0.218814	-3011.5987169	420.52 <i>i</i>
2	0.217919	-3011.6472977	
3	0.579117	-4076.4038352	
TS2	0.577956	-4076.3624738	488.75 <i>i</i>
TS2'	0.578248	-4076.3368522	182.86 <i>i</i>
4	0.585989	-4076.4403378	
TS3	0.579538	-4076.3859435	170.28 <i>i</i>
5	0.57532	-3966.8160886	
TS4	0.573178	-3966.8126182	302.31 <i>i</i>
6	0.571034	-3966.8458549	
TS5	0.574321	-3966.8337783	206.56 <i>i</i>
7	0.583227	-3966.9464366	
TS6	1.086722	-3680.3316476	455.28 <i>i</i>
8	0.21864	-2902.0743981	
9	0.727527	-2506.0531443	
Rh₂(esp)₂	0.605876	-2067.7854497	

Rh₂(pfb)₄	0.122128	-4230.3535864	
5a	0.452287	-1503.1095273	
4a	0.451383	-1503.1098969	
10	0.734252	-2615.5983734	
TS7	0.728658	-2615.5690391	383.91 <i>i</i>
11	0.727706	-2615.6258763	
12	0.76875	-2659.0211176	
TS8	0.765301	-2658.9641277	343.63 <i>i</i>
13	0.770682	-2658.9943343	
TS9	0.768142	-2658.9731902	841.74 <i>i</i>
14	0.769066	-2659.0283812	
2a'	0.094683	-438.2452787	
TS8'	0.718236	-2505.9171685	1423.60 <i>i</i>
TS8''	0.785834	-2735.4328771	719.04 <i>i</i>
TS8_Cu	0.25867	-3054.9827918	486.98 <i>i</i>
15	0.968263	-3242.1203559	
TS10	0.962269	-3242.1059337	452.10 <i>i</i>
16	0.957834	-3132.5615814	
17	1.076147	-3570.8178495	
TS11	1.07909	-3570.8159026	71.50 <i>i</i>
18	1.083522	-3570.8538729	
TS12	1.085605	-3570.8424504	344.65 <i>i</i>
19	1.088775	-3570.922133	
TS13	1.081503	-3570.8147342	19.02 <i>i</i>
TS14	0.598895	-5733.3883151	51.67 <i>i</i>
TS15	0.602683	-5733.3993493	362.33 <i>i</i>
2s	0.21888	-3011.6472893	
3s	0.576645	-4076.4058313	
TS2's	0.579577	-4076.3448162	284.02 <i>i</i>

3_Rh	1.089205	-3680.3908451	
4_Rh	1.093518	-3680.4127466	
12s	0.78927	-2735.5031871	
TS8s	0.787269	-2735.4581801	482.93 <i>i</i>
13s	0.789265	-2735.4586325	
12_Cu	0.259926	-3055.0440578	
13_Cu	0.266813	-3055.0202921	
TS9_Cu	0.261935	-3055.001932	781.33 <i>i</i>
14_Cu	0.266767	-3055.0609435	
TS8_N	0.719322	-2505.9045053	1813.39 <i>i</i>
TS8_O	0.722572	-2505.9874765	846.60 <i>i</i>
12_O	0.724401	-2505.9929603	
13_O	0.723559	-2505.9900976	
TS9_O	0.716531	-2505.9599186	1667.51 <i>i</i>
16'	0.958805	-3132.5626147	
20	0.484656	-5404.6875977	
TS16	0.482721	-5404.6645234	360.0438 <i>i</i>
21	0.471573	-5295.1290769	
21'	0.475235	-5295.1291148	
22	0.605534	-5733.439721	
TS17	0.603677	-5733.4298887	226.8529 <i>i</i>
23	0.606831	-5733.496821	

7. Cartesian coordinates of all optimized structures

Cu(CH₃CN)₄BF₄

Cu	-1.53062600	-0.07669200	-0.00925500
N	-0.88976600	-1.88053300	-0.67552500
N	-3.47550600	0.17450600	0.09024100
N	-0.55902500	1.22341600	-1.20572600
N	-0.50295800	0.08536200	1.71432500

C	-0.07853100	-2.66253200	-0.94494900
C	-4.61986100	0.34597600	0.12459200
C	0.32498300	1.81626900	-1.66255500
C	0.39095500	0.18703800	2.44344900
C	-6.05477400	0.56336500	0.16333100
H	-6.52509900	0.06698500	-0.69033200
H	-6.46564300	0.15349200	1.09033000
H	-6.26569400	1.63572800	0.11808300
C	1.44755600	2.54573500	-2.22271800
H	1.52959100	3.52005100	-1.73256800
H	2.36550500	1.97817900	-2.04568500
H	1.29698200	2.69314900	-3.29576400
C	0.98315400	-3.59808700	-1.26505100
H	1.93523600	-3.08069300	-1.11866700
H	0.92913500	-4.46770400	-0.60424900
H	0.89589500	-3.92557700	-2.30463700
C	1.52921200	0.30826100	3.33541600
H	1.66886700	1.35843900	3.60679600
H	1.35755300	-0.27980700	4.24111400
H	2.42279400	-0.04718200	2.81507300
B	3.02019000	0.20206000	0.02218100
F	2.17096000	-0.79660400	-0.49856200
F	2.24558300	1.26655100	0.52493500
F	3.79549000	-0.33841700	1.06386000
F	3.85426700	0.68550500	-1.00293200

CH₃CN

N	0.00000000	0.00000000	1.43818900
C	0.00000000	0.00000000	0.27730400
C	0.00000000	0.00000000	-1.17924600
H	0.00000000	1.02812000	-1.55189300
H	0.89037800	-0.51406000	-1.55189300
H	-0.89037800	-0.51406000	-1.55189300

N₂

N	0.00000000	0.00000000	0.55251400
N	0.00000000	0.00000000	-0.55251400

1a

C	-0.90916500	2.01881000	-0.42376700
H	-1.80731100	2.57697500	-0.64215700
H	0.05222700	2.50713100	-0.52254000
C	-0.98512900	0.73651100	-0.03419600
C	-2.24202700	-0.01401100	0.13493900

N	-2.11980600	-1.27542200	0.48883700
N	-1.99987400	-2.36142300	0.79598500
C	-3.60362000	0.48759500	-0.05858600
O	-3.88257800	1.62761300	-0.38681200
O	-4.51935800	-0.47729500	0.17159300
C	-5.89443300	-0.08177000	0.00124600
H	-6.48114000	-0.97266200	0.22308700
H	-6.15096500	0.72403500	0.69279300
H	-6.07504300	0.24630600	-1.02501600
O	0.07202400	-0.06188300	0.26544800
Si	1.73665400	0.12338000	-0.07187400
C	2.43317800	1.56693300	0.95371000
H	2.33982100	2.45412600	0.31015400
C	2.41114000	-1.55845000	0.47713700
H	3.50192800	-1.51014600	0.34684900
C	1.95711600	0.47546100	-1.92658300
H	1.82166400	1.56106300	-2.03549300
C	0.91097300	-0.20849500	-2.82223600
H	-0.10629800	0.09855500	-2.56401900
H	1.07881600	0.05452100	-3.87461100
H	0.95985500	-1.29919900	-2.74908300
C	3.38701400	0.13994400	-2.39028700
H	3.59664900	-0.93176800	-2.30107500
H	3.52554100	0.41171800	-3.44429800
H	4.14850500	0.67535900	-1.81323300
C	1.63427100	1.84270300	2.23911200
H	2.06013500	2.69788100	2.77943800
H	0.58656000	2.07275200	2.02534200
H	1.65289400	0.98560800	2.92007400
C	3.92956900	1.38092500	1.26639000
H	4.53014600	1.22916900	0.36336800
H	4.32931700	2.26381300	1.78090400
H	4.09653100	0.51951500	1.92201900
C	2.11921600	-1.82862500	1.96418400
H	2.52052900	-2.80477300	2.26514600
H	2.56379100	-1.07443400	2.61999800
H	1.04059100	-1.84452200	2.15660000
C	1.87837600	-2.71606700	-0.38481300
H	2.17319000	-2.62177500	-1.43366700
H	2.26284200	-3.67714100	-0.01981600
H	0.78424600	-2.76775200	-0.34761100
2a			
C	-2.08529600	1.22919400	-0.24423200

C	-2.61422300	0.12258000	0.67344200
C	-1.70060600	-1.06656100	0.35277900
H	-2.55194500	1.19477300	-1.23671000
H	-2.20020700	2.24421600	0.14133700
H	-2.49016400	0.41239800	1.72113800
H	-3.66564000	-0.11593700	0.50469800
H	-1.55950500	-1.75256700	1.18874600
H	-2.05912300	-1.64031700	-0.50807700
N	-0.41995500	-0.41167300	0.01931500
C	0.70886500	-1.22605800	-0.18715500
O	0.56511000	-2.43598700	-0.34416400
C	2.03666700	-0.63973200	-0.15544100
H	2.89529400	-1.24920300	-0.40384300
C	-0.61407700	0.89946700	-0.43060300
O	0.24104000	1.61772600	-0.91887200
N	2.29723100	0.52455100	0.37549500
N	2.52188400	1.53560500	0.84008500

3a

O	0.26248900	2.70393000	-0.46033400
C	1.38853700	2.05580700	-0.09258200
C	0.16485300	4.06947300	-0.02263600
O	2.28304100	2.62098200	0.52414100
C	1.43793300	0.65010200	-0.52151300
H	0.95226200	4.67829100	-0.47506900
H	0.24042700	4.13858800	1.06509400
H	-0.81450600	4.41291100	-0.35516900
C	2.79577600	-0.04637200	-0.70064900
C	0.45322100	-1.61509000	-0.98113800
N	3.10716200	-0.90960300	0.46416200
C	4.06658700	0.78689400	-0.87785500
H	-0.07469000	-1.77261300	-1.92820200
H	-0.05340900	-2.22481500	-0.22592900
C	2.64738100	-2.16744500	0.22646500
C	4.33512100	-0.54140300	1.17099700
H	3.87458100	1.79130200	-1.25243100
H	4.68000300	0.24776200	-1.60558000
C	4.74016900	0.79203100	0.50949300
O	2.80993700	-3.16927700	0.90954100
H	5.08440900	-1.32773000	1.02434400
H	4.16002100	-0.43536800	2.24497900
H	5.82591100	0.89063000	0.43961600
H	4.34888300	1.62599900	1.09136500
C	0.33858500	-0.14856700	-0.62594100

O	-0.89591400	0.31902500	-0.43929800
Si	-2.37209500	-0.35234900	0.10442100
C	-2.03738900	-1.46111000	1.61652000
H	-1.81726100	-2.45785200	1.20759000
C	-3.35867400	1.20632300	0.52819900
H	-4.34380900	0.86654100	0.87837300
C	-3.12412800	-1.37576800	-1.30962500
H	-2.63037200	-2.35655400	-1.24417800
C	-3.56892600	2.10311900	-0.70437500
H	-2.61117900	2.38199000	-1.15646800
H	-4.17253300	1.61261500	-1.47330400
H	-4.08534100	3.02988200	-0.42300600
C	-2.69256100	2.00384800	1.66330500
H	-3.24914700	2.92840700	1.86349200
H	-2.65094900	1.43760200	2.59789300
H	-1.66931200	2.28423700	1.39571200
C	-2.84150800	-0.80627400	-2.71000900
H	-3.35681000	0.14587900	-2.86792500
H	-1.77588800	-0.62944100	-2.88126900
H	-3.19368200	-1.49935500	-3.48432500
C	-4.63443100	-1.60014600	-1.11099400
H	-5.03876100	-2.23830800	-1.90670000
H	-4.86346300	-2.08559300	-0.15687600
H	-5.18518400	-0.65327100	-1.14266800
C	-3.29205200	-1.60069000	2.50044300
H	-3.10726800	-2.30762800	3.31882300
H	-3.57230500	-0.64449700	2.95495900
H	-4.15886400	-1.96817100	1.94202700
C	-0.82716500	-1.02776000	2.46306700
H	0.10126600	-0.98848200	1.88599000
H	-0.97700900	-0.03788600	2.90513200
H	-0.66867500	-1.73334400	3.28809900
C	1.91411600	-2.05248600	-1.12853400
H	2.01284400	-2.97248200	-1.70488700
O	2.64248800	-0.99791900	-1.76984500

1

Cu	-0.27687100	0.21906000	0.31450200
N	0.82604300	-0.07179600	1.85836200
N	-1.12478300	1.84472000	-0.34620500
N	-0.70472500	-1.33518800	-0.84194600
C	1.60416500	-0.31704200	2.67916800
C	-2.07504500	2.45749200	-0.59942400
C	-1.53564600	-2.07292500	-1.17174700

C	-3.31028500	3.16117900	-0.88122600
H	-3.57065300	3.04311100	-1.93677800
H	-4.09280400	2.71452700	-0.26071600
H	-3.20660400	4.22387100	-0.64629600
C	2.62497800	-0.63624800	3.65719100
H	2.38524200	-1.58522100	4.14536700
H	3.58348000	-0.72491900	3.13669800
H	2.68362900	0.15431100	4.41073600
C	-2.61842900	-2.96816100	-1.52826400
H	-2.97775100	-2.73434300	-2.53413900
H	-2.27848300	-4.00665600	-1.49360200
H	-3.42862100	-2.81482700	-0.80889900
B	-3.81392700	-0.22727700	0.62894100
F	-2.58210200	-0.25603800	1.34427000
F	-3.56229100	-0.04811900	-0.74355600
F	-4.47835600	-1.44794200	0.82365500
F	-4.58836700	0.84285800	1.10192600
C	3.49929800	1.93935200	0.60908400
C	2.38577800	2.69593400	-0.12162000
C	2.22528700	1.91635400	-1.43189400
H	4.49554600	2.30847000	0.33501300
H	3.42689900	1.95478900	1.69862600
H	1.45832300	2.64129200	0.45501200
H	2.62110800	3.74626000	-0.30206900
H	1.21147600	1.93928000	-1.83125100
H	2.91516500	2.26476700	-2.20719600
N	2.57721600	0.53598400	-1.03872500
C	2.39528300	-0.48786400	-1.98746200
O	2.15285100	-0.18745700	-3.15406100
C	2.46685400	-1.88231000	-1.58952100
H	2.45228000	-2.64677900	-2.35550300
C	3.39270600	0.51518200	0.09526000
O	3.93946300	-0.47165900	0.56265200
N	2.25762100	-2.30255700	-0.37161400
N	2.06184500	-2.69457100	0.67542500

TS1

Cu	-0.32840000	0.88717700	0.68040900
N	0.55283600	0.07832400	2.31374600
N	-0.16428500	-0.83612100	-0.53517700
N	1.21737300	1.93858400	-0.04470900
C	1.33806500	-0.51381200	2.92445200
C	0.31200600	-1.64703800	-1.21096700
C	2.22033700	2.26248200	-0.52305200

C	0.91986600	-2.66171000	-2.05282200
H	0.92590800	-2.31651900	-3.09047000
H	1.95018800	-2.82618800	-1.72638100
H	0.34822300	-3.59138200	-1.98481900
C	2.35421300	-1.26451700	3.63788900
H	3.15332000	-1.49843300	2.92943200
H	2.75311100	-0.66744700	4.46251400
H	1.92716900	-2.19006300	4.03367200
C	3.49031800	2.63683200	-1.11608300
H	3.35925200	2.79327700	-2.19060800
H	3.85662600	3.55974200	-0.65810900
H	4.20541500	1.82518500	-0.95487500
B	3.77233000	-0.95568100	-0.64231800
F	3.19593500	-0.89954900	0.64345800
F	2.89622000	-0.37339700	-1.58116100
F	4.98524600	-0.24267300	-0.64358300
F	3.99775200	-2.29885000	-0.99486100
C	-3.98660800	-2.35905200	0.61928500
C	-3.90514900	-2.59180700	-0.89964900
C	-3.93786200	-1.17564700	-1.50653700
H	-5.02438900	-2.31471600	0.97255800
H	-3.45734900	-3.09801300	1.22369100
H	-2.95474400	-3.07274800	-1.14765200
H	-4.71483300	-3.21521100	-1.28159200
H	-3.32307400	-1.06893700	-2.40056300
H	-4.95445100	-0.84197200	-1.73774900
N	-3.38352900	-0.35224800	-0.42189900
C	-2.88546200	0.93107200	-0.63263000
O	-2.95252300	1.44453600	-1.74498900
C	-2.16171600	1.50606400	0.53947200
H	-2.76637200	1.87146800	1.36674200
C	-3.38113300	-0.98539900	0.80410800
O	-2.95772500	-0.45753700	1.82648700
N	-1.35530100	4.13857600	-0.46167400
N	-1.90676800	3.22026700	-0.17936100

2

Cu	0.36418600	1.01082100	-0.33645700
N	-0.95391200	1.53188500	-1.74595900
N	0.52681800	-1.10351300	-0.78507200
N	-0.68710400	0.99956500	1.33884600
C	-1.96699000	1.52357600	-2.30754500
C	0.07337800	-2.17035500	-0.82269100
C	-1.44019600	0.77589800	2.18851700

C	-0.49017300	-3.50767900	-0.87285700
H	-0.18840800	-4.06321600	0.01962100
H	-1.58106400	-3.43965600	-0.89420700
H	-0.12707700	-4.02855600	-1.76319800
C	-3.26137900	1.46398300	-2.96027600
H	-3.84507900	0.68090400	-2.46842100
H	-3.77582800	2.42380100	-2.86037300
H	-3.14052300	1.22559100	-4.02056100
C	-2.40900800	0.47365500	3.22557200
H	-1.95529200	-0.18603100	3.97071300
H	-2.73394000	1.39725000	3.71263200
H	-3.26369100	-0.03198700	2.76753600
B	-3.27375200	-1.62248300	0.35933700
F	-3.05282700	-0.59754000	-0.58242900
F	-2.10127100	-1.83390900	1.11342300
F	-4.31945100	-1.25118500	1.22379600
F	-3.60606600	-2.81170900	-0.31706000
C	4.01918900	-1.68552900	-1.17959200
C	3.98690700	-2.48712100	0.15716600
C	3.84255200	-1.43544800	1.29405900
H	5.03854800	-1.51050200	-1.54279700
H	3.44711600	-2.15062500	-1.98485100
H	3.11480100	-3.14421000	0.16119100
H	4.87935400	-3.09920200	0.28798600
H	3.13628600	-1.73360000	2.06980500
H	4.79588600	-1.17157000	1.75943100
N	3.32285300	-0.27788600	0.56171400
C	2.78850900	1.02448000	0.90458800
O	2.71543700	1.44678700	2.05218900
C	2.37579800	1.52876800	-0.38910100
H	2.52083300	2.56461300	-0.67327600
C	3.42238600	-0.39698700	-0.74546800
O	2.98452700	0.63663700	-1.39012400
N	-0.15428000	4.18828600	0.16216500
N	-1.20345500	4.11935500	0.50102200

3

Cu	2.18284000	-0.72219400	0.56513900
N	2.45511000	-2.22632800	-0.75351100
N	2.98463300	0.85500400	-0.67756500
N	3.59622300	-0.97518800	1.89937100
C	3.05233600	-2.89004100	-1.49185300
C	3.85259600	1.43929900	-1.17727900
C	4.61819400	-1.05453800	2.43797800

C	4.93903600	2.16947500	-1.80575800
H	5.28141000	2.96175900	-1.13415600
H	5.76923000	1.48467100	-1.99726500
H	4.59270400	2.61431800	-2.74276500
C	3.85698100	-3.68733600	-2.39889400
H	4.88694300	-3.32588700	-2.33494000
H	3.81742000	-4.74084100	-2.10854800
H	3.48957300	-3.57956800	-3.42314200
C	5.91844500	-1.15701700	3.07360500
H	6.16588300	-0.20747100	3.55684800
H	5.90384500	-1.95081400	3.82573800
H	6.66645700	-1.37748100	2.30686700
B	6.64697800	-0.67962700	-0.47620800
F	5.62417800	-1.55354400	-0.89747500
F	6.09804400	0.33887500	0.33013500
F	7.60031300	-1.39596000	0.26967500
F	7.25503600	-0.09571200	-1.60406800
C	0.12304300	2.86608100	-1.52997200
C	0.79496100	4.04726000	-0.76345400
C	0.74160600	3.68423000	0.74967100
H	-0.91126900	3.08415200	-1.81545400
H	0.66418600	2.56248900	-2.42859200
H	1.83657300	4.13512100	-1.07806700
H	0.29590300	4.99513400	-0.96493000
H	1.68032600	3.87809500	1.27028700
H	-0.07836300	4.16944900	1.28299900
N	0.48732200	2.24291200	0.70204600
C	0.45737100	1.15629500	1.65693600
O	0.61754000	1.30805900	2.86157400
C	0.27110900	0.00047700	0.80213400
H	-0.41771800	-0.78511200	1.08319700
C	0.14598900	1.80499900	-0.49137400
O	-0.09000300	0.53377900	-0.52543500
C	-2.93539100	0.56706200	1.85304400
H	-2.50378400	1.39419700	2.39622800
H	-3.02282300	-0.39323800	2.34563900
C	-3.35387400	0.73064400	0.58867100
C	-3.28293700	2.00703200	-0.14846300
N	-3.65715600	1.97101100	-1.41052000
N	-3.97787600	1.92676000	-2.49840300
C	-2.86650500	3.30737400	0.37340800
O	-2.49053200	3.51079500	1.51591000
O	-2.93914200	4.26639100	-0.57676100
C	-2.60793200	5.60152800	-0.14591300

H	-2.69945300	6.22233500	-1.03659400
H	-3.30677600	5.93649200	0.62425200
H	-1.58926800	5.64273700	0.24332800
O	-3.90946100	-0.22161200	-0.20214200
Si	-4.23083900	-1.88439400	0.02798800
C	-5.29474100	-2.14069400	1.58579800
H	-4.57392600	-2.28393600	2.40457800
C	-5.17663900	-2.27889000	-1.56795100
H	-5.43495400	-3.34682700	-1.52433900
C	-2.55979200	-2.75490200	0.25950400
H	-2.15505700	-2.28124600	1.16691900
C	-1.55248300	-2.51168200	-0.87801100
H	-1.52605700	-1.46670200	-1.19831300
H	-0.53852300	-2.78753700	-0.56352800
H	-1.79517600	-3.12208600	-1.75359700
C	-2.69710700	-4.25918300	0.55193100
H	-3.17813800	-4.78886200	-0.27928300
H	-1.70879500	-4.71440400	0.69670800
H	-3.28150200	-4.45440000	1.45616900
C	-6.17760600	-0.93528000	1.95480800
H	-6.72757600	-1.13585500	2.88347200
H	-5.58760200	-0.02778000	2.10825700
H	-6.92023300	-0.72326900	1.17901200
C	-6.14465200	-3.42319400	1.49046200
H	-5.54759600	-4.31001300	1.25589200
H	-6.65733700	-3.61564200	2.44140800
H	-6.91698700	-3.33346500	0.71893500
C	-6.48677200	-1.47134700	-1.63904900
H	-7.02380100	-1.69154100	-2.57055400
H	-7.16266500	-1.69601100	-0.80988300
H	-6.28490000	-0.39436300	-1.62370900
C	-4.35033500	-2.03472900	-2.84327900
H	-3.48393800	-2.69629300	-2.91273900
H	-4.96671700	-2.20448900	-3.73557400
H	-3.98757300	-1.00151500	-2.89029100

TS2

Cu	-2.91744500	0.27787200	-0.58896100
N	-2.81812300	-1.62859200	-0.98562200
N	-2.81982500	0.77403000	1.30150600
N	-4.23258600	1.28164600	-1.62292100
C	-3.37158300	-2.64386300	-0.89752400
C	-3.43383300	0.74144500	2.28562100
C	-5.37309700	1.39197100	-1.80506500

C	-4.24462700	0.68858800	3.48458500
H	-5.29041700	0.77220700	3.17734600
H	-4.09149100	-0.26731300	3.99250200
H	-3.98296900	1.50988400	4.15698700
C	-4.11965300	-3.87824200	-0.77204400
H	-3.88763400	-4.35729600	0.18300600
H	-5.18203100	-3.62217600	-0.80299900
H	-3.87330200	-4.55704200	-1.59279000
C	-6.80623900	1.46943600	-2.00261700
H	-7.03205300	1.75002300	-3.03480700
H	-7.22029000	0.48203100	-1.78136900
H	-7.23610000	2.20552600	-1.31821700
B	-6.21555800	-1.06414700	0.79462600
F	-6.20789800	-1.39197600	-0.58362000
F	-6.15149500	0.34203500	0.93051600
F	-7.38524500	-1.54409800	1.38766500
F	-5.08811200	-1.64350600	1.41335000
C	0.50220500	0.80429100	1.75649200
C	0.23213500	2.33836200	1.85055600
C	-0.29550200	2.79593700	0.45810100
H	1.42578200	0.50502900	2.25653900
H	-0.32033000	0.21710000	2.17716000
H	-0.48865300	2.56765000	2.63646500
H	1.15815100	2.86702800	2.08423400
H	-1.37717300	2.95176400	0.45312200
H	0.19260100	3.70116600	0.09261300
N	0.02126000	1.65517600	-0.39168700
C	-0.21983400	1.30651200	-1.72902500
O	-0.67231000	2.04051800	-2.61398600
C	0.28765100	-0.05532500	-1.74685700
H	0.08775800	-0.81295600	-2.48900400
C	0.56765400	0.60848600	0.28161500
O	0.39479100	-0.50648800	-0.44079400
C	2.43736800	0.49351500	-1.79236100
H	2.40858800	1.37268400	-2.42013700
H	2.67274400	-0.44048200	-2.28543900
C	2.76399200	0.64620800	-0.44597800
C	3.17257300	1.94157000	0.14733500
N	3.74099600	1.89952300	1.32834400
N	4.24622400	1.85638700	2.35085800
C	2.95303500	3.26984500	-0.42054000
O	2.45848100	3.48451000	-1.51537200
O	3.36161100	4.24540900	0.42242400
C	3.20520800	5.59123500	-0.06426800

H	3.59178500	6.23240400	0.72770600
H	3.77719400	5.73726400	-0.98378000
H	2.15227800	5.81493400	-0.25233500
O	3.20839400	-0.39528400	0.34143100
Si	3.96990800	-1.86385100	-0.04511300
C	5.33071100	-1.56562700	-1.34903700
H	4.82299800	-1.64606500	-2.32145600
C	4.66714900	-2.38127400	1.64532000
H	5.02519900	-3.41573400	1.53173600
C	2.66972600	-3.05398600	-0.76897200
H	2.17947000	-2.45633800	-1.55045000
C	1.57704200	-3.49115100	0.22001700
H	1.14816500	-2.64614200	0.76324500
H	0.75821400	-3.99367300	-0.31184600
H	1.97117500	-4.20516200	0.95125300
C	3.28897100	-4.28466800	-1.45500800
H	3.86228000	-4.89629600	-0.74770800
H	2.50316500	-4.92800500	-1.87196800
H	3.95627600	-4.00981400	-2.27717600
C	5.96413100	-0.16521100	-1.27270200
H	6.74450000	-0.05508000	-2.03717500
H	5.22840500	0.62595700	-1.43802700
H	6.43454000	0.01543300	-0.30097200
C	6.42065300	-2.65516900	-1.31472500
H	6.00950800	-3.66690100	-1.37402900
H	7.11199600	-2.53282600	-2.15841600
H	7.01824900	-2.59789200	-0.39946200
C	5.86011400	-1.50632200	2.07602200
H	6.24064100	-1.83273500	3.05261300
H	6.69320200	-1.54507800	1.37066700
H	5.56179100	-0.45731100	2.18034200
C	3.60586200	-2.35474200	2.76139900
H	2.77366400	-3.03629000	2.57513000
H	4.05532000	-2.63588600	3.72269700
H	3.19232000	-1.34675700	2.87628800

TS2'

Cu	-2.20591200	-0.37078200	-0.25931500
N	-2.71962600	-0.44435500	1.69358800
N	-3.23098900	1.23321300	-0.94849300
N	-3.15618200	-1.93321500	-1.10583500
C	-3.46083500	-0.49910200	2.58172400
C	-4.21531400	1.81753800	-1.12625400
C	-4.10452300	-2.56751100	-1.30569100

C	-5.45827200	2.53885100	-1.31728800
H	-6.01561100	2.09234600	-2.14423700
H	-6.04335600	2.44466500	-0.39969500
H	-5.25508700	3.59106000	-1.53340000
C	-4.41157100	-0.55282500	3.67539300
H	-5.25263100	0.09549400	3.42009400
H	-4.77289000	-1.57725500	3.79392800
H	-3.93974600	-0.21779700	4.60279600
C	-5.30747100	-3.34694600	-1.52242100
H	-5.04974800	-4.36368500	-1.83012100
H	-5.86767000	-3.36467100	-0.58470200
H	-5.91667500	-2.86971800	-2.29375000
B	-6.38590800	-0.49873800	0.54464600
F	-5.77433100	-1.63826400	1.11301000
F	-6.07627800	-0.44220100	-0.83025200
F	-7.77055600	-0.56539900	0.71935400
F	-5.87987500	0.66159100	1.18065800
C	-0.15307700	2.81128200	0.76832600
C	-0.71299500	3.60805800	-0.43937600
C	-0.28280000	2.84954200	-1.72217900
H	0.43824500	3.43054100	1.44602400
H	-0.95498300	2.35326700	1.35079600
H	-1.80137500	3.66299000	-0.37950000
H	-0.31885800	4.62438500	-0.45063700
H	-1.12815000	2.54411600	-2.34357900
H	0.40427100	3.44254800	-2.32697300
N	0.37120100	1.63292700	-1.23602300
C	0.02558300	0.32922900	-1.63889900
O	-0.20491700	-0.00128700	-2.80614400
C	-0.10510700	-0.41294100	-0.40346800
H	0.09735400	-1.47015600	-0.28721700
C	0.66418800	1.66108600	0.16014300
O	0.30630500	0.38027800	0.67715000
C	3.74341600	1.13579400	-1.57998500
H	3.76126700	2.15470500	-1.94291400
H	4.25664900	0.38829400	-2.17301700
C	3.06403700	0.79476600	-0.47530700
C	2.25583800	1.81933200	0.30164300
N	2.57622400	1.49626800	1.85757900
N	2.11819400	0.61046100	2.42180100
C	2.74520100	3.23602400	0.03636200
O	2.20162800	4.01713000	-0.71689800
O	3.85793400	3.49291500	0.72278900
C	4.43982300	4.79976100	0.50685000

H	5.31414500	4.83410200	1.15491400
H	4.73137600	4.91125000	-0.53980600
H	3.72705000	5.58094900	0.77811800
O	2.96310600	-0.44580100	0.03281400
Si	4.06358200	-1.75941700	-0.08850900
C	5.81868200	-1.07131800	0.14261600
H	6.06886400	-0.59177200	-0.81422400
C	3.48423900	-2.93046800	1.28074500
H	3.99125700	-3.88389500	1.07407700
C	3.89000500	-2.54096000	-1.81648600
H	4.66635600	-2.06081700	-2.43127300
C	2.53009400	-2.25913400	-2.47902500
H	2.33025800	-1.19074700	-2.58479700
H	2.49349900	-2.70393900	-3.48180600
H	1.70390500	-2.68985700	-1.90367800
C	4.18194200	-4.05280100	-1.79726900
H	3.41919300	-4.59556900	-1.22817300
H	4.17890100	-4.45959400	-2.81629200
H	5.15523500	-4.28868700	-1.35366500
C	5.94711200	0.00052600	1.23838800
H	6.98471600	0.35268800	1.30457600
H	5.32151200	0.87401100	1.03431300
H	5.67108500	-0.38358900	2.22438200
C	6.82787700	-2.21594000	0.35669000
H	6.81487500	-2.93716400	-0.46744400
H	7.84923500	-1.82136100	0.42844400
H	6.62682000	-2.76647500	1.28243100
C	3.87723900	-2.48944500	2.70066600
H	3.49118100	-3.20199700	3.44111000
H	4.96154600	-2.43539300	2.83232500
H	3.45935100	-1.50814700	2.94747900
C	1.96537900	-3.17329800	1.20058200
H	1.65124500	-3.54192300	0.21891100
H	1.65422500	-3.91544600	1.94673900
H	1.41704000	-2.24864700	1.40566900

4

Cu	-2.06198700	-0.02391100	-0.01819800
N	-2.65654200	0.83614200	-1.66944900
N	-2.76114400	-1.87493200	0.06946100
N	-2.65111600	1.03843700	1.55298400
C	-3.49944700	1.22801400	-2.36174100
C	-3.69666000	-2.55158400	0.17615900
C	-3.53403000	1.52647900	2.12482500

C	-4.89780300	-3.34800900	0.32798100
H	-5.61466600	-2.75536200	0.90222400
H	-5.32095700	-3.57139500	-0.65483300
H	-4.67209800	-4.27998900	0.85304000
C	-4.59421800	1.71238000	-3.17903000
H	-5.00107700	0.88995300	-3.77334500
H	-5.36866100	2.08740100	-2.50541200
H	-4.25105300	2.51061400	-3.84241000
C	-4.66680500	2.13450300	2.79447200
H	-4.34789100	3.02011200	3.35052600
H	-5.39467600	2.41081400	2.02756200
H	-5.12077300	1.41344300	3.47891800
B	-6.08427500	0.19240800	-0.07216300
F	-5.61327300	1.52450700	-0.18356800
F	-5.62345400	-0.35419200	1.14741400
F	-7.48151600	0.18352900	-0.09694600
F	-5.57917000	-0.56852900	-1.14556700
C	0.71826400	-0.97449300	-1.89851400
C	0.83040700	-2.46488500	-2.30056000
C	0.32636500	-3.25571800	-1.07465900
H	1.42900700	-0.33108200	-2.41786000
H	-0.29160200	-0.59684500	-2.08448700
H	0.25206700	-2.69473900	-3.19768600
H	1.87563500	-2.71995400	-2.49907800
H	-0.75440100	-3.43208000	-1.11508900
H	0.83563700	-4.21495400	-0.95268400
N	0.63698800	-2.34968500	0.02557700
C	0.21621900	-2.30846300	1.32167900
O	-0.23408500	-3.20554300	2.01314500
C	0.45454100	-0.81904800	1.67912000
H	-0.14487900	-0.43809800	2.50131100
C	0.95145500	-0.99201700	-0.40348000
O	0.07610600	-0.18698500	0.41874000
C	1.97184800	-0.54376700	1.71818700
H	2.51052200	-1.29317600	2.29351500
H	2.16730500	0.44024400	2.13916200
C	2.33543400	-0.56872500	0.19746700
C	3.43978100	-1.55208600	-0.17511900
N	4.13817400	-1.23104000	-1.23578400
N	4.74098000	-0.91896100	-2.14698400
C	3.72608200	-2.84820200	0.43372500
O	3.21576400	-3.27161300	1.45839100
O	4.64933000	-3.53172600	-0.27821400
C	5.03397500	-4.80745800	0.26823900

H	5.77824600	-5.20546100	-0.42123900
H	5.46599200	-4.68549100	1.26448300
H	4.17241700	-5.47716600	0.32496000
O	2.68549000	0.66429000	-0.37020300
Si	2.80755300	2.27478300	0.13626900
C	3.98818000	2.39940300	1.63148800
H	3.35497600	2.23691500	2.51688400
C	3.51004200	3.09646200	-1.42829500
H	3.42494400	4.18222100	-1.27027200
C	1.08601800	2.90770800	0.64985300
H	0.73738900	2.16209600	1.37712500
C	0.05513000	2.93711300	-0.48983300
H	0.04720200	2.01011400	-1.06662500
H	-0.95573700	3.08059200	-0.08858900
H	0.25310100	3.76630700	-1.17799200
C	1.12362000	4.26812400	1.36705700
H	1.53734400	5.05522700	0.72501900
H	0.10882300	4.58179300	1.64554700
H	1.71787200	4.23784600	2.28491000
C	5.07995800	1.31509300	1.63692300
H	5.72195300	1.41815100	2.52140900
H	4.66324000	0.30421400	1.65163300
H	5.72559100	1.38783500	0.75614200
C	4.61656900	3.79880900	1.78344300
H	3.86973100	4.59738300	1.79718100
H	5.18380400	3.86442100	2.72066000
H	5.31441100	4.01790400	0.96966100
C	4.99522900	2.76052000	-1.66220000
H	5.35776800	3.24707200	-2.57708100
H	5.64102700	3.08402700	-0.84269700
H	5.13899800	1.68236800	-1.79209000
C	2.71446100	2.73008500	-2.69561500
H	1.65979500	3.00523300	-2.63178200
H	3.13714600	3.23724200	-3.57261500
H	2.76658000	1.65230400	-2.88415000

TS3

Cu	-1.97243800	0.03817700	0.11322100
N	-2.56415300	-0.76738300	1.78041400
N	-2.75100100	1.83604400	-0.15914300
N	-2.43944300	-1.14638300	-1.43897000
C	-3.40188100	-1.17499900	2.46974500
C	-3.71787200	2.45425600	-0.32476300
C	-3.28937300	-1.70253000	-1.99882300

C	-4.95508400	3.17529000	-0.54580500
H	-5.62482500	2.51595600	-1.10389400
H	-5.41409400	3.42517000	0.41434700
H	-4.76574500	4.09024300	-1.11345700
C	-4.48689800	-1.68360800	3.28494700
H	-4.98103500	-0.85331500	3.79630300
H	-5.20230800	-2.17150200	2.61827600
H	-4.10892600	-2.39715500	4.02181200
C	-4.38009400	-2.39489100	-2.65649700
H	-4.00683800	-3.27745100	-3.18264000
H	-5.09852200	-2.68767900	-1.88687800
H	-4.86821500	-1.72136000	-3.36528300
B	-5.95995200	-0.40185500	0.06464900
F	-5.42321600	-1.69863200	0.26031000
F	-5.49301100	0.10207200	-1.17127300
F	-7.35571300	-0.46689200	0.05274900
F	-5.52788100	0.44178500	1.10760200
C	0.86735700	1.10024300	1.81116600
C	0.88924100	2.60630500	2.16137600
C	0.33863700	3.32067200	0.91227700
H	1.62458200	0.51827200	2.33613100
H	-0.11099100	0.66259800	2.03249700
H	0.29639600	2.83072300	3.05025400
H	1.91540600	2.93462300	2.34258800
H	-0.75248000	3.41414900	0.93861300
H	0.77574500	4.31004200	0.76479100
N	0.72089900	2.40568300	-0.16578300
C	0.22725000	2.29089700	-1.43872700
O	-0.26654100	3.15101200	-2.14374600
C	0.45332200	0.78702300	-1.73144700
H	-0.18355700	0.36402000	-2.50385200
C	1.06015800	1.07035500	0.31025200
O	0.14845100	0.22366000	-0.42886400
C	1.96386200	0.50778200	-1.85250000
H	2.46721500	1.21609600	-2.50933200
H	2.15145400	-0.50178200	-2.21243100
C	2.42763600	0.60186800	-0.33558400
C	3.57916000	1.52009500	-0.32793100
N	4.05069600	1.43665200	1.68794500
N	4.81663500	1.18589100	2.44764900
C	3.44055500	2.92693700	-0.63116000
O	3.37700700	3.26336000	-1.81273600
O	3.54756200	3.78581400	0.39676200
C	3.59363700	5.18145000	0.02800700

H	3.62622700	5.72633500	0.97093100
H	4.48818500	5.39163600	-0.56312400
H	2.70480600	5.45859600	-0.54227500
O	2.77077600	-0.60970200	0.27588500
Si	2.84311500	-2.25185800	-0.11730400
C	3.93741200	-2.52737100	-1.65684900
H	3.25515100	-2.41477100	-2.51369900
C	3.61675600	-2.96380100	1.46726400
H	3.54286500	-4.05889200	1.39043000
C	1.08898400	-2.88687700	-0.51121100
H	0.70507400	-2.15978400	-1.23963800
C	0.12693300	-2.87143600	0.68674500
H	0.13908200	-1.91570900	1.21490400
H	-0.90328100	-3.04927300	0.35505200
H	0.37898300	-3.66045100	1.40406100
C	1.06626500	-4.26850100	-1.18760600
H	1.50584400	-5.04275200	-0.54729400
H	0.03204000	-4.57362400	-1.39585000
H	1.60490800	-4.27580600	-2.13968300
C	5.06548900	-1.49463700	-1.82580200
H	5.58558800	-1.64615100	-2.78072200
H	4.70136500	-0.46408700	-1.80174100
H	5.81344600	-1.58662600	-1.03157600
C	4.51250000	-3.95666800	-1.72655300
H	3.74388500	-4.72953200	-1.64063100
H	5.03122900	-4.11503700	-2.68077000
H	5.24362400	-4.13198700	-0.93093300
C	5.10502400	-2.58634100	1.59363700
H	5.52334800	-2.97813900	2.52996800
H	5.71277400	-2.97724900	0.77409400
H	5.23137100	-1.49815000	1.61124500
C	2.88026300	-2.51797700	2.74415200
H	1.82798500	-2.80855200	2.75137100
H	3.35292200	-2.95719400	3.63230500
H	2.92565900	-1.42917500	2.85378600

5

Cu	-1.81485400	0.01226100	0.14966600
N	-2.44876600	-0.81861000	1.79416800
N	-2.64273500	1.79273300	-0.10638800
N	-2.15206700	-1.15707200	-1.43152400
C	-3.31036400	-1.26747100	2.42622100
C	-3.62691300	2.37096600	-0.31020800
C	-2.92580700	-1.74225500	-2.06641500

C	-4.88221000	3.04093500	-0.58332300
H	-5.49159200	2.36332100	-1.18690600
H	-5.40093600	3.25252500	0.35537400
H	-4.70504500	3.97370600	-1.12532500
C	-4.42190000	-1.83087000	3.16617900
H	-4.98093900	-1.02922200	3.65589300
H	-5.07342500	-2.33846600	2.45034600
H	-4.06080900	-2.53920600	3.91642700
C	-3.92430800	-2.47271500	-2.82173700
H	-3.45977400	-3.30048600	-3.36393300
H	-4.66511600	-2.85311600	-2.11425700
H	-4.41589600	-1.79843500	-3.52742000
B	-5.72637800	-0.59012300	-0.14448300
F	-5.12887200	-1.85783200	0.06219500
F	-5.22261600	-0.03582400	-1.34364000
F	-7.11339800	-0.73350800	-0.23618700
F	-5.40006800	0.25702500	0.93415900
C	0.94183200	1.12772000	2.00619800
C	0.92845700	2.62274300	2.39765400
C	0.35042500	3.35187300	1.16983200
H	1.70305900	0.54681400	2.52617700
H	-0.03366500	0.66618600	2.18903500
H	0.33842900	2.80867200	3.29706300
H	1.94963700	2.96824800	2.57489100
H	-0.74423200	3.39154000	1.19073400
H	0.74063400	4.36424300	1.05382800
N	0.78159300	2.48729700	0.06825600
C	0.33870700	2.39758000	-1.22454800
O	-0.16757900	3.25627000	-1.92116100
C	0.64905000	0.91652600	-1.55629300
H	0.06450900	0.48736400	-2.36641200
C	1.17132300	1.15805400	0.51044500
O	0.33517100	0.29232500	-0.28846600
C	2.17476500	0.71665800	-1.65407300
H	2.65189500	1.46334400	-2.28939000
H	2.43759900	-0.27363300	-2.01870000
C	2.59088600	0.77346500	-0.08960200
C	3.66398700	1.72466700	-0.16755700
C	3.45458400	3.12643000	-0.42207700
O	3.43080100	3.58580000	-1.56060400
O	3.47660300	3.86136400	0.70521300
C	3.45632100	5.29375200	0.51493300
H	3.42948700	5.71637600	1.51864300
H	4.35612000	5.62150500	-0.01098600

H	2.57187900	5.59529100	-0.04973900
O	2.96593800	-0.44413200	0.48018700
Si	3.11598800	-2.06569100	0.01622400
C	4.22865300	-2.23922100	-1.52670400
H	3.54700100	-2.14357700	-2.38608100
C	3.92609900	-2.81515700	1.56265600
H	3.97848000	-3.90148500	1.39668200
C	1.39179300	-2.75226900	-0.42136900
H	1.00413000	-2.02394300	-1.14686600
C	0.40045600	-2.78819500	0.75272500
H	0.40016700	-1.86031300	1.32885600
H	-0.62102800	-2.94758000	0.38724900
H	0.63240000	-3.61222000	1.43610600
C	1.42409400	-4.12101500	-1.12287700
H	1.87193400	-4.89433200	-0.48726600
H	0.40368700	-4.45128200	-1.35901100
H	1.98237000	-4.09528900	-2.06308700
C	5.31187600	-1.15570600	-1.67158500
H	5.83583700	-1.26336100	-2.63027700
H	4.90848000	-0.14066900	-1.62225300
H	6.06427300	-1.23552100	-0.88044900
C	4.87065300	-3.63884000	-1.61561100
H	4.13808300	-4.44785200	-1.55006300
H	5.40513900	-3.75663300	-2.56690500
H	5.60070300	-3.79168300	-0.81438200
C	5.36134500	-2.28640900	1.74768600
H	5.80546300	-2.69087400	2.66651500
H	6.01963600	-2.55807600	0.91865100
H	5.36829500	-1.19387000	1.83266600
C	3.12239500	-2.56135300	2.85066900
H	2.12737000	-3.00977900	2.82315400
H	3.64927500	-2.97785400	3.71905300
H	2.99905400	-1.48721300	3.02832500

TS4

Cu	-1.90549500	-0.03432300	0.19241400
N	-2.44308100	-0.95603900	1.81331200
N	-2.60460000	1.79710400	-0.01490000
N	-2.14043700	-1.08372900	-1.46500100
C	-3.31407200	-1.46407400	2.38603700
C	-3.56314200	2.41181900	-0.23506800
C	-2.89343300	-1.60885500	-2.17324900
C	-4.78938200	3.12402700	-0.52956500
H	-5.40687100	2.46921600	-1.15035900

H	-5.32005100	3.34854100	0.39960100
H	-4.57063800	4.05293200	-1.06307100
C	-4.44014700	-2.09698200	3.04190500
H	-4.96154300	-1.36861000	3.66880600
H	-5.11561700	-2.45304900	2.25938500
H	-4.10088400	-2.93516100	3.65634300
C	-3.87038900	-2.26710700	-3.01675300
H	-3.40698700	-3.09686500	-3.55697500
H	-4.66939800	-2.63825400	-2.36995500
H	-4.28598300	-1.54967100	-3.72892300
B	-5.70990100	-0.54630000	-0.21231300
F	-5.14222900	-1.83886600	-0.08847300
F	-5.19404200	0.07042000	-1.37608300
F	-7.09954600	-0.64957300	-0.30803600
F	-5.36021300	0.22304600	0.91591900
C	0.81977200	1.29127400	2.19338100
C	0.88581400	2.80675000	2.49943500
C	0.29295800	3.49896500	1.25147100
H	1.57580600	0.69862500	2.70685900
H	-0.16912000	0.87738300	2.42254100
H	0.34139600	3.06815000	3.40807500
H	1.92922800	3.10893100	2.61792200
H	-0.79547800	3.60179400	1.31280000
H	0.74401800	4.46856600	1.04696700
N	0.61442100	2.53355600	0.19751300
C	0.31516700	2.40967600	-1.13391900
O	-0.06432400	3.26223700	-1.91429400
C	0.64750200	0.92214900	-1.39061800
H	0.05376200	0.44881700	-2.16712900
C	0.98453000	1.27542900	0.70544300
O	0.34728000	0.33452100	-0.09187200
C	2.18673600	0.73102600	-1.48733700
H	2.65492300	1.52763300	-2.06657600
H	2.40428800	-0.21456500	-1.98109400
C	2.68858400	0.71947000	-0.02876200
C	3.45547400	1.73440600	0.54212700
C	3.66858100	2.97407100	-0.14370400
O	4.47963800	3.01121000	-1.07287100
O	3.09012900	4.07235300	0.38202300
C	3.36031700	5.30819000	-0.30749300
H	2.83195000	6.07781200	0.25511500
H	4.43193900	5.51888200	-0.32004600
H	2.98325300	5.26793600	-1.33286700
O	2.82391900	-0.52794400	0.55063000

Si	3.08614000	-2.09646300	-0.02694400
C	4.33397700	-2.07888400	-1.47348700
H	3.72660700	-1.95253600	-2.38264800
C	3.79488200	-2.94945900	1.51699300
H	3.92841700	-4.01194200	1.26542800
C	1.43063500	-2.79490500	-0.66320300
H	1.07595200	-2.02314800	-1.36166800
C	0.34590400	-2.95722300	0.41487300
H	0.26973300	-2.08081600	1.06243300
H	-0.63630800	-3.11099000	-0.04812400
H	0.54764400	-3.82996600	1.04493000
C	1.58344900	-4.09760700	-1.46736800
H	2.00449600	-4.90394600	-0.85492800
H	0.60574000	-4.44459700	-1.82738100
H	2.22744500	-3.97128600	-2.34279300
C	5.35130400	-0.92414200	-1.43082800
H	6.01860500	-0.97270900	-2.30137300
H	4.88463100	0.06430100	-1.43658200
H	5.98147900	-0.97464900	-0.53773700
C	5.06859400	-3.42813900	-1.60965000
H	4.38367500	-4.27880100	-1.67231700
H	5.68765000	-3.43831300	-2.51583000
H	5.73659900	-3.60690100	-0.76110900
C	5.17169300	-2.36139700	1.88253700
H	5.55663100	-2.82571200	2.79983000
H	5.91941900	-2.51525400	1.10040300
H	5.09882800	-1.28344200	2.06578900
C	2.86682200	-2.85526400	2.74188700
H	1.91255400	-3.36310400	2.58936000
H	3.34613800	-3.30801800	3.61965900
H	2.65317400	-1.80967000	2.99016900

6

Cu	-2.39061000	-0.78782200	-0.16228200
N	-2.94406400	-0.93223900	1.65594200
N	-2.74108700	1.22370700	-0.63764000
N	-1.77909400	-1.74112400	-1.67840900
C	-3.75317700	-1.02547000	2.47920600
C	-3.68431800	1.82443100	-0.95118700
C	-1.39724900	-2.34027700	-2.59153300
C	-4.87659000	2.54083000	-1.35535600
H	-5.54177700	1.82520000	-1.84447500
H	-5.37679100	2.95121700	-0.47506000
H	-4.61522800	3.34738400	-2.04540900

C	-4.80282000	-1.14466000	3.46857600
H	-5.12592500	-0.14965700	3.78625900
H	-5.63998400	-1.66396500	2.99478900
H	-4.44891300	-1.71231600	4.33320500
C	-0.90333500	-3.09619200	-3.72567600
H	0.06614200	-3.53678200	-3.47599900
H	-1.61059400	-3.89467400	-3.96744200
H	-0.79352300	-2.43587300	-4.59060000
B	-6.07677600	-0.68481000	-0.10132400
F	-5.71997400	-1.90569700	0.50943900
F	-5.38944700	-0.57213600	-1.33631300
F	-7.45390600	-0.64286300	-0.32555100
F	-5.69517600	0.38600700	0.73748000
C	-0.27429400	1.48957400	2.19500700
C	-0.07759800	3.01329600	2.43660200
C	-0.30053500	3.69603400	1.06063400
H	0.40574000	0.84535500	2.75545700
H	-1.30222300	1.15224800	2.37986000
H	-0.75977600	3.39923300	3.19335000
H	0.95037300	3.19002300	2.75649600
H	-1.32576100	4.04212100	0.90877700
H	0.40880400	4.49408100	0.85547400
N	-0.04457400	2.57621300	0.14020200
C	0.14528300	2.40869800	-1.24888700
O	0.08691900	3.25966200	-2.09731400
C	0.45041000	0.91720700	-1.38606400
H	-0.22536700	0.43540100	-2.09045200
C	-0.02882600	1.40048500	0.74264400
O	0.12273300	0.38187900	-0.04012600
C	1.93771100	0.62484800	-1.66015500
H	2.25215600	1.31178600	-2.45198600
H	2.00681100	-0.39047100	-2.05861300
C	2.78974900	0.83072200	-0.41575100
C	3.34359400	1.97420300	-0.02895300
C	3.33766000	3.13988700	-0.84205600
O	4.03814900	3.38391300	-1.83173700
O	2.49860900	4.13958400	-0.34039300
C	2.47537100	5.34434100	-1.10555000
H	1.75507500	6.00333600	-0.61437500
H	3.45803300	5.82662700	-1.12307600
H	2.15761700	5.16138500	-2.13626400
O	2.85947700	-0.31425100	0.39585200
Si	3.16712400	-1.93026700	0.06817600
C	4.25421900	-2.15704400	-1.48928400

H	3.54456000	-2.22407500	-2.32873900
C	4.07380100	-2.52684700	1.63048400
H	4.33082800	-3.58537300	1.48047900
C	1.49096700	-2.78472100	-0.27155900
H	1.05936900	-2.16224400	-1.06941500
C	0.49932200	-2.75572600	0.90322800
H	0.45108200	-1.77489500	1.38248900
H	-0.51192100	-3.00870300	0.55985400
H	0.77307400	-3.49027600	1.66701800
C	1.60985600	-4.21452700	-0.82453700
H	2.10721700	-4.88197300	-0.11038700
H	0.61636900	-4.64071500	-1.01946700
H	2.17389700	-4.25411000	-1.76160100
C	5.21304900	-0.99123000	-1.79134200
H	5.76066100	-1.17831000	-2.72493100
H	4.69943800	-0.03203900	-1.89026800
H	5.95854900	-0.86922700	-0.99887200
C	5.03905100	-3.48339100	-1.44606700
H	4.39981500	-4.35002400	-1.25249500
H	5.55413900	-3.66100600	-2.39920000
H	5.80639300	-3.46135400	-0.66468100
C	5.38238700	-1.73125500	1.80173400
H	5.89238800	-2.01671100	2.73127400
H	6.08232100	-1.90037900	0.97845600
H	5.18219500	-0.65552700	1.84851000
C	3.22800300	-2.41964700	2.91219100
H	2.39983100	-3.13218200	2.92413400
H	3.84528500	-2.61898900	3.79840600
H	2.80705900	-1.41643800	3.02968200

TS5

Cu	-1.98229700	-1.18092500	-0.57943900
N	-2.35077000	-1.50537400	1.27688800
N	-2.76728000	0.56081300	-1.16581700
N	-1.06181900	-2.12297600	-1.96700900
C	-2.96226200	-1.63398500	2.25105400
C	-3.69334200	1.24095800	-1.31686000
C	-0.46650600	-2.65932800	-2.80221500
C	-4.87976900	2.05596700	-1.48481300
H	-5.75413500	1.41486100	-1.33698100
H	-4.88812200	2.85443800	-0.73764500
H	-4.89621100	2.49352900	-2.48655500
C	-3.79590400	-1.77807000	3.42737800
H	-3.70303300	-0.88914200	4.05775100

H	-4.83094000	-1.87943100	3.08649500
H	-3.49905400	-2.66257000	3.99731300
C	0.29769200	-3.32162600	-3.84202100
H	1.31630300	-2.92396400	-3.85351000
H	0.33176000	-4.39692600	-3.64714800
H	-0.17172700	-3.14318600	-4.81379200
B	-5.74137900	-0.94255600	0.36979600
F	-6.30075900	-1.78052800	1.35083000
F	-4.85774400	-1.69531300	-0.43885200
F	-6.75363700	-0.39483700	-0.43924200
F	-5.04189200	0.10544100	1.00237300
C	-0.51861400	1.53978600	2.01654200
C	-0.98247000	3.01959300	2.03398100
C	-1.28158500	3.37426200	0.55703500
H	0.19019300	1.28197100	2.80168400
H	-1.36542900	0.84247000	2.05726200
H	-1.85612200	3.16756400	2.66943100
H	-0.16417300	3.64755800	2.38743900
H	-2.31766900	3.15920300	0.27854200
H	-1.03198400	4.39997600	0.29773900
N	-0.41578700	2.42703900	-0.15507000
C	-0.11834900	2.14426300	-1.47733000
O	-0.38188900	2.80610900	-2.45872800
C	0.67284100	0.83087600	-1.37662600
H	0.36665800	0.09991700	-2.11947800
C	0.06309600	1.44119000	0.65142200
O	0.30246600	0.33316500	-0.05535500
C	2.23227400	1.06167400	-1.35680700
H	2.46821600	1.95464200	-1.93775200
H	2.71149700	0.20041700	-1.82367500
C	2.60056800	1.25518500	0.09471600
C	2.32289700	2.38618100	0.79902100
C	2.33971800	3.64702200	0.11216600
O	3.19303900	4.02357200	-0.70119700
O	1.38180200	4.53476500	0.55273800
C	1.37738700	5.80327300	-0.10606200
H	0.58776200	6.38690700	0.37172600
H	2.33692500	6.31475900	0.00900600
H	1.16326100	5.69560100	-1.17467300
O	2.92387000	0.12897500	0.77518900
Si	3.54400700	-1.40854600	0.39546400
C	4.87952600	-1.25118900	-0.95902800
H	4.33478200	-1.30269200	-1.91429300
C	4.25685200	-1.95182300	2.06919500

H	4.57344400	-2.99941800	1.95516200
C	2.11513300	-2.48209300	-0.26457600
H	1.65539300	-1.85375300	-1.04011500
C	1.02662600	-2.79689300	0.77364600
H	0.70190600	-1.90756800	1.31882500
H	0.14401900	-3.22576400	0.28532700
H	1.38393600	-3.53303800	1.50119500
C	2.58245000	-3.77808600	-0.94888400
H	3.11961700	-4.43174400	-0.25155000
H	1.72067300	-4.34748400	-1.32068900
H	3.24194300	-3.58661200	-1.80043800
C	5.65096400	0.08072700	-0.93639400
H	6.35110600	0.13077200	-1.78019000
H	4.99603300	0.95424900	-1.00146800
H	6.23925900	0.18741800	-0.01990800
C	5.86235900	-2.43909600	-0.93674000
H	5.35602000	-3.40784300	-0.97646600
H	6.54395200	-2.38961500	-1.79542300
H	6.48129500	-2.42883100	-0.03411400
C	5.49210200	-1.11414700	2.45362300
H	5.87702000	-1.42967800	3.43187500
H	6.30958700	-1.20835300	1.73474100
H	5.23637400	-0.05142000	2.53152300
C	3.22724700	-1.87519600	3.21259600
H	2.38890100	-2.56034600	3.07472300
H	3.70304800	-2.12454900	4.16985100
H	2.82110500	-0.86171100	3.30228300

7

Cu	-1.24176100	1.35553700	-1.81337200
N	-0.78601600	-0.53647100	-1.97029300
N	-3.14416700	1.50650200	-1.47230100
N	-0.01834500	2.67742900	-2.51876300
C	-0.81415800	-1.69342200	-1.97244200
C	-4.23597000	1.35230100	-1.12146300
C	0.75480200	3.41233800	-2.96868600
C	-5.59164600	1.13568800	-0.65542000
H	-5.78920300	0.06010200	-0.62386400
H	-5.69822400	1.55322700	0.35025300
H	-6.30079200	1.62780800	-1.32680300
C	-0.88473100	-3.14131500	-1.99699100
H	0.08601200	-3.56349000	-1.73169600
H	-1.63603500	-3.46746000	-1.27527300
H	-1.17168800	-3.47194000	-2.99924000

C	1.73691800	4.32532300	-3.52312600
H	2.74120700	3.91546300	-3.38145500
H	1.54977500	4.45902000	-4.59251600
H	1.66572800	5.29428100	-3.02083000
B	-4.08971200	-2.18739300	-0.67664100
F	-3.65775400	-3.47314300	-0.28880100
F	-3.73352000	-1.95563300	-2.01548100
F	-5.48641500	-2.09040200	-0.53105200
F	-3.47146800	-1.22555800	0.14989700
C	-2.44674100	1.18227800	1.99242400
C	-2.45171100	1.23029200	3.53335800
C	-1.21996900	2.07447300	3.92468700
H	-2.94862200	0.31006000	1.58479100
H	-2.91281100	2.08456900	1.58570200
H	-3.37438900	1.66471500	3.92508200
H	-2.35132900	0.22109900	3.93292600
H	-1.46872100	3.12695700	4.10129000
H	-0.71801200	1.68989900	4.81663000
N	-0.35667300	1.98030700	2.74600600
C	0.50633200	2.92925700	2.29796300
O	1.10131700	3.77515900	2.95194200
C	0.53591500	2.72506600	0.77160600
H	0.67810500	3.66836200	0.24574300
C	-0.97122600	1.27451700	1.59698500
O	-0.78853200	2.22974400	0.51797000
C	1.54439200	1.65841900	0.34360800
H	2.50382900	1.82114200	0.84574800
H	1.72262200	1.73933300	-0.73132000
C	1.04167500	0.25772700	0.61802300
C	-0.16733900	0.02581500	1.20655300
C	-0.62302500	-1.35314200	1.44756600
O	-0.26488700	-2.34639200	0.83239600
O	-1.49159900	-1.43518700	2.47899500
C	-2.08654600	-2.72834700	2.68688500
H	-2.82430200	-2.58425300	3.47713900
H	-2.56858200	-3.07691100	1.77309000
H	-1.33129000	-3.45124500	3.00727900
O	1.83707500	-0.73482600	0.22072200
Si	3.52352500	-0.85133600	-0.04796300
C	4.43161500	-0.15971000	1.47838400
H	4.61748600	0.90283500	1.26172600
C	3.77774500	-2.71548500	-0.24612400
H	4.86667800	-2.86770700	-0.24274200
C	3.96604800	0.15788100	-1.59926900

H	3.97507100	1.20558500	-1.26482300
C	2.93480000	0.04053700	-2.73629000
H	1.91219900	0.22680300	-2.39721800
H	3.16060600	0.75828000	-3.53577500
H	2.94745500	-0.95654500	-3.18577100
C	5.38249300	-0.17720100	-2.10123800
H	5.46271000	-1.22736800	-2.40289400
H	5.63918900	0.43288400	-2.97668300
H	6.14631700	0.00886500	-1.33908900
C	3.60961900	-0.23511800	2.77853700
H	4.18352000	0.18108500	3.61612900
H	2.66991700	0.32178400	2.72121300
H	3.35823800	-1.26867900	3.03735700
C	5.80249100	-0.83638200	1.67727600
H	6.42947700	-0.79171000	0.78071400
H	6.35643300	-0.34992500	2.48975900
H	5.68804600	-1.89166500	1.94831800
C	3.17929700	-3.48495600	0.94613300
H	3.34960900	-4.56327000	0.83198400
H	3.62717000	-3.18162000	1.89770700
H	2.09979600	-3.31770400	1.01553600
C	3.23126700	-3.26524100	-1.57410000
H	3.75954800	-2.85337200	-2.43846000
H	3.33757800	-4.35704000	-1.61181600
H	2.16771100	-3.03643200	-1.69421500

TS6

Rh	-1.14575200	0.07059100	-0.01094700
O	-1.65855700	0.99387300	1.72844200
O	-1.26089300	-1.73697100	0.96464200
O	-0.74780000	-0.86333900	-1.79007100
O	-1.17175100	1.87486100	-0.97079100
Rh	-3.46410000	-0.13450300	-0.49731700
C	-2.26169200	2.31093900	-1.46207800
O	-3.37787200	1.69552000	-1.41828800
C	-1.71860900	-1.21079100	-2.54109200
O	-2.94666800	-1.02512200	-2.26993800
C	-2.88198400	1.10136100	2.05265000
O	-3.85900000	0.73194600	1.32181800
O	-3.45026200	-1.93865100	0.45194100
C	-2.38287400	-2.34403000	1.01046500
C	-3.20717900	1.70760900	3.41973400
C	-2.24694500	3.66869700	-2.17118700
C	-1.35824900	-1.89176100	-3.86429300

C	-2.44406700	-3.65454600	1.80012900
C	-4.09577000	2.97249700	3.20310300
H	-4.27701200	3.40975000	4.19064000
H	-5.06120500	2.64606300	2.80551300
C	-1.92129400	2.06336700	4.17683000
H	-2.18247800	2.46912800	5.15997000
H	-1.28852000	1.18402200	4.32074400
H	-1.33389300	2.81348500	3.64350500
C	-4.00967200	0.66213700	4.21926900
H	-4.27532600	1.07142700	5.19932100
H	-4.92872600	0.38480100	3.69663800
H	-3.41427200	-0.24317500	4.37908000
C	-3.29881800	4.60047000	-1.49330500
H	-3.24704200	5.56531000	-2.00895300
H	-4.29238000	4.18194600	-1.67666400
C	-2.66244400	3.43542300	-3.63791200
H	-2.66353400	4.38829100	-4.17688600
H	-1.95762000	2.76289600	-4.13877300
H	-3.66189100	2.99774400	-3.70088500
C	-0.84992100	4.29648500	-2.12687300
H	-0.12844100	3.66819800	-2.65193900
H	-0.87526700	5.27385300	-2.61992800
H	-0.49441500	4.43335900	-1.10403000
C	-2.61914200	-2.23209000	-4.66663600
H	-2.33191100	-2.71885500	-5.60440300
H	-3.28011800	-2.90489000	-4.11674600
H	-3.18306400	-1.32732500	-4.90945100
C	-0.47114700	-0.92063700	-4.66921600
H	0.43593200	-0.66491000	-4.11703500
H	-0.18404700	-1.38472200	-5.61838000
H	-1.01098600	0.00552800	-4.89372900
C	-0.53107100	-3.17920300	-3.55568500
H	-0.32127700	-3.65944600	-4.51729500
H	0.42796400	-2.87080000	-3.12902400
C	-1.45060400	-4.67187300	1.15762100
H	-0.43447200	-4.31234900	1.33477400
H	-1.56393300	-5.61592700	1.70066800
C	-1.99986500	-3.35723800	3.24597600
H	-2.70484700	-2.67524000	3.73335400
H	-1.97247200	-4.28683900	3.82372000
H	-1.01049900	-2.89630800	3.27428300
C	-3.86758600	-4.22441500	1.80351200
H	-3.88271100	-5.15418600	2.38166600
H	-4.56877800	-3.52332700	2.26417800

H	-4.22020100	-4.44073700	0.79322300
C	-3.48987500	4.00176900	2.27762900
C	-3.69813300	3.90548600	0.89580500
C	-2.68085800	5.03928000	2.75986500
C	-3.09845100	4.79105600	-0.00795400
H	-4.33364200	3.11479500	0.51312600
C	-2.09192900	5.94469400	1.87509500
H	-2.52099300	5.14316900	3.82942500
C	-2.29323800	5.81969000	0.49949100
H	-1.47756300	6.75401500	2.25987900
H	-1.83417300	6.52888600	-0.18350300
C	-1.64907900	-4.89134100	-0.32418800
C	-1.02035700	-4.03757400	-1.23831200
C	-2.47046100	-5.91087400	-0.82205000
C	-1.20247100	-4.15897800	-2.62077700
H	-0.38158000	-3.25153400	-0.85910200
C	-2.65395300	-6.05786400	-2.19866400
H	-2.95640200	-6.59536000	-0.13236800
C	-2.02819400	-5.18765700	-3.09383200
H	-3.28267000	-6.85941200	-2.57630300
H	-2.17109900	-5.31447200	-4.16331800
C	2.09922200	-1.96442500	-0.33338700
C	2.29475000	-3.21559800	0.58113300
C	1.95284400	-2.78691500	2.04242600
H	2.96070900	-1.76271800	-0.97493800
H	1.21812300	-2.03956500	-0.97606000
H	1.64615100	-4.03166500	0.25898700
H	3.32527300	-3.57014400	0.52748700
H	1.03602900	-3.24736600	2.41345900
H	2.75954500	-3.01030000	2.74308200
N	1.74351800	-1.34823200	1.92415900
C	1.28520300	-0.32139600	2.77550700
O	1.04422300	-0.43150900	3.98265000
C	1.28644000	0.80810600	1.87292700
H	0.74922800	1.73413900	1.99272000
C	1.91401300	-0.88855100	0.66918900
O	1.31633000	0.31067300	0.55688100
C	3.47394500	1.22551200	1.74627500
H	3.66316100	1.22053800	2.80928100
H	3.27406100	2.18622200	1.28793300
C	4.02124700	0.22196400	0.95858900
C	4.77874600	-0.91338300	1.52535500
N	5.37604200	-1.71391600	0.67386900
N	5.91183300	-2.38997600	-0.07224100

C	4.88314700	-1.27738800	2.93921600
O	4.50381200	-0.58374600	3.86729300
O	5.45418200	-2.49388800	3.09600200
C	5.64023600	-2.91862900	4.45999800
H	6.10792500	-3.90082700	4.39579400
H	6.29108200	-2.22237600	4.99446400
H	4.67970100	-2.98798400	4.97578600
O	4.27272200	0.33641000	-0.38802500
Si	4.60477300	1.66459100	-1.39181900
C	5.61963800	2.98312000	-0.46114200
H	4.87449800	3.59204900	0.07218500
C	5.57769800	0.84721300	-2.80703500
H	5.65860900	1.59916800	-3.60627000
C	2.92698600	2.39856100	-1.89868500
H	2.44101600	2.62091800	-0.93651300
C	2.01971600	1.40599600	-2.64678200
H	2.00547000	0.41970000	-2.17691200
H	0.98651000	1.76650600	-2.66604300
H	2.34854700	1.28270400	-3.68440900
C	3.04310700	3.71960300	-2.67894300
H	3.61939200	3.59373200	-3.60378600
H	2.05160800	4.08951900	-2.96645700
H	3.52411700	4.50581100	-2.08952400
C	6.59304900	2.42057400	0.58981200
H	7.12169300	3.23936300	1.09519500
H	6.07859600	1.83826700	1.35796800
H	7.35302600	1.77704400	0.13614800
C	6.36734800	3.91802500	-1.43302100
H	5.70801200	4.37230500	-2.17780600
H	6.85154200	4.73489300	-0.88275800
H	7.15446700	3.38420800	-1.97540800
C	7.00312800	0.45034100	-2.37674000
H	7.53368100	-0.03043400	-3.20883600
H	7.60420400	1.30469600	-2.05651100
H	6.97942300	-0.26989800	-1.55112100
C	4.86832500	-0.39363000	-3.38222400
H	3.88689400	-0.16472900	-3.80248700
H	5.47365100	-0.84375300	-4.17972300
H	4.73147100	-1.15581100	-2.60702100
8			
Cu	-0.38043400	-1.30197000	0.03651900
N	0.73173200	-2.03137200	-1.49624700
N	-0.44163000	0.77087800	-0.52382000

N	0.85419200	-1.26848100	1.56342500
C	1.66329200	-2.06016200	-2.18499500
C	0.01979800	1.83000600	-0.62258200
C	1.72598900	-1.02277800	2.28464600
C	0.59303900	3.15794900	-0.75085800
H	0.45774000	3.70429600	0.18669500
H	1.66288900	3.07042100	-0.95723800
H	0.09541000	3.69856200	-1.56075400
C	2.85481700	-2.04973100	-3.01301500
H	3.51332200	-1.26192500	-2.63719300
H	3.36315800	-3.01588700	-2.95120100
H	2.58900900	-1.84552200	-4.05385300
C	2.83875000	-0.69785000	3.15700200
H	2.53010900	0.06930100	3.87274300
H	3.15918000	-1.59088100	3.70071400
H	3.65988300	-0.31094100	2.54694600
B	3.45327600	1.18123400	0.08762400
F	3.04432500	0.14229800	-0.77359000
F	2.41266100	1.48653500	0.98917400
F	4.58642000	0.77243900	0.81323000
F	3.75114900	2.32696500	-0.67335000
C	-3.81192400	1.38594600	-1.48090500
C	-3.85904600	2.38336900	-0.28333700
C	-3.86757000	1.51670900	1.00876400
H	-4.80087000	1.19894300	-1.91508400
H	-3.14213000	1.69697200	-2.28514500
H	-2.96020900	3.00321500	-0.29616300
H	-4.72877700	3.03870500	-0.33190400
H	-3.21026500	1.90117000	1.78976800
H	-4.86883600	1.37104300	1.42221200
N	-3.35603200	0.23703100	0.51190400
C	-2.90849100	-1.00916700	1.09713700
O	-2.94998900	-1.24717800	2.29843000
C	-2.41107100	-1.72530400	-0.06005000
H	-2.59283700	-2.78594200	-0.19330700
C	-3.32943400	0.15690900	-0.80163400
O	-2.88480100	-0.97737900	-1.23861400

9

Rh	-0.20103100	0.02272400	0.61590500
O	-1.68223600	-1.36835600	0.83963700
O	1.17782700	-1.49176600	0.43539800
O	1.25865500	1.42968700	0.24200500
O	-1.60215700	1.51995600	0.62793600

Rh	-0.51029600	-0.14738600	-1.78605300
C	-2.13297900	1.88531900	-0.46974500
O	-1.88323000	1.38386900	-1.61198300
C	1.53087500	1.74496600	-0.96524100
O	0.97092600	1.25984900	-1.99435100
C	-2.22623800	-1.87627700	-0.19288100
O	-1.94692900	-1.57380600	-1.39644900
O	0.89704900	-1.64081800	-1.80295500
C	1.43345000	-1.99417500	-0.70766300
C	-3.30238700	-2.94780100	0.02073800
C	-3.15192000	3.03125100	-0.42461000
C	2.61211000	2.81502600	-1.16041000
C	2.46226600	-3.13119900	-0.72677000
C	-4.61576500	-2.48444700	-0.68399700
H	-5.36844300	-3.25887200	-0.50105500
H	-4.42910400	-2.45563800	-1.76130100
C	-3.54156700	-3.19844500	1.51412400
H	-4.31651700	-3.96265500	1.63662300
H	-2.62931100	-3.55399500	2.00077600
H	-3.86658400	-2.29252600	2.02967300
C	-2.81375000	-4.24609500	-0.65182300
H	-3.56558300	-5.03289300	-0.52977700
H	-2.63883800	-4.09481800	-1.72006600
H	-1.88111000	-4.59337700	-0.19423500
C	-4.48920700	2.53641700	-1.05735600
H	-5.20112800	3.36646900	-0.99413500
H	-4.30808000	2.33854100	-2.11757700
C	-2.59682900	4.18653500	-1.28170700
H	-3.30370800	5.02292000	-1.28122300
H	-1.64424400	4.54740700	-0.87836700
H	-2.43480600	3.86821600	-2.31470200
C	-3.37503700	3.51734800	1.01211000
H	-2.44479500	3.89391300	1.44631200
H	-4.10707000	4.33199900	1.01163400
H	-3.74910700	2.71938000	1.65652200
C	2.90349000	3.03761100	-2.64860300
H	3.68036400	3.80169000	-2.75815500
H	3.25004500	2.12247100	-3.13336400
H	2.00902000	3.38088900	-3.17499300
C	2.09166000	4.12244700	-0.52949300
H	1.87589300	3.98876500	0.53387900
H	2.84274600	4.91202700	-0.63702500
H	1.17471600	4.45563300	-1.02710700
C	3.90279000	2.37760900	-0.40340100

H	4.65452800	3.15591400	-0.57227800
H	3.67739600	2.36871500	0.66513000
C	3.76539000	-2.64672900	-0.01994200
H	3.52535800	-2.45912900	1.03006000
H	4.47696000	-3.47881200	-0.05221000
C	1.87057000	-4.30063900	0.08661300
H	0.94209100	-4.66083600	-0.36961400
H	2.58155000	-5.13325300	0.11153600
H	1.65347400	-3.99228800	1.11232500
C	2.75425900	-3.58776000	-2.16009200
H	3.49017700	-4.39863100	-2.14228600
H	1.84727900	-3.95980300	-2.64374300
H	3.15302400	-2.77493400	-2.77073700
C	-5.13129200	-1.13990200	-0.22636700
C	-4.66765200	0.03147800	-0.83827200
C	-6.04811400	-1.02484200	0.82720200
C	-5.06953300	1.30195700	-0.40698400
H	-3.96571000	-0.04641100	-1.66064900
C	-6.47610800	0.23253800	1.25707300
H	-6.43435500	-1.92203100	1.30302800
C	-5.98638700	1.39000700	0.64916400
H	-7.19749400	0.31052600	2.06589400
H	-6.32461100	2.36584400	0.98672300
C	4.38670900	-1.41055800	-0.62711100
C	3.94865500	-0.13990500	-0.23205700
C	5.37944600	-1.49843300	-1.61195300
C	4.45136500	1.03112600	-0.81433200
H	3.18290400	-0.06424100	0.52986200
C	5.90721600	-0.34150600	-2.18815900
H	5.74333700	-2.47432400	-1.92128200
C	5.44354100	0.91576500	-1.79696700
H	6.68444400	-0.41998100	-2.94329600
H	5.85716100	1.81263400	-2.24992100
C	3.10179000	2.09164700	3.49511200
C	4.24821900	1.04392500	3.37811600
C	3.58505800	-0.34872600	3.56798200
H	3.01691700	2.51404600	4.50368400
H	3.18285000	2.91998500	2.78912400
H	4.68778200	1.09825200	2.38047800
H	5.03448900	1.21606300	4.11296700
H	3.96682700	-1.10230100	2.87896300
H	3.65645100	-0.72450900	4.59192600
N	2.18061000	-0.05060100	3.26263700
C	0.94529100	-0.80071600	3.19531100

O	0.86393800	-2.00030100	3.38638300
C	-0.01374900	0.22486000	2.79819000
H	-1.00996100	0.24798100	3.22565500
C	1.91371000	1.24051400	3.23803400
O	0.66142200	1.50904000	3.05957100

Rh₂(esp)₂

Rh	-0.04787600	-0.00022700	-1.18584100
O	-1.48444800	1.45074200	-1.08023900
O	1.36984900	1.47846500	-1.17353900
O	1.37087800	-1.47786300	-1.17372100
O	-1.48347500	-1.45216900	-1.08018400
Rh	0.04786700	-0.00021900	1.18584800
C	-1.83474300	-1.89324700	0.06055200
O	-1.37087000	-1.47787300	1.17372500
C	1.83475900	-1.89322400	-0.06054600
O	1.48347900	-1.45215300	1.08018800
C	-1.83458300	1.89297100	0.06040000
O	-1.36985900	1.47846700	1.17354900
O	1.48442400	1.45076100	1.08024900
C	1.83456700	1.89297800	-0.06039300
C	-2.88135000	3.00878000	0.11637900
C	-2.88189300	-3.00869000	0.11663700
C	2.88189500	-3.00867900	-0.11662600
C	2.88135500	3.00876800	-0.11637400
C	-4.08729700	2.51721600	0.97776100
H	-4.83110300	3.32096400	0.97200000
H	-3.74056200	2.39751300	2.00812600
C	-3.33755400	3.40230000	-1.29322800
H	-4.09111900	4.19340800	-1.22290900
H	-2.49838200	3.78117200	-1.88302100
H	-3.77337500	2.55724600	-1.82949200
C	-2.23910600	4.22471100	0.81409300
H	-2.96828900	5.03853200	0.88074100
H	-1.90734400	3.97103900	1.82406900
H	-1.37583300	4.58781800	0.24612800
C	-4.08770900	-2.51670400	0.97794700
H	-4.83171400	-3.32026800	0.97228200
H	-3.74096000	-2.39696000	2.00829900
C	-2.23999100	-4.22472100	0.81451300
H	-2.96942000	-5.03830900	0.88131900
H	-1.37685200	-4.58818100	0.24657300
H	-1.90812100	-3.97099100	1.82444400
C	-3.33818800	-3.40224400	-1.29293000

H	-2.49913900	-3.78148000	-1.88265700
H	-4.09203500	-4.19307500	-1.22252600
H	-3.77370400	-2.55710100	-1.82931200
C	3.33819000	-3.40222900	1.29294300
H	4.09202900	-4.19306800	1.22254200
H	3.77371600	-2.55708700	1.82931800
H	2.49913900	-3.78145400	1.88267300
C	2.23997000	-4.22470800	-0.81449000
H	1.90810500	-3.97098100	-1.82442300
H	2.96938500	-5.03831000	-0.88128600
H	1.37682600	-4.58814400	-0.24654400
C	4.08771200	-2.51671700	-0.97794500
H	4.83171300	-3.32028500	-0.97226600
H	3.74096400	-2.39698800	-2.00829900
C	4.08728000	2.51720500	-0.97778300
H	3.74052700	2.39749900	-2.00814100
H	4.83108600	3.32095400	-0.97203900
C	2.23911100	4.22471900	-0.81405700
H	1.37584800	4.58782100	-0.24607300
H	2.96829900	5.03853600	-0.88069800
H	1.90733400	3.97106800	-1.82403400
C	3.33759000	3.40226100	1.29323000
H	4.09117000	4.19335400	1.22290800
H	2.49843600	3.78114200	1.88304100
H	3.77340400	2.55719100	1.82947700
C	-4.70983900	1.22482200	0.50282800
C	-4.21300900	0.00027900	0.96629300
C	-5.75893500	1.21147800	-0.42595300
C	-4.70998800	-1.22422600	0.50287800
H	-3.41291900	0.00024000	1.69821300
C	-6.28262700	0.00037100	-0.88179900
H	-6.17132600	2.15066200	-0.78381600
C	-5.75908000	-1.21078200	-0.42590800
H	-7.10555300	0.00040700	-1.59121100
H	-6.17159700	-2.14992700	-0.78372700
C	4.70983800	1.22481500	-0.50285800
C	4.21300700	0.00026700	-0.96631100
C	5.75894700	1.21148000	0.42591000
C	4.70999600	-1.22423400	-0.50289600
H	3.41290700	0.00022200	-1.69821900
C	6.28264900	0.00037700	0.88175400
H	6.17133700	2.15066700	0.78376400
C	5.75910100	-1.21078000	0.42587700
H	7.10558500	0.00041900	1.59115600

H	6.17162500	-2.14992200	0.78369700
Rh₂(pfb)₄			
Rh	-0.04962100	-0.00920700	-1.20025700
O	0.72968400	-1.90140400	-1.14845700
O	-1.93856700	-0.77173800	-1.05061300
O	-0.81700500	1.88203700	-1.12302400
O	1.84159100	0.76838500	-1.22020200
Rh	0.04953800	0.00921600	1.20041600
C	2.37879500	1.01215700	-0.10757700
O	1.93845400	0.77180700	1.05076900
C	-1.02478100	2.37612900	0.01973800
O	-0.72973400	1.90142900	1.14860800
C	1.02475100	-2.37609600	-0.01958600
O	0.81691600	-1.88203200	1.12317700
O	-1.84164800	-0.76843600	1.22035700
C	-2.37888000	-1.01214400	0.10773100
C	3.46281200	3.25920600	0.26521300
C	-3.46274500	-3.25924900	-0.26511500
C	3.71245000	1.78046900	-0.13838800
F	4.58449800	1.22977400	0.73650400
F	4.24981200	1.74346300	-1.37809700
F	2.33527500	3.68679100	-0.36382800
F	3.25905300	3.31436400	1.59853200
C	4.61201900	4.23118800	-0.09094500
F	4.38969800	5.41176300	0.49575400
F	5.77753600	3.73803700	0.34916400
F	4.68069900	4.40958500	-1.41359000
C	-1.83082900	3.68763400	0.01746900
F	-1.70909700	4.31767000	1.20733000
F	-1.38822700	4.50643800	-0.96301900
C	-3.32877000	3.36597800	-0.23873700
C	-4.30708400	4.51481700	0.10240500
F	-3.66850400	2.28537300	0.51370000
F	-3.48167100	3.04889700	-1.54220500
F	-4.39032000	4.67785500	1.42626700
F	-5.51986800	4.21878600	-0.37638500
F	-3.88432900	5.65655100	-0.45640600
C	-3.71248400	-1.78054400	0.13854000
C	1.83083200	-3.68758500	-0.01735900
F	-4.24983100	-1.74359800	1.37825800
F	-4.58457700	-1.22988600	-0.73633000
F	-3.25890400	-3.31432000	-1.59842600
F	-2.33521700	-3.68680000	0.36396200

C	-4.61190500	-4.23133200	0.09091400
F	-4.68066200	-4.40982500	1.41354200
F	-5.77742900	-3.73824100	-0.34924500
F	-4.38945500	-5.41185300	-0.49584500
F	1.70890100	-4.31772400	-1.20714600
F	1.38846300	-4.50632900	0.96327500
C	3.32881700	-3.36587700	0.23850900
F	3.66836400	-2.28528300	-0.51402400
F	3.48199000	-3.04878000	1.54194400
C	4.30707800	-4.51469900	-0.10284300
F	5.51998200	-4.21861700	0.37561400
F	4.38994200	-4.67777100	-1.42672300
F	3.88451400	-5.65643800	0.45610300

5a

O	3.24767300	-1.06576100	1.69196500
C	2.46555200	-0.44067400	0.67658700
C	3.96984300	-2.13946800	1.08793000
N	3.10813900	-0.81219100	-0.58952600
C	2.49773900	1.11841500	0.69642100
C	4.09009300	-1.74145900	-0.38003900
H	3.44376700	-3.09927000	1.19422100
H	4.95854800	-2.22204000	1.54541400
C	3.27621800	0.34775900	-1.47130200
C	0.23370300	0.41619500	0.47162400
C	3.44041400	1.50021000	-0.47008500
H	2.87988900	1.48219700	1.65485400
O	4.90544100	-2.14695900	-1.19505200
H	4.14197000	0.18038700	-2.11427500
H	2.38972100	0.47489700	-2.09943400
H	4.47542800	1.52426600	-0.11418200
H	3.19558500	2.47660500	-0.88933900
O	-1.08397200	0.43908600	0.31278200
Si	-2.20600500	-0.79558500	-0.08913700
C	-2.29858400	-2.00972500	1.36798100
H	-1.43444200	-2.67674500	1.23399300
C	-1.60186600	-1.68970900	-1.65612700
C	-3.77901000	0.21352900	-0.37666100
H	-4.54581600	-0.49670200	-0.71797300
C	-4.28915800	0.88613900	0.90932600
H	-3.52998500	1.54854200	1.33990800
H	-5.17536900	1.49785900	0.69740200
H	-4.56996100	0.15580700	1.67360300
C	-3.57009200	1.26359300	-1.48394600

H	-3.34051100	0.80458300	-2.45010800
H	-4.47576100	1.86934500	-1.61484800
H	-2.74722700	1.94019000	-1.23095700
C	-2.16015000	-1.34440100	2.74758400
H	-2.10199200	-2.10559000	3.53572400
H	-1.26393100	-0.72149800	2.82079100
H	-3.01941700	-0.70655700	2.97516900
C	-3.56850600	-2.87848000	1.30289200
H	-3.58037100	-3.60793400	2.12231400
H	-4.47415500	-2.26890100	1.39691400
H	-3.64192700	-3.44033200	0.36580300
C	-2.77801900	-2.27834500	-2.45930700
H	-3.41921900	-1.48890700	-2.86537100
H	-2.40733100	-2.86624800	-3.30806300
H	-3.40894000	-2.93824500	-1.85486900
H	-0.99421500	-2.53429200	-1.29985100
C	-0.70739800	-0.82283700	-2.55954500
H	-1.23713500	0.06163300	-2.92693600
H	0.19082100	-0.47393000	-2.04291900
H	-0.37923600	-1.39608000	-3.43563200
C	0.98416500	-0.86034400	0.74655800
H	0.75175600	-1.65767000	0.03570800
H	0.74555000	-1.22349300	1.75234700
C	1.05024000	1.50452100	0.47681600
C	0.68633000	2.91177200	0.34218700
O	1.48783900	3.83140700	0.46273600
O	-0.62299900	3.12442400	0.07274100
C	-1.00934500	4.50200100	-0.05302400
H	-2.08011400	4.48812300	-0.25694600
H	-0.80897300	5.04976700	0.87152400
H	-0.47475600	4.98402800	-0.87596400

4a

O	-2.89755700	-0.04572100	1.69635100
C	-2.34542600	-0.54728800	0.47126500
C	-4.28864300	0.21510800	1.52282400
N	-3.49495800	-0.78151800	-0.39243400
C	-1.25949400	0.36354100	-0.05129500
C	-1.64659200	-1.92972500	0.56585500
C	-4.66765800	-0.45170400	0.20843300
H	-4.48814600	1.29300900	1.49038800
H	-4.86342000	-0.23161200	2.34108800
C	-3.30998300	-1.91824800	-1.29047700
C	-0.04311200	-0.23181100	0.10062100

C	-1.47806800	1.72862900	-0.52096000
C	-0.15013200	-1.62006100	0.69432400
C	-2.01580600	-2.60380200	-0.77903900
H	-2.04954500	-2.48276100	1.41650800
O	-5.79668300	-0.68330100	-0.20662200
H	-4.19548500	-2.55660400	-1.22533300
H	-3.20582800	-1.58984100	-2.32842000
O	-2.78201100	2.08946700	-0.38803400
O	-0.63774200	2.48390200	-0.98508200
H	0.48199900	-2.33992200	0.16709200
H	0.17992500	-1.59742800	1.73873900
H	-2.15208200	-3.68127100	-0.66425500
H	-1.20891300	-2.45030300	-1.50081900
C	-3.10693200	3.41409700	-0.83520800
H	-2.55526800	4.16472100	-0.26298500
H	-4.17836800	3.52625900	-0.66806200
H	-2.87626900	3.53385200	-1.89700100
O	1.11376300	0.33153300	-0.20391400
Si	2.74376100	-0.13409300	0.07558100
C	3.11288100	-1.69749000	-0.94470200
H	2.84550700	-2.54048500	-0.29101300
C	2.94369000	-0.48536800	1.93141600
C	3.68269100	1.38750200	-0.53641600
H	4.75166100	1.14541000	-0.44491000
C	3.38154100	1.68097100	-2.01749600
H	2.31369300	1.86961100	-2.17052900
H	3.92536500	2.57451600	-2.34907800
H	3.67565300	0.85646500	-2.67332500
C	3.40092400	2.63571100	0.31827700
H	3.73440500	2.51327000	1.35261300
H	3.92456600	3.50759700	-0.09402200
H	2.33166000	2.87268700	0.33277800
C	2.26801200	-1.81442900	-2.22495000
H	2.46445700	-2.76960600	-2.72805700
H	1.19432700	-1.76247000	-2.02318500
H	2.50320400	-1.01772700	-2.93721500
C	4.61249000	-1.82294400	-1.27383500
H	4.81637200	-2.77155800	-1.78584900
H	4.94176200	-1.01750600	-1.93880200
H	5.24370700	-1.79250200	-0.37983900
C	4.42610000	-0.47541300	2.34839300
H	4.87541300	0.51388400	2.20762400
H	4.53061100	-0.73215600	3.40993000
H	5.02215100	-1.19560900	1.77887900

H	2.56960200	-1.51039600	2.06830100
C	2.11459300	0.43662600	2.84281300
H	2.47179200	1.46975000	2.80310300
H	1.05332900	0.44955900	2.57737500
H	2.18957600	0.10662000	3.88654900

10

Rh	0.09974000	-0.02922200	0.52885300
O	-1.18832700	-1.54726600	0.98036900
O	1.61020600	-1.17400600	1.29550100
O	1.40503800	1.44489700	-0.05766800
O	-1.40846100	1.04430700	-0.32566000
Rh	0.48339400	-1.07058500	-1.57411300
C	-1.65427800	0.89183900	-1.56371800
O	-1.03554900	0.08434300	-2.33287500
C	1.97656900	1.36731200	-1.19463000
O	1.79499400	0.42807500	-2.03300500
C	-1.37843600	-2.47939500	0.13786900
O	-0.82584700	-2.54212100	-1.00924200
O	1.99509800	-2.14238600	-0.70537700
C	2.23480600	-1.98292900	0.53429600
C	-2.33011300	-3.61585200	0.51901900
C	-2.76612900	1.73968100	-2.18637600
C	2.94084300	2.49763600	-1.56504600
C	3.34297600	-2.81918300	1.17910000
C	-3.46424500	-3.69538800	-0.54993200
H	-4.14453800	-4.49256400	-0.23238700
H	-3.01492100	-4.00570800	-1.49767000
C	-2.91308800	-3.39337300	1.91943300
H	-3.58807300	-4.21929600	2.16630800
H	-2.12066600	-3.36242900	2.67233400
H	-3.47508100	-2.45970500	1.97968100
C	-1.52854300	-4.93267100	0.49045700
H	-2.18660800	-5.77036500	0.74290700
H	-1.10015700	-5.11257500	-0.49879100
H	-0.71373100	-4.90806000	1.22207200
C	-3.82710400	0.78472000	-2.81591300
H	-4.62264200	1.41684500	-3.22412900
H	-3.35849200	0.26333700	-3.65553300
C	-2.13887500	2.59333100	-3.30650800
H	-2.91241000	3.20668000	-3.77991000
H	-1.37338600	3.26511500	-2.90313700
H	-1.67711100	1.96397500	-4.07149200
C	-3.40632600	2.65341400	-1.13479200

H	-2.66788600	3.34524800	-0.72391500
H	-4.20359500	3.24074800	-1.60188200
H	-3.83370300	2.08526700	-0.30700400
C	3.58462700	2.24251400	-2.93264500
H	4.27652300	3.05858200	-3.16505400
H	4.14088500	1.30335900	-2.95026900
H	2.82681900	2.20239200	-3.71978300
C	2.13409300	3.81109900	-1.60779900
H	1.68297600	4.02920400	-0.63795800
H	2.79617000	4.64044900	-1.87676900
H	1.33721000	3.75589300	-2.35726600
C	4.02468600	2.61438800	-0.44859100
H	4.70268600	3.42087500	-0.74695000
H	3.52778600	2.92675400	0.47423700
C	4.36675200	-1.85304600	1.85368600
H	3.85915400	-1.34296900	2.67715900
H	5.15474600	-2.47710200	2.28805800
C	2.69329300	-3.69255300	2.27186600
H	1.95269100	-4.37289400	1.83779900
H	3.46141400	-4.29719800	2.76498800
H	2.19808200	-3.07592900	3.02634200
C	4.03196800	-3.71319100	0.14214900
H	4.82187400	-4.29249400	0.63116200
H	3.32088100	-4.41343600	-0.30460900
H	4.48160300	-3.12807600	-0.66249800
C	-4.22733300	-2.40700900	-0.75201400
C	-3.76386100	-1.45906000	-1.67251400
C	-5.38580000	-2.11527000	-0.01992800
C	-4.40464300	-0.22744900	-1.85420300
H	-2.87677100	-1.68099900	-2.25497500
C	-6.04986500	-0.90124100	-0.20312800
H	-5.77375900	-2.84483900	0.68554700
C	-5.55960800	0.04156600	-1.10813800
H	-6.95363200	-0.68903500	0.36121800
H	-6.08123000	0.98457100	-1.24563500
C	4.96910000	-0.82830400	0.92046500
C	4.31569500	0.39204000	0.70615400
C	6.16237700	-1.07736000	0.22928500
C	4.80346000	1.34411400	-0.19787900
H	3.40079600	0.60162600	1.24849400
C	6.67602900	-0.12958200	-0.65768800
H	6.69487300	-2.00972300	0.39537900
C	5.99903600	1.07145900	-0.87614200
H	7.60948400	-0.32629300	-1.17774400

H	6.40463100	1.80554900	-1.56683300
C	-1.99009300	4.86508300	1.66958300
C	-0.60442900	4.78178200	1.02151300
C	0.16447100	3.82724900	1.94449200
H	-2.03498300	5.64846400	2.43668500
H	-2.81648600	5.02970400	0.97541400
H	-0.68278300	4.34301000	0.02231700
H	-0.10817000	5.74993600	0.93315100
H	0.92028200	3.23568500	1.42986100
H	0.62933000	4.35520800	2.78391600
N	-0.89861600	2.93263200	2.44164800
C	-0.52633300	1.79283000	3.17201200
O	0.61473700	1.71432100	3.63403000
C	-1.45373700	0.68849600	3.32770900
H	-1.18400700	-0.15190400	3.95372600
C	-2.15788600	3.53180600	2.37830500
O	-3.18646800	3.07844800	2.85266600
N	-2.54368400	0.52846800	2.61590100
N	-3.48353500	0.35040500	2.01121900

TS7

Rh	-0.01620400	-0.10216200	0.55383200
O	-1.35718100	-1.59088700	0.95822600
O	1.46391800	-1.34777900	1.24854600
O	1.31358000	1.33519700	-0.04739100
O	-1.45557000	1.06761200	-0.30472200
Rh	0.32507400	-1.12189800	-1.62752100
C	-1.69870300	0.95613200	-1.55040000
O	-1.15931900	0.11311200	-2.33420500
C	1.85974700	1.27946200	-1.20026300
O	1.67177400	0.36465300	-2.05721900
C	-1.56111400	-2.50991800	0.09624700
O	-1.02691900	-2.56034000	-1.05421300
O	1.82185700	-2.24919500	-0.79159400
C	2.07191000	-2.13388300	0.44505400
C	-2.53950100	-3.62994300	0.46488200
C	-2.74296100	1.90264000	-2.15145200
C	2.81129100	2.43085700	-1.53799400
C	3.18330200	-2.99481900	1.05446500
C	-3.78359500	-3.50597900	-0.47303000
H	-4.51664500	-4.24346500	-0.12881600
H	-3.47562900	-3.79464400	-1.48218900
C	-2.95875300	-3.54059300	1.93635000
H	-3.63831800	-4.36738300	2.16845400

H	-2.08945600	-3.61698700	2.59613900
H	-3.46738900	-2.60223500	2.15725000
C	-1.85451700	-4.98423500	0.20242700
H	-2.55339200	-5.79889700	0.41836900
H	-1.53069900	-5.06895100	-0.83744400
H	-0.97882100	-5.10849400	0.84864900
C	-3.96476200	1.04152800	-2.60470800
H	-4.75068800	1.73805000	-2.91568300
H	-3.66525500	0.46865100	-3.48721700
C	-2.13257500	2.58944900	-3.38725000
H	-2.87522100	3.24969800	-3.84734400
H	-1.26686000	3.19887400	-3.10503300
H	-1.81032200	1.85624800	-4.13021700
C	-3.16821200	2.96559300	-1.13255600
H	-2.31383500	3.58832300	-0.85330000
H	-3.92965100	3.61360400	-1.57955400
H	-3.56826200	2.52326000	-0.22054100
C	3.42071500	2.24828000	-2.93193400
H	4.10090200	3.07986500	-3.14369200
H	3.98194700	1.31516200	-3.00977800
H	2.64209000	2.23927900	-3.69969300
C	1.99924500	3.74083300	-1.49038500
H	1.55020400	3.88650300	-0.50548100
H	2.65402700	4.59159600	-1.70563900
H	1.19855300	3.73026500	-2.23802800
C	3.91935500	2.48795800	-0.43974400
H	4.60643000	3.29381700	-0.71905400
H	3.44278400	2.76754700	0.50365600
C	4.23469800	-2.05215300	1.72008700
H	3.75325600	-1.55186400	2.56510300
H	5.02620700	-2.69262900	2.12370900
C	2.55197900	-3.88056500	2.14706200
H	1.79087700	-4.54243300	1.71989700
H	3.32387200	-4.50523200	2.60849600
H	2.08446300	-3.27291600	2.92606200
C	3.83701100	-3.87825100	-0.01430200
H	4.63136700	-4.47588300	0.44473500
H	3.10674000	-4.56146200	-0.45662500
H	4.27376300	-3.28400000	-0.81918800
C	-4.40202000	-2.12831000	-0.51837800
C	-3.98410000	-1.21514500	-1.49374300
C	-5.36881300	-1.71762800	0.40924600
C	-4.48778800	0.08990600	-1.55399400
H	-3.24052400	-1.52546900	-2.22053000

C	-5.88809900	-0.42268400	0.35972200
H	-5.72433500	-2.41624900	1.16117400
C	-5.45051700	0.47807800	-0.61331900
H	-6.64507400	-0.11698200	1.07666100
H	-5.86667600	1.48085500	-0.65121400
C	4.82656600	-1.01498200	0.79353000
C	4.19658400	0.22660100	0.63931700
C	5.98729700	-1.27264300	0.05159300
C	4.67655600	1.19341300	-0.25409900
H	3.30754400	0.44431900	1.22045800
C	6.49242000	-0.31195300	-0.82618900
H	6.50157900	-2.22227800	0.17058100
C	5.83941700	0.91177800	-0.98360900
H	7.40055300	-0.51624500	-1.38667300
H	6.23875500	1.65577300	-1.66736900
C	-2.01654900	4.81466400	1.84346600
C	-0.65472700	5.37548400	1.42787100
C	0.33862000	4.50781000	2.20864200
H	-2.37374600	5.26912400	2.77669100
H	-2.80763400	4.91198100	1.09890800
H	-0.50185300	5.22920400	0.35395600
H	-0.53328100	6.43597800	1.65403200
H	1.29495400	4.37147100	1.70660400
H	0.52397400	4.89555900	3.21622000
N	-0.36048100	3.20725500	2.30162400
C	0.38162300	2.08771100	2.61923600
O	1.58047100	2.19765800	2.88389400
C	-0.04557000	0.67690800	2.42722500
H	0.41224800	0.04928800	3.19397700
C	-1.74852800	3.35039100	2.13582500
O	-2.57812600	2.46989100	2.25454500
N	-1.75131200	0.33794500	3.18691200
N	-2.58536300	-0.38620900	3.28577300

11

Rh	-0.01893600	0.00567300	0.56736000
O	-1.50570400	-1.32359500	1.06491300
O	1.33498800	-1.39942800	1.19652400
O	1.45067200	1.28756600	-0.09460600
O	-1.38443800	1.33011800	-0.21357200
Rh	0.07203700	-1.04624300	-1.61788400
C	-1.73389300	1.22546200	-1.43215600
O	-1.30897600	0.34740400	-2.24899700
C	1.92579200	1.15424900	-1.27098500

O	1.56721400	0.27487800	-2.11146900
C	-1.86330100	-2.20378500	0.21800900
O	-1.40198300	-2.32214700	-0.96225200
O	1.45558800	-2.35324100	-0.85021100
C	1.77840400	-2.26732700	0.37485200
C	-2.93903900	-3.21474900	0.63605900
C	-2.75148100	2.23848300	-1.97255300
C	3.01526600	2.15379300	-1.67677000
C	2.78382700	-3.27953100	0.93585400
C	-4.14811200	-3.08084200	-0.34210300
H	-4.92119600	-3.77411800	0.00643300
H	-3.82149800	-3.42172200	-1.32865300
C	-3.38651800	-2.99010300	2.08379100
H	-4.12754100	-3.74923400	2.35639600
H	-2.54186800	-3.07184400	2.77342800
H	-3.83627300	-2.00652400	2.22012000
C	-2.34232100	-4.62876800	0.49331900
H	-3.09470800	-5.37822400	0.76070600
H	-2.01200000	-4.81643500	-0.53129700
H	-1.48390300	-4.75721600	1.16182500
C	-3.99193400	1.45952200	-2.51150200
H	-4.71616000	2.20700100	-2.85274200
H	-3.67352100	0.88776000	-3.38777700
C	-2.09495100	2.99166000	-3.14613700
H	-2.80186600	3.71436800	-3.56723300
H	-1.20923100	3.54119800	-2.80830200
H	-1.79037900	2.30152900	-3.93686100
C	-3.16572000	3.23814100	-0.88686800
H	-2.30276000	3.81402700	-0.54015600
H	-3.90013000	3.93957200	-1.29704800
H	-3.60499600	2.73910300	-0.02248500
C	3.49577000	1.89193400	-3.10829400
H	4.27402600	2.61644100	-3.37068000
H	3.90817800	0.88742400	-3.21904000
H	2.67386100	1.99925100	-3.82150400
C	2.41879800	3.57152700	-1.57978600
H	2.06317000	3.77701700	-0.56782600
H	3.17911800	4.31528400	-1.84042600
H	1.57759300	3.68955800	-2.27167100
C	4.19467900	2.03824700	-0.66141300
H	4.97234300	2.73588700	-0.99106700
H	3.83505300	2.37971300	0.31333100
C	4.00423200	-2.49666600	1.51384600
H	3.65706000	-1.92692500	2.37978000

H	4.72248700	-3.24165900	1.87313400
C	2.09895100	-4.04273600	2.08678400
H	1.22310800	-4.59116900	1.72294900
H	2.79693500	-4.76708700	2.51978400
H	1.77456300	-3.35773100	2.87417700
C	3.22860600	-4.26862300	-0.14743500
H	3.94886700	-4.97601100	0.27724100
H	2.37643700	-4.83728500	-0.52993700
H	3.69970900	-3.76083800	-0.99136000
C	-4.71678600	-1.68518200	-0.46043000
C	-4.17563300	-0.79016800	-1.39163600
C	-5.77191100	-1.24616300	0.35062700
C	-4.64053600	0.52506700	-1.51569200
H	-3.36753600	-1.12383800	-2.03235200
C	-6.26078900	0.05578200	0.22894800
H	-6.21858800	-1.92935300	1.06790300
C	-5.69761200	0.93880800	-0.69426700
H	-7.08731700	0.38267000	0.85397700
H	-6.08561700	1.94962500	-0.78548900
C	4.67104200	-1.55965800	0.53352100
C	4.21162400	-0.24189000	0.40919200
C	5.73002600	-1.98049600	-0.28211900
C	4.76543500	0.64623200	-0.52138800
H	3.40693400	0.09734900	1.05181000
C	6.30551900	-1.10156300	-1.20165000
H	6.11165000	-2.99343800	-0.18754600
C	5.82460900	0.20319900	-1.32505400
H	7.13561800	-1.43262800	-1.81976300
H	6.27929800	0.88428600	-2.03928300
N	-3.49407100	0.41886000	2.87936000
N	-3.82565000	1.20214100	2.17541300
C	-0.53803100	4.57011500	2.17156700
C	0.88718200	5.14362100	1.90587100
C	1.89739700	4.07481700	2.41479600
H	-1.00193000	4.97806600	3.07704700
H	-1.23349200	4.71573600	1.34209800
H	1.02236000	5.28887700	0.83232700
H	1.03830200	6.10145900	2.40353000
H	2.72347500	3.90246500	1.72442100
H	2.29655900	4.29788500	3.40746600
N	1.05354000	2.87861000	2.49225300
C	1.24793800	1.48237800	2.79423100
O	2.32689700	0.99485300	3.08592300
C	-0.08463000	0.92423500	2.57628500

H	-0.49257100	0.19029000	3.26244400
C	-0.23373600	3.13440400	2.38496500
O	-0.98262100	2.08949900	2.51085500

12

Rh	0.04176600	-0.00399800	-0.44210400
O	1.46370800	-1.13197300	-1.39342600
O	-1.40128800	-1.10640700	-1.39181300
O	-1.34190000	1.04387800	0.65466100
O	1.49135700	1.00199700	0.60900900
Rh	0.01631300	-1.66003000	1.32370300
C	1.87436200	0.54135800	1.73354500
O	1.46093400	-0.53646000	2.26671300
C	-1.76173200	0.57740500	1.76351800
O	-1.40230400	-0.52534700	2.27968800
C	1.84915500	-2.22461100	-0.86679500
O	1.43246600	-2.69540600	0.23939300
O	-1.45980200	-2.63330100	0.27476500
C	-1.84535000	-2.16866000	-0.84200600
C	2.90024000	-3.04956400	-1.61952500
C	2.92019400	1.34158400	2.51901200
C	-2.77915700	1.44779300	2.50903400
C	-2.92776600	-2.92939700	-1.61612300
C	4.14091500	-3.23805000	-0.69109900
H	4.88669700	-3.80041900	-1.26328500
H	3.83721200	-3.86018600	0.15549000
C	3.29979800	-2.36783700	-2.93293600
H	4.05789100	-2.97246500	-3.44197400
H	2.43784100	-2.26911700	-3.59863800
H	3.71052100	-1.37088000	-2.76261600
C	2.29320900	-4.43487600	-1.91690900
H	3.02759500	-5.05822400	-2.43780100
H	1.99809100	-4.94201600	-0.99482600
H	1.41025600	-4.34270600	-2.55869900
C	4.15979300	0.42518800	2.76210600
H	4.90916000	1.02928500	3.28489800
H	3.85605700	-0.37967100	3.43709000
C	2.30597700	1.71927500	3.88125100
H	3.03755500	2.27458600	4.47762600
H	1.42453500	2.35607900	3.74657900
H	2.00546700	0.82884600	4.43887600
C	3.32218900	2.61464800	1.76676800
H	2.45859100	3.26965200	1.62448700
H	4.07322000	3.16072300	2.34733200

H	3.74269200	2.38751100	0.78557400
C	-3.23062900	0.77727600	3.81061100
H	-3.96550800	1.41408400	4.31438800
H	-3.68768400	-0.19656000	3.62543700
H	-2.38456000	0.63011300	4.48756500
C	-2.10094900	2.79608000	2.82543400
H	-1.76436200	3.28962000	1.90989600
H	-2.80696200	3.45698600	3.33920800
H	-1.23383000	2.65174200	3.47932200
C	-3.99024500	1.70985300	1.55944800
H	-4.71557100	2.30916300	2.12073600
H	-3.63288100	2.31390900	0.72132700
C	-4.12152400	-1.96079000	-1.88596900
H	-3.77280300	-1.17659400	-2.56348700
H	-4.88848500	-2.53760800	-2.41426800
C	-2.32754600	-3.36043100	-2.96938200
H	-1.47488900	-4.03206700	-2.82090200
H	-3.08195400	-3.89481700	-3.55640000
H	-1.98881000	-2.49428900	-3.54358300
C	-3.38941200	-4.16744200	-0.83891300
H	-4.16509400	-4.68854800	-1.41004800
H	-2.55864700	-4.86021200	-0.67915200
H	-3.79935900	-3.90338500	0.13788000
C	4.74083200	-1.95003300	-0.17683800
C	4.26894400	-1.39019800	1.01673200
C	5.74663600	-1.27327400	-0.88004000
C	4.75098700	-0.16889400	1.50464400
H	3.49838300	-1.91215000	1.57272000
C	6.25362400	-0.06476300	-0.39894000
H	6.14076900	-1.70050000	-1.79789900
C	5.75664500	0.48805300	0.78291800
H	7.04406400	0.44463700	-0.94331900
H	6.15925000	1.42644000	1.15438300
C	-4.70730400	-1.32871200	-0.64482800
C	-4.17717700	-0.12764600	-0.15539400
C	-5.75753500	-1.93385100	0.05867200
C	-4.64633400	0.45590300	1.02889200
H	-3.37780600	0.36100800	-0.70152600
C	-6.25307900	-1.35235800	1.22701300
H	-6.19417000	-2.85588900	-0.31536400
C	-5.69767000	-0.16792600	1.71417200
H	-7.07696300	-1.82193300	1.75747300
H	-6.08667200	0.28041200	2.62429000
C	1.90491100	4.44598600	-1.13161000

C	0.87427900	5.26967000	-0.30592900
C	-0.52427700	4.75221000	-0.73598900
H	2.18044500	4.94388700	-2.06811000
H	2.81447100	4.19244500	-0.58628000
H	1.02175300	5.06998800	0.75821200
H	0.97588600	6.34152900	-0.47581100
H	-1.23835100	4.68941900	0.08526600
H	-0.95923800	5.32861600	-1.55623200
N	-0.19537800	3.41268200	-1.23149300
C	-0.92538400	2.34039400	-1.83413800
O	-2.15043300	2.32442700	-1.95785900
C	0.11593200	1.38999300	-2.15138000
H	0.09775700	0.78841300	-3.05175300
C	1.09186500	3.25983100	-1.48468200
O	1.37070700	2.13645400	-2.05983200
O	0.27557700	4.34863700	-4.01230500
H	0.40066300	3.56765200	-4.56864000
H	-0.69844500	4.46463200	-3.97463600
O	-2.48267400	4.47861900	-3.68338400
H	-2.81682500	5.25459000	-3.21094400
H	-2.57813500	3.73675300	-3.05233600

TS8

Rh	0.00060500	-0.03743000	-0.43670900
O	1.33478400	-1.26908900	-1.39275700
O	-1.52167300	-0.96808500	-1.46381200
O	-1.31109000	1.08788400	0.67064500
O	1.48605300	0.78541100	0.70061500
Rh	-0.23066400	-1.76391700	1.27755500
C	1.79268700	0.26113900	1.81824600
O	1.28509800	-0.79864400	2.30462800
C	-1.81329900	0.61888800	1.74329800
O	-1.57904300	-0.52992000	2.22766400
C	1.61271500	-2.40414200	-0.89002700
O	1.13190300	-2.87436200	0.18975900
O	-1.75790400	-2.54922700	0.13783500
C	-2.08028000	-1.99760000	-0.95836800
C	2.61675700	-3.28703800	-1.64492800
C	2.87283300	0.96311200	2.65125100
C	-2.77019700	1.55596800	2.49138800
C	-3.22918800	-2.60584400	-1.77428000
C	3.82890300	-3.57504600	-0.70495400
H	4.54692700	-4.16979700	-1.28031500
H	3.47336200	-4.19766600	0.12082800

C	3.08256200	-2.61081600	-2.93968100
H	3.80075200	-3.25969800	-3.45260400
H	2.23937600	-2.43470700	-3.61344400
H	3.56274200	-1.65021500	-2.74427500
C	1.92501100	-4.62306100	-1.97804100
H	2.62460100	-5.28599100	-2.49820800
H	1.57946800	-5.12478700	-1.07073600
H	1.06156600	-4.46097200	-2.63259600
C	4.05355200	-0.03405100	2.86563600
H	4.83649300	0.50329500	3.41177700
H	3.69822400	-0.84250500	3.51079900
C	2.26715400	1.31789200	4.02261600
H	3.02266800	1.80209400	4.65065800
H	1.42644200	2.01109100	3.90748900
H	1.90695800	0.42403300	4.53799300
C	3.35547900	2.24092500	1.95463500
H	2.53202900	2.94942800	1.83222700
H	4.13217800	2.71829300	2.56194100
H	3.76592900	2.03212400	0.96571300
C	-3.38006200	0.86254000	3.71384200
H	-4.06217800	1.55087400	4.22426200
H	-3.93986300	-0.03161300	3.43243400
H	-2.60166600	0.56502300	4.42171100
C	-1.95616400	2.78629900	2.94120000
H	-1.50928500	3.29439000	2.08240200
H	-2.60661200	3.49392400	3.46635500
H	-1.15237400	2.49254600	3.62516100
C	-3.87884200	2.02806700	1.50019000
H	-4.55009300	2.69087500	2.05742600
H	-3.39734300	2.62046900	0.71752700
C	-4.26789300	-1.48633900	-2.09341700
H	-3.77795700	-0.74264400	-2.72815100
H	-5.06730900	-1.94856300	-2.68313400
C	-2.63711300	-3.11923000	-3.10269500
H	-1.88595500	-3.89533600	-2.92005800
H	-3.43006100	-3.55365600	-3.72088600
H	-2.16499100	-2.30734700	-3.66234500
C	-3.88784600	-3.76612300	-1.02039700
H	-4.70541000	-4.17629100	-1.62280900
H	-3.16771800	-4.56640400	-0.83020000
H	-4.29608300	-3.44385900	-0.06035900
C	4.50291800	-2.34254800	-0.14758400
C	4.05344600	-1.78816200	1.05701900
C	5.56187600	-1.71463300	-0.81750200

C	4.61409600	-0.62107200	1.59123100
H	3.23736000	-2.26904300	1.58461800
C	6.14309100	-0.55891900	-0.29265000
H	5.93838400	-2.13914000	-1.74406000
C	5.67077600	-0.01170000	0.90186700
H	6.97268800	-0.08731900	-0.81237800
H	6.13188700	0.88450600	1.30808400
C	-4.85120100	-0.80520900	-0.87635900
C	-4.19245200	0.28832500	-0.29903400
C	-6.03381500	-1.26495000	-0.28110700
C	-4.66596100	0.90303500	0.86788500
H	-3.28401400	0.66172300	-0.75728000
C	-6.53318500	-0.64833700	0.86732300
H	-6.56717500	-2.10167800	-0.72399100
C	-5.85120600	0.42514800	1.44308400
H	-7.45763700	-1.00416800	1.31401500
H	-6.24325800	0.90036800	2.33829900
C	2.55198600	4.14600500	-1.23066300
C	1.85656600	5.17953800	-0.33522900
C	0.33895900	4.81879400	-0.44142000
H	1.80353400	4.72343700	-2.79374300
H	3.62442500	4.06335600	-1.34424500
H	2.18988200	5.09029000	0.70564600
H	2.03608900	6.21208200	-0.64791000
H	-0.17231600	4.82240100	0.52191700
H	-0.20079800	5.48830200	-1.11853200
N	0.38424500	3.45996800	-0.99241400
C	-0.51668600	2.60552000	-1.58637900
O	-1.72494200	2.87579300	-1.76639600
C	0.26988000	1.43753200	-1.97483300
H	0.06040600	0.99462100	-2.94639800
C	1.66700200	3.11394700	-1.38023200
O	1.66859900	1.92903200	-1.97216700
O	-1.16255800	4.75166700	-3.49416000
H	-1.50378600	4.08625400	-2.80855800
H	-1.48265000	4.45249200	-4.36318000
O	1.23063300	5.09976700	-3.56973700
H	0.06763400	4.90542400	-3.50649100
H	1.42143100	6.05157100	-3.64607400

13

Rh	0.26237100	-1.20211100	-1.57080100
Rh	0.12585700	-0.21020800	0.65352300
O	1.70401000	-1.39667300	1.20566600

C	2.19716300	-2.21338800	0.36270000
O	1.81750400	-2.34854800	-0.84336100
C	3.34200600	-3.12138600	0.83138700
C	3.70977800	-2.83948400	2.29241800
C	2.87360100	-4.58310200	0.68698500
C	4.57078700	-2.89771600	-0.10364200
H	4.53158600	-3.49704200	2.59554900
H	4.02467500	-1.80431100	2.43839800
H	2.85891200	-3.02945000	2.95244800
H	2.60298900	-4.80868000	-0.34760200
H	3.67575400	-5.26268100	0.99365900
H	2.00268100	-4.77751600	1.32242500
H	5.37833000	-3.53793200	0.26756200
H	4.30294600	-3.25198900	-1.10310000
C	5.03857100	-1.46352300	-0.18695700
C	4.46353800	-0.59592900	-1.12376100
C	6.01882600	-0.95838400	0.67773500
C	4.81863800	0.75651000	-1.19683500
H	3.71012900	-0.97928200	-1.80226400
C	6.39948200	0.38296600	0.60671000
H	6.49053700	-1.61913000	1.39990300
C	4.12376800	1.66418200	-2.18453600
C	5.80038500	1.23789100	-0.32018500
H	7.16969500	0.76230500	1.27270500
C	2.81267200	2.31991800	-1.65180600
H	3.87517800	1.09849700	-3.08697100
H	4.79211900	2.48000200	-2.48084700
H	6.10307000	2.28009000	-0.37252200
C	1.85128700	1.20697300	-1.20812100
C	2.14857100	3.09085000	-2.80971900
C	3.11563700	3.28455700	-0.49967600
O	1.54428600	0.33303500	-2.08032000
O	1.42501100	1.23707300	-0.00976000
H	1.23682300	3.59264300	-2.47046800
H	2.83218800	3.86039800	-3.18368900
H	1.89270100	2.42161800	-3.63499600
H	3.81393900	4.05457400	-0.84481600
H	2.20539900	3.78059000	-0.15633100
H	3.55967000	2.77061300	0.35434300
O	-1.03195600	-2.65937000	-0.93178300
C	-1.43825500	-2.64882000	0.26930500
O	-1.13644300	-1.77043900	1.14442600
C	-2.36197600	-3.78293300	0.73299000
C	-3.67647400	-3.16288600	1.29780700

C	-1.64493100	-4.53933200	1.86898600
C	-2.66766300	-4.74886500	-0.41763200
H	-4.32277800	-3.99492000	1.59748700
H	-3.42406600	-2.60178400	2.20227600
C	-4.40829600	-2.25820500	0.33353400
H	-2.28146500	-5.35198800	2.23460800
H	-0.70685100	-4.97820500	1.51205600
H	-1.41734000	-3.87199000	2.70420200
H	-1.75021500	-5.20491200	-0.79931400
H	-3.32343000	-5.54850800	-0.05713400
H	-3.16462800	-4.24477800	-1.24894200
C	-4.06112500	-0.90425800	0.24939700
C	-5.41697800	-2.74160100	-0.51029000
C	-4.67448700	-0.03526600	-0.66085000
H	-3.28163400	-0.52426800	0.89775000
C	-6.05092800	-1.88675700	-1.41419600
H	-5.71215400	-3.78561500	-0.45151600
C	-4.22903100	1.40595200	-0.74629500
C	-5.68132900	-0.54280000	-1.49293500
H	-6.84015000	-2.26851900	-2.05598200
C	-3.02096400	1.66021900	-1.69875100
H	-5.05357400	2.03311500	-1.10182100
H	-3.95590100	1.76442300	0.25008600
H	-6.18177700	0.11820500	-2.19519700
C	-1.83907400	0.78354000	-1.25934100
C	-3.40589600	1.37338800	-3.15405300
C	-2.59215300	3.13364000	-1.55608500
O	-1.33514900	-0.01498300	-2.10558900
O	-1.44093800	0.93682900	-0.05574000
H	-4.25126400	2.00797500	-3.44033300
H	-2.57252000	1.58869400	-3.82843300
H	-3.69336100	0.33001100	-3.29751000
H	-3.41045100	3.79323200	-1.86277500
H	-2.32892100	3.36974600	-0.52243600
H	-1.73162500	3.33912700	-2.20243100
H	-2.08690900	5.39675100	1.77323900
O	-1.67208600	6.64024500	0.94793500
H	-1.12902200	7.27679100	1.43643300
H	-1.09575800	6.28946300	0.22351900
O	-0.10580700	5.34799000	-0.82576200
H	-0.56151200	5.15131100	-1.65862700
H	-0.06215700	4.49742300	-0.35622700
C	0.02404400	0.52586000	2.76561000
C	-1.36057400	0.24642600	3.39769400

C	-2.25481400	1.43965100	2.95194700
H	0.90105100	0.06480000	3.21124300
H	-1.78308800	-0.70272000	3.06821800
H	-1.28930200	0.23294300	4.49287900
H	-2.79603100	1.22831400	2.02947600
H	-2.94940500	1.78114600	3.72029900
N	-1.23880500	2.46261500	2.67784800
C	-1.18180000	3.79033000	2.28612000
O	-2.29216000	4.50164200	2.20952500
C	0.13985700	4.05687300	2.06095800
H	0.70693700	4.95605500	1.90064300
C	-0.00328900	1.93070900	2.61483000
O	0.87621700	2.87402100	2.30660900

TS9

Rh	0.27715600	-1.12480600	-1.58026000
Rh	0.13148600	-0.15652500	0.64728400
O	1.72499200	-1.32870300	1.18474000
C	2.21586800	-2.14444000	0.33978900
O	1.83429200	-2.27350600	-0.86658900
C	3.35592700	-3.05962900	0.80472400
C	3.73050800	-2.77902700	2.26428700
C	2.87526600	-4.51777000	0.66320300
C	4.58289400	-2.84568100	-0.13465600
H	4.54965100	-3.44117100	2.56442600
H	4.05206100	-1.74565400	2.40862400
H	2.88104900	-2.96397800	2.92751500
H	2.59989000	-4.74253700	-0.37033000
H	3.67323700	-5.20293500	0.96822200
H	2.00497100	-4.70465400	1.30165300
H	5.38662100	-3.49244500	0.23321400
H	4.30880300	-3.19696200	-1.13351300
C	5.06036400	-1.41482000	-0.21678000
C	4.47685000	-0.53726900	-1.13893900
C	6.05629000	-0.92192200	0.63679100
C	4.83855700	0.81334400	-1.20723100
H	3.71242000	-0.91124900	-1.81012900
C	6.44430500	0.41755000	0.56928100
H	6.53401800	-1.59064900	1.34758600
C	4.13462900	1.73142400	-2.17819300
C	5.83635800	1.28266000	-0.34214400
H	7.22661200	0.78754600	1.22634500
C	2.83387700	2.39104200	-1.62492800
H	3.87275200	1.17455000	-3.08226800

H	4.80279600	2.54690200	-2.47580600
H	6.14390200	2.32356300	-0.39119500
C	1.85904100	1.28413100	-1.19451200
C	2.17522600	3.18532100	-2.77066900
C	3.15629000	3.33218500	-0.45899700
O	1.55297100	0.41731900	-2.07509800
O	1.41796400	1.31069500	-0.00148600
H	1.26152800	3.68292000	-2.43026100
H	2.86133300	3.96060500	-3.12739500
H	1.92123600	2.53226000	-3.60948500
H	3.85935800	4.10100800	-0.79712300
H	2.25562800	3.82921400	-0.09477100
H	3.60627900	2.79696800	0.37892300
O	-0.99756800	-2.60438400	-0.96263300
C	-1.38737300	-2.62316000	0.24391800
O	-1.09997700	-1.74661300	1.12531600
C	-2.26938100	-3.79169700	0.70224400
C	-3.60612000	-3.22045000	1.26659300
C	-1.52688300	-4.52829900	1.83456900
C	-2.53976200	-4.76211100	-0.45365400
H	-4.22765500	-4.07563800	1.55275800
H	-3.37826200	-2.66144600	2.17899700
C	-4.35725000	-2.32871600	0.30539800
H	-2.13711200	-5.36173400	2.19801600
H	-0.57617200	-4.93621700	1.47443200
H	-1.31878800	-3.85721300	2.67171300
H	-1.60609200	-5.18160800	-0.83804600
H	-3.16470000	-5.58750200	-0.09660100
H	-3.05605200	-4.27269700	-1.28189500
C	-4.04633600	-0.96532300	0.23593000
C	-5.34405200	-2.83214200	-0.55214700
C	-4.67467600	-0.10501000	-0.67174000
H	-3.28454300	-0.57025300	0.89585900
C	-5.99207800	-1.98680800	-1.45516400
H	-5.61105600	-3.88430200	-0.50516800
C	-4.27196300	1.34950700	-0.73499100
C	-5.65898200	-0.63256000	-1.51844900
H	-6.76422200	-2.38425900	-2.10808800
C	-3.07145900	1.65884100	-1.68145000
H	-5.11467500	1.95603000	-1.08365400
H	-4.01215400	1.70279100	0.26689200
H	-6.17122400	0.02078000	-2.21933100
C	-1.85865300	0.81872800	-1.25175000
C	-3.44319600	1.37929500	-3.14147400

C	-2.70495700	3.14546100	-1.51288000
O	-1.33101200	0.04624300	-2.10856100
O	-1.46086200	0.96909600	-0.04778900
H	-4.30688900	1.99142500	-3.42166900
H	-2.61530800	1.62909400	-3.81065700
H	-3.69842900	0.32967800	-3.29932800
H	-3.55685900	3.77601000	-1.78621400
H	-2.43740200	3.36306300	-0.47701300
H	-1.87068200	3.41051100	-2.17350300
H	-2.27187000	5.44020900	1.30221700
O	-2.10306900	6.09674000	0.48044600
H	-1.92772000	6.99109800	0.81747800
H	-1.15366800	5.65115700	-0.03960300
O	-0.12787500	5.02772700	-0.39573000
H	-0.35123300	4.36298100	-1.06764000
H	0.06237100	4.49307700	0.52162700
C	0.04119800	0.50800700	2.82181900
C	-1.32757800	0.15568200	3.44101300
C	-2.26500100	1.31369300	2.99491500
H	0.94498500	0.04477400	3.20364400
H	-1.70563200	-0.80821500	3.10160100
H	-1.26111700	0.13585300	4.53660700
H	-2.78803800	1.08442400	2.06625500
H	-2.98237900	1.61878100	3.75760300
N	-1.29627000	2.38324200	2.73813300
C	-1.31922800	3.70861800	2.36192300
O	-2.38493700	4.37553600	2.22883500
C	0.04820400	4.05400800	2.08726700
H	0.48539100	4.94672700	2.52709800
C	-0.02426200	1.90150600	2.68085600
O	0.82924200	2.86753400	2.41801500

14

Rh	0.39591100	-1.04605800	-1.60674400
Rh	0.19190300	-0.21642300	0.64947700
O	1.81191500	-1.36473700	1.14732400
C	2.37669100	-2.07414200	0.25368200
O	2.01180600	-2.14413900	-0.96265800
C	3.58468200	-2.92298800	0.66446000
C	3.92789600	-2.71402800	2.14370000
C	3.22468300	-4.40202500	0.41769100
C	4.79309100	-2.54433000	-0.24783500
H	4.79311800	-3.33113200	2.40751900
H	4.16989800	-1.67149900	2.35952000

H	3.09124800	-3.00706800	2.78381400
H	2.97759400	-4.57788200	-0.63240900
H	4.07305300	-5.03964600	0.68705400
H	2.36700200	-4.70156500	1.02975800
H	5.64412900	-3.14996900	0.08156600
H	4.55109300	-2.84639400	-1.27066400
C	5.16004800	-1.07820200	-0.22952800
C	4.53962200	-0.19059600	-1.11777200
C	6.09585000	-0.56728900	0.67996500
C	4.80544600	1.18455700	-1.09845900
H	3.82307500	-0.57789000	-1.83315800
C	6.38881800	0.79747000	0.69993800
H	6.60356200	-1.24163900	1.36403000
C	4.05363700	2.11120900	-2.02628000
C	5.74480200	1.67015600	-0.17896800
H	7.12598500	1.18182900	1.39952200
C	2.69826700	2.62755300	-1.45116000
H	3.84937800	1.59746100	-2.97015800
H	4.66178300	2.99263700	-2.25554800
H	5.97789700	2.73111600	-0.15933700
C	1.83393800	1.41594300	-1.08636100
C	1.95584000	3.42130100	-2.54469600
C	2.92640100	3.53098600	-0.23323100
O	1.56944600	0.59003300	-2.01950300
O	1.43207700	1.31505400	0.11571000
H	1.00126800	3.79557100	-2.16109900
H	2.55801200	4.28344800	-2.85001400
H	1.76265900	2.80166500	-3.42412800
H	3.56880600	4.36992500	-0.52137500
H	1.97994700	3.93679700	0.13079700
H	3.40546200	2.99376800	0.58712900
O	-0.82205600	-2.60550400	-1.09834300
C	-1.28263200	-2.67377400	0.08241200
O	-1.03075300	-1.84087100	1.01609500
C	-2.19603600	-3.85360300	0.43328800
C	-3.52385000	-3.31289700	1.04400800
C	-1.46993300	-4.69936300	1.49961700
C	-2.48099000	-4.71268500	-0.80413000
H	-4.14234700	-4.18384400	1.28488200
H	-3.28410600	-2.81335400	1.98731100
C	-4.29699300	-2.36414700	0.15555100
H	-2.09384800	-5.55293700	1.78433300
H	-0.52247400	-5.08699400	1.10995400
H	-1.25884600	-4.10937100	2.39553100

H	-1.55642700	-5.12278700	-1.21858900
H	-3.13193900	-5.54770700	-0.52498200
H	-2.97738200	-4.13764900	-1.58870500
C	-3.95684200	-1.00678200	0.12393400
C	-5.35267800	-2.80276100	-0.65423200
C	-4.62785800	-0.08504100	-0.68756900
H	-3.13925900	-0.66089800	0.74029000
C	-6.04021600	-1.89820200	-1.46668500
H	-5.64379800	-3.84955900	-0.63893100
C	-4.19261200	1.36277500	-0.70040800
C	-5.68184400	-0.54856200	-1.48595100
H	-6.86490900	-2.24587000	-2.08275300
C	-2.99170000	1.66568400	-1.64670200
H	-5.02253600	1.99947800	-1.02429900
H	-3.91740200	1.67718100	0.31019000
H	-6.22737200	0.14978600	-2.11479900
C	-1.79075300	0.81175100	-1.22337000
C	-3.37025500	1.39400200	-3.10691800
C	-2.58746000	3.14345500	-1.48126900
O	-1.24892100	0.06805000	-2.09699600
O	-1.40385900	0.91836200	-0.00946100
H	-4.23026300	2.01477000	-3.37903600
H	-2.54380400	1.64164400	-3.77840100
H	-3.63627900	0.34749900	-3.26936200
H	-3.41988700	3.79221300	-1.77224400
H	-2.32202400	3.36645000	-0.44867400
H	-1.72947800	3.37837200	-2.11989000
H	-2.93387000	5.08463200	1.41097300
O	-2.71822100	5.93204200	0.96413500
H	-2.52748300	6.54855700	1.68579900
H	-1.26448200	5.74089100	-0.04608200
O	-0.43834000	5.55616800	-0.54696000
H	-0.74625000	5.33699100	-1.43618500
H	-0.43925000	3.94849600	0.97875500
C	0.18335800	0.28928100	2.99808500
C	-1.04607000	-0.35165400	3.64883600
C	-2.22684800	0.59082900	3.26729700
H	1.19625400	-0.03234600	3.19685500
H	-1.22927400	-1.36560800	3.29372000
H	-0.92256600	-0.38375900	4.73792800
H	-2.80288300	0.21243500	2.42327100
H	-2.90218700	0.80134900	4.09733100
N	-1.52554200	1.81293500	2.85894600
C	-1.86534200	3.02779400	2.36686000

O	-2.99497500	3.49337200	2.22686000
C	-0.53008900	3.69251400	2.03855700
H	-0.36357900	4.58509600	2.64683100
C	-0.16600600	1.58683500	2.73483400
O	0.47509900	2.69745100	2.38671700

2a'

C	0.44861300	0.87584600	-0.00003300
C	1.13628300	-1.37597600	0.00003200
C	1.77950500	0.99044100	0.00007200
H	1.09837000	-2.01215100	0.88745800
H	1.09845900	-2.01238900	-0.88722400
H	2.34917100	1.90773100	0.00017100
C	2.37388400	-0.41253100	-0.00002600
H	3.00228200	-0.59424200	-0.87964800
H	3.00241100	-0.59431900	0.87948600
O	-0.60527000	1.72389200	-0.00000500
C	-1.81442600	0.91911000	0.00000600
H	-2.40456300	1.14603700	0.89291000
H	-2.40456600	1.14604600	-0.89289800
C	-1.34699300	-0.54311800	0.00000300
O	-2.04819800	-1.54515900	0.00004000
N	0.00356900	-0.44845900	-0.00012200

TS8'

Rh	-0.18781900	0.00230300	0.54352600
O	-1.59389500	-1.47447500	0.57444500
O	1.21550500	-1.42491000	0.15518100
O	1.19206200	1.51012500	0.41682100
O	-1.63528700	1.41697900	0.82858500
Rh	-0.51018300	0.20141700	-1.80333400
C	-2.19379300	1.93498900	-0.19064800
O	-1.92930400	1.62937100	-1.39920700
C	1.45606900	2.02207100	-0.72140900
O	0.91144500	1.67411100	-1.81637600
C	-2.13790900	-1.83242500	-0.51923700
O	-1.89322900	-1.31423100	-1.65771100
O	0.94530200	-1.21686800	-2.07331900
C	1.49213800	-1.73635000	-1.04866000
C	-3.15758400	-2.97380400	-0.47726000
C	-3.25821600	3.01321700	0.03271600
C	2.49719300	3.14433200	-0.74454800
C	2.54944700	-2.82595700	-1.23885200
C	-4.50351500	-2.46135800	-1.07760800

H	-5.21924900	-3.28730700	-1.00838600
H	-4.34337300	-2.25330200	-2.13931300
C	-3.35518800	-3.48124000	0.95614300
H	-4.09183900	-4.29129600	0.95556000
H	-2.41917700	-3.87182900	1.36489700
H	-3.71196500	-2.69208700	1.62086500
C	-2.62072000	-4.11664400	-1.36251300
H	-3.32999400	-4.95067500	-1.35912600
H	-2.47888500	-3.78426200	-2.39398700
H	-1.66170900	-4.48532800	-0.98263000
C	-4.58424300	2.55540200	-0.65301700
H	-5.33019100	3.33220600	-0.45427200
H	-4.41566000	2.53097000	-1.73338500
C	-2.77063800	4.30595800	-0.65189000
H	-3.51745100	5.09606600	-0.52273500
H	-1.83056500	4.65136200	-0.20825400
H	-2.61107100	4.14998000	-1.72180400
C	-3.47477600	3.26893500	1.52857100
H	-2.55393500	3.62060200	2.00198200
H	-4.24205100	4.03924600	1.65838500
H	-3.79971000	2.36708000	2.05103000
C	2.75672300	3.62298600	-2.17734800
H	3.50552700	4.42166900	-2.16363400
H	3.12587600	2.81607400	-2.81335900
H	1.84303600	4.01905700	-2.62854000
C	1.94490400	4.30973500	0.10175000
H	1.75888100	3.99590600	1.13223400
H	2.66699500	5.13261000	0.11266000
H	1.00679900	4.68717500	-0.31934000
C	3.81052900	2.62337200	-0.08214000
H	4.53536200	3.44338600	-0.12417100
H	3.59998100	2.42359000	0.97231200
C	3.85576700	-2.39434600	-0.49847500
H	3.64670600	-2.37960700	0.57435800
H	4.59507400	-3.18203100	-0.67954800
C	2.01746900	-4.11047000	-0.56954900
H	1.07058400	-4.42435300	-1.02237700
H	2.74218800	-4.92034700	-0.70328800
H	1.86299400	-3.95611100	0.50090900
C	2.81383900	-3.07935700	-2.72672900
H	3.57770100	-3.85646800	-2.83342900
H	1.90636200	-3.42073100	-3.23269000
H	3.16541700	-2.17877200	-3.23464300
C	-5.05887900	-1.22976300	-0.40044400

C	-4.65929000	0.04217100	-0.82956800
C	-5.94724300	-1.32188700	0.67932200
C	-5.09670600	1.21044400	-0.19320300
H	-3.98272000	0.12386000	-1.67271600
C	-6.41097100	-0.16710500	1.31215500
H	-6.28368500	-2.29841700	1.01637600
C	-5.98507600	1.09147800	0.88392000
H	-7.11060900	-0.24810900	2.13946300
H	-6.35136800	1.98640700	1.37919500
C	4.40704100	-1.05616400	-0.93070700
C	3.95343900	0.11701000	-0.31372700
C	5.34645800	-0.94741300	-1.96474200
C	4.38593500	1.38364200	-0.72686500
H	3.24061000	0.04052600	0.49881500
C	5.80664600	0.30596900	-2.37272500
H	5.72497400	-1.84672100	-2.44282600
C	5.32516700	1.46612500	-1.76357300
H	6.54494500	0.37871000	-3.16658900
H	5.68594200	2.43902800	-2.08578600
C	1.59667500	0.82572400	4.53083200
C	3.08909200	0.82418200	4.82742100
C	3.68339200	-0.05612100	3.67436600
H	1.06248400	-0.58984400	4.70342300
H	0.88949900	1.47223100	5.04048600
H	3.50050300	1.83653600	4.79619300
H	3.29319900	0.41500400	5.82010100
H	4.38421400	0.49773300	3.04881200
H	4.16846200	-0.96921100	4.02243000
N	2.49765100	-0.44670900	2.87682300
C	1.96530600	-1.78565300	2.97689300
O	2.64311300	-2.80437900	2.94249000
C	0.57365400	-1.55754900	3.32162400
H	-0.22498900	-2.27018700	3.15956000
C	1.44698600	0.37330500	3.21345000
O	0.26650100	-0.20136600	2.88009400

TS8''

Rh	0.04745100	-0.06174900	-0.34325200
O	1.47947500	-1.05394200	-1.42165000
O	-1.37636200	-1.03995300	-1.43886200
O	-1.35004800	0.82682800	0.86305700
O	1.48187900	0.81281600	0.81382300
Rh	0.02006700	-1.89886300	1.19231300
C	1.86252300	0.23550400	1.87995000

O	1.44840100	-0.89896600	2.28878100
C	-1.79627400	0.22018900	1.88785300
O	-1.43185100	-0.93760700	2.27044100
C	1.87006100	-2.19909500	-1.02826300
O	1.44930900	-2.79464900	0.01578500
O	-1.43414600	-2.75746700	0.02569400
C	-1.82267600	-2.16055900	-1.02760600
C	2.92521800	-2.92485500	-1.86963300
C	2.89954100	0.95222100	2.75054300
C	-2.84216800	0.97201500	2.71637200
C	-2.89771300	-2.82105000	-1.89614800
C	4.16858700	-3.20513700	-0.96893900
H	4.91957200	-3.68999500	-1.60195400
H	3.87262100	-3.92476200	-0.20046000
C	3.31481200	-2.09314600	-3.09759800
H	4.06927900	-2.63407600	-3.67846800
H	2.44803400	-1.91915600	-3.74127600
H	3.72677000	-1.12209900	-2.81638500
C	2.32936700	-4.27186600	-2.32399200
H	3.06999400	-4.82406200	-2.91177700
H	2.03795400	-4.88422500	-1.46701400
H	1.44626000	-4.11432200	-2.95277700
C	4.15360900	0.03266900	2.88523800
H	4.89527900	0.58556300	3.47168600
H	3.86660200	-0.84966800	3.46460000
C	2.28444100	1.16004600	4.14848300
H	3.00986400	1.65459900	4.80284400
H	1.39241900	1.79324700	4.09029500
H	2.00153300	0.20621100	4.60083300
C	3.27490400	2.30885000	2.14407700
H	2.39860700	2.95725200	2.07059400
H	4.01581400	2.80097300	2.78312500
H	3.69561700	2.20263900	1.14308000
C	-3.36564400	0.10359500	3.86515000
H	-4.11316800	0.66457000	4.43593900
H	-3.82975800	-0.81459200	3.50000100
H	-2.55491600	-0.17390000	4.54435300
C	-2.15930900	2.23197000	3.28591500
H	-1.77203700	2.86169500	2.48171500
H	-2.88003000	2.81331500	3.87040400
H	-1.32693400	1.96121700	3.94461400
C	-3.99799100	1.41549600	1.76587100
H	-4.72630000	1.95924600	2.37735500
H	-3.58163200	2.11391600	1.03501900

C	-4.06371400	-1.80522300	-2.10900100
H	-3.67376500	-0.96036500	-2.68323200
H	-4.81502900	-2.30715500	-2.72828100
C	-2.26114500	-3.13270800	-3.26648500
H	-1.42136200	-3.82752900	-3.15711100
H	-3.00403300	-3.59878900	-3.92212400
H	-1.89634400	-2.22137700	-3.74776500
C	-3.40433100	-4.11700400	-1.25374600
H	-4.17408400	-4.56353700	-1.89178500
H	-2.59201100	-4.84002300	-1.14080500
H	-3.83640200	-3.93654100	-0.26741500
C	4.75387600	-1.97812900	-0.30945000
C	4.27997500	-1.56642200	0.94239100
C	5.74843700	-1.21175900	-0.93177700
C	4.74882200	-0.40407500	1.56691300
H	3.51876600	-2.15820900	1.43826800
C	6.24198300	-0.06060700	-0.31515200
H	6.14429200	-1.52445700	-1.89403900
C	5.74319800	0.34512700	0.92402100
H	7.02352500	0.51873500	-0.79905400
H	6.13380500	1.23957900	1.40115600
C	-4.69635800	-1.29905300	-0.83303300
C	-4.15841400	-0.18218500	-0.17915700
C	-5.80073600	-1.94500500	-0.26114600
C	-4.67106600	0.27089700	1.04398900
H	-3.32186400	0.34479900	-0.62515300
C	-6.34363800	-1.48562200	0.93997400
H	-6.24140700	-2.80164900	-0.76392700
C	-5.77851800	-0.38925400	1.59338200
H	-7.20984800	-1.98312100	1.36762800
H	-6.20236700	-0.03880100	2.53052900
C	1.74573700	4.60120300	-0.40308200
C	0.74225300	5.29948700	0.51508100
C	-0.63201000	4.66348300	0.12998600
H	0.72706700	5.30075700	-2.35210100
H	2.80599500	4.80630000	-0.43662600
H	0.96312900	5.09972900	1.57269400
H	0.71865700	6.38611300	0.39126200
H	-1.25151400	4.42758100	0.99531400
H	-1.20769500	5.31031500	-0.53916500
N	-0.22449300	3.44035300	-0.57007200
C	-0.86443300	2.52370700	-1.38923100
O	-2.10094300	2.45713900	-1.55786100
C	0.21657400	1.83710000	-2.05997900

H	0.28847400	0.83402100	-2.46096600
C	1.13316600	3.48369200	-0.85917700
O	1.47053100	2.44445700	-1.64027500
O	-2.36661900	4.95698600	-2.57511800
H	-2.44307300	4.04674800	-2.19046300
H	-2.87315800	4.93745800	-3.40138600
O	0.33031600	3.22000100	-4.34089100
H	1.21667700	3.03806000	-4.70262900
H	0.17404800	2.53867700	-3.51343100
O	0.16283100	5.32654000	-3.15873500
H	-0.80586100	5.29029800	-2.87445600
H	0.31919800	4.23942000	-3.83761400

TS8_Cu

Cu	-0.07230300	-0.95823000	0.47085000
N	-1.42295000	-0.75414200	2.00334400
N	-0.17883200	1.17644800	-0.17603600
N	-1.28421300	-1.70337000	-0.87296600
C	-2.44531400	-0.54512300	2.50650400
C	-0.85186200	2.02688100	-0.58732000
C	-2.17820800	-1.96037000	-1.56209300
C	-1.69892700	3.08051600	-1.11808800
H	-2.45267500	2.61951800	-1.75990300
H	-2.20347500	3.59276900	-0.29584100
H	-1.09779800	3.79552500	-1.68605800
C	-3.74003400	-0.29597500	3.11280100
H	-4.50989600	-0.60419100	2.40216500
H	-3.83404600	-0.85968000	4.04472800
H	-3.84976600	0.77197800	3.31597700
C	-3.31744800	-2.27738500	-2.40228400
H	-3.33707000	-1.60193000	-3.26086100
H	-3.25348100	-3.31241500	-2.74847400
H	-4.22385300	-2.12845000	-1.81171500
B	-4.26785000	0.65214700	-0.38692000
F	-3.52090200	1.36258700	0.57538100
F	-3.55153200	0.62779900	-1.60505500
F	-4.45736300	-0.67653600	0.06109600
F	-5.50766300	1.26794000	-0.57891600
C	3.69455000	2.08107500	0.70820600
C	3.93769000	2.40505200	-0.77398600
C	3.66372600	1.05323800	-1.51037500
H	5.04161400	0.92137400	0.87685100
H	3.70461700	2.82530100	1.49376300
H	3.24236400	3.17216600	-1.13630500

H	4.95108900	2.76254000	-0.97827300
H	3.07118900	1.17165000	-2.41863800
H	4.58789000	0.52760500	-1.77044000
N	2.91156200	0.30491100	-0.49908900
C	2.53383400	-1.01589400	-0.31722600
O	2.83506800	-1.93086700	-1.13155300
C	1.88476700	-1.05283800	0.97073400
H	2.12614100	-1.88125600	1.63320300
C	2.90773600	0.95351900	0.71425900
O	2.29185900	0.22307100	1.62961600
O	5.35301900	-1.72004200	-0.63176900
H	4.38115200	-1.86566300	-0.93106600
H	5.63603600	-2.52766800	-0.16967400
O	5.78720000	0.19395800	0.78445400
H	5.53604400	-0.74003600	0.08320500
H	6.59791200	0.64064100	0.48521400

15

Rh	-2.20434100	1.73446500	0.83580500
O	-2.81798300	0.24477600	2.08752700
O	-0.77710100	2.24002400	2.21730200
O	-1.53275700	3.15225700	-0.49738200
O	-3.55812300	1.11843600	-0.58291800
Rh	-0.62801100	0.21312200	-0.12580200
C	-3.20434700	0.25748700	-1.44691100
O	-2.05341300	-0.28875200	-1.50360300
C	-0.62888000	2.83803400	-1.33633300
O	-0.05755000	1.70280400	-1.39761400
C	-2.25079800	-0.89195700	2.01432600
O	-1.31396200	-1.19157400	1.20488900
O	0.70227700	0.79520100	1.30677900
C	0.35190600	1.64685500	2.18215700
C	-2.70406200	-1.99439700	2.97578300
C	-4.20885500	-0.16773000	-2.52080200
C	-0.19211600	3.91519900	-2.33307600
C	1.36371100	2.00643600	3.27353200
C	-3.08137400	-3.25919200	2.14483700
H	-3.41064200	-4.02317400	2.85696700
H	-2.16940000	-3.62560900	1.66737900
C	-3.88555100	-1.52730700	3.83321800
H	-4.18813700	-2.33670800	4.50573800
H	-3.60864600	-0.66259800	4.44219800
H	-4.74588900	-1.24868300	3.22112800
C	-1.50447000	-2.34048800	3.88188300

H	-1.78427800	-3.14091000	4.57469600
H	-0.64789600	-2.67314900	3.29034500
H	-1.19977100	-1.47036600	4.47330600
C	-4.33954900	-1.72268200	-2.49048200
H	-5.06739300	-1.99750100	-3.26138200
H	-3.37467200	-2.14760000	-2.78080700
C	-3.63108500	0.25324500	-3.88770400
H	-4.31650100	-0.04597200	-4.68741100
H	-3.50393300	1.34014500	-3.93843200
H	-2.65994500	-0.21552300	-4.06607200
C	-5.56763400	0.50525900	-2.29956800
H	-5.47681800	1.59354300	-2.35188800
H	-6.26598600	0.18177700	-3.07833900
H	-5.99185900	0.24731800	-1.32715900
C	0.75771600	3.33652200	-3.38818000
H	1.00540400	4.11525200	-4.11700600
H	1.68664800	2.97840300	-2.94299500
H	0.29162900	2.50262900	-3.92124800
C	-1.44621100	4.48343900	-3.02301100
H	-2.15006900	4.88928500	-2.29268800
H	-1.15690800	5.28383100	-3.71180000
H	-1.95771500	3.70628700	-3.60124900
C	0.50526200	5.06139500	-1.53041800
H	0.91668500	5.76054100	-2.26650200
H	-0.26558400	5.59471900	-0.96663300
C	1.77222300	3.50224600	3.07668500
H	0.91782000	4.12585000	3.35588600
H	2.57837600	3.71010200	3.78845300
C	0.68545500	1.85253700	4.64717200
H	0.37769600	0.81453100	4.81386500
H	1.38915600	2.12867300	5.43938100
H	-0.19743500	2.49119600	4.72789800
C	2.58917900	1.09010000	3.19199400
H	3.30984200	1.37341100	3.96644300
H	2.30660900	0.04550800	3.35002800
H	3.07496900	1.15798400	2.22024000
C	-4.14844700	-3.03089200	1.09909900
C	-3.79642400	-2.57102900	-0.17678000
C	-5.50464300	-3.24104400	1.38255000
C	-4.76050800	-2.28774800	-1.15319500
H	-2.75055800	-2.41799600	-0.41212600
C	-6.47715200	-2.98587800	0.41407400
H	-5.79649500	-3.61377200	2.36048900
C	-6.10968000	-2.50600700	-0.84422700

H	-7.52489800	-3.16401700	0.63987800
H	-6.87062100	-2.30761900	-1.59392600
C	2.20345300	3.85177600	1.67155700
C	1.25544900	4.32144700	0.75426100
C	3.52426200	3.68085200	1.23720100
C	1.58494100	4.60212700	-0.57736500
H	0.23084000	4.46140400	1.08328300
C	3.87426200	3.96539600	-0.08385300
H	4.27954400	3.33206200	1.93522400
C	2.91262700	4.42100800	-0.98779700
H	4.90334000	3.83792200	-0.40809100
H	3.19607200	4.65235900	-2.01064200
C	2.86178000	0.41759600	-1.65163500
H	2.18919700	1.01432900	-2.25088800
H	3.87503900	0.77188500	-1.51846500
C	2.43744700	-0.69744200	-1.03985400
C	1.05261200	-1.25339600	-1.25498500
N	0.56459400	-0.98068200	-2.47879000
N	0.14433500	-0.69119200	-3.48204000
C	0.61062700	-2.57636900	-0.72509000
O	0.98702400	-3.07022400	0.31483500
O	-0.27565500	-3.15342800	-1.56396300
C	-0.77621700	-4.44385600	-1.16054400
H	-1.52986000	-4.70550100	-1.90223400
H	0.03321900	-5.17799600	-1.16466500
H	-1.22186300	-4.39229100	-0.16705300
O	3.18305400	-1.45981200	-0.21608000
Si	4.77725000	-2.02361900	-0.45555700
C	6.03010100	-0.63661900	-0.07476500
H	6.20265300	-0.12966400	-1.03623900
C	4.92571900	-3.44235400	0.78716000
H	5.98738200	-3.72932500	0.78265400
C	4.94624300	-2.53980400	-2.27870800
H	5.04011200	-1.59452300	-2.83276900
C	3.73185100	-3.28608900	-2.85703700
H	2.81779100	-2.68937800	-2.80482000
H	3.90223200	-3.52460300	-3.91504000
H	3.54067500	-4.22974900	-2.33797800
C	6.24073900	-3.34208000	-2.50872600
H	6.23743400	-4.28228900	-1.94535000
H	6.35306100	-3.59908700	-3.56977800
H	7.13359100	-2.78141800	-2.21436600
C	5.50901500	0.41723900	0.91752300
H	6.24176400	1.22611900	1.03847300

H	4.57016100	0.86604800	0.58714700
H	5.33563600	-0.01418900	1.90855000
C	7.38186700	-1.19715800	0.40722800
H	7.81325600	-1.92426900	-0.28813500
H	8.11310900	-0.38818100	0.53074700
H	7.27779500	-1.69241600	1.37876800
C	4.56857700	-2.97024400	2.20925500
H	4.66884400	-3.79556000	2.92611500
H	5.21622700	-2.15709700	2.55135100
H	3.53458500	-2.61325600	2.25624900
C	4.09891100	-4.68179800	0.40576000
H	4.43064700	-5.11701800	-0.54178200
H	4.19631000	-5.45921800	1.17522500
H	3.03615900	-4.43601900	0.31590400

TS10

Rh	-2.33858000	1.77785900	0.55663200
O	-3.06028800	0.36991200	1.85747700
O	-1.08403800	2.44859400	2.05114800
O	-1.51809800	3.08119600	-0.82309300
O	-3.49568900	0.99565100	-0.94595400
Rh	-0.61362700	0.19532300	-0.07393000
C	-3.02859300	0.07769400	-1.68591800
O	-1.86697000	-0.43972000	-1.56861400
C	-0.51770400	2.70861200	-1.51091400
O	0.07692900	1.58742500	-1.39126800
C	-2.48325500	-0.75822500	1.93600800
O	-1.45815800	-1.11119100	1.26368900
O	0.48985200	0.93427600	1.47678400
C	0.03690100	1.87018900	2.20972400
C	-3.02766700	-1.79247300	2.92638000
C	-3.89283000	-0.46489300	-2.82862200
C	0.04339900	3.67960100	-2.55432200
C	0.92988500	2.34541300	3.36086000
C	-3.26638000	-3.13565200	2.17051000
H	-3.65952300	-3.84965600	2.90208200
H	-2.29406700	-3.50655200	1.83728600
C	-4.31731600	-1.29542100	3.58840200
H	-4.68537300	-2.05571200	4.28524400
H	-4.13840100	-0.37482000	4.15026700
H	-5.09961200	-1.09499200	2.85333000
C	-1.94258800	-2.01792400	3.99969600
H	-2.28864800	-2.76179200	4.72492000
H	-1.01293800	-2.37391500	3.54896000

H	-1.73162400	-1.08884400	4.54017200
C	-3.99314600	-2.01618200	-2.69084200
H	-4.61836500	-2.37046100	-3.51743300
H	-2.99215600	-2.43314200	-2.83252800
C	-3.17622700	-0.13359400	-4.15378100
H	-3.77218100	-0.49827000	-4.99682500
H	-3.05095600	0.94840800	-4.26961400
H	-2.18985700	-0.60176700	-4.19735100
C	-5.28267700	0.18112700	-2.81765500
H	-5.21070100	1.26259900	-2.96126300
H	-5.88331100	-0.23332400	-3.63393900
H	-5.80736700	-0.00018100	-1.87747100
C	1.11449100	2.99419400	-3.41316300
H	1.50425000	3.70801900	-4.14647400
H	1.94692500	2.62763200	-2.80995300
H	0.69291200	2.14233300	-3.95472800
C	-1.11029500	4.16490600	-3.45029200
H	-1.89515900	4.64228400	-2.85900300
H	-0.73377500	4.88917500	-4.18003500
H	-1.55346100	3.32776100	-4.00040300
C	0.64422000	4.90566600	-1.79524900
H	1.13720200	5.53517200	-2.54373400
H	-0.18493600	5.48268200	-1.37526300
C	1.37396400	3.81060600	3.05281900
H	0.50049700	4.45941000	3.16584700
H	2.09708900	4.09545200	3.82462400
C	0.10475100	2.33983900	4.66057300
H	-0.22184500	1.32417400	4.90854200
H	0.71604000	2.71149200	5.48950100
H	-0.78016200	2.97415800	4.56888200
C	2.14854200	1.42679100	3.51671700
H	2.77089500	1.78494800	4.34372400
H	1.83657500	0.40326200	3.73993900
H	2.75624600	1.39730400	2.61119700
C	-4.20366900	-3.03175800	0.98974400
C	-3.71000100	-2.67207700	-0.27138100
C	-5.58066200	-3.25090700	1.13101100
C	-4.55801800	-2.48897200	-1.37141100
H	-2.64543800	-2.51525700	-0.39714300
C	-6.43663000	-3.09872900	0.03895200
H	-5.98025400	-3.54802200	2.09669300
C	-5.93109000	-2.71267900	-1.20354700
H	-7.50097200	-3.28297100	0.15630700
H	-6.60197300	-2.59133400	-2.04951000

C	1.96357700	4.01313800	1.67665500
C	1.12629300	4.38084400	0.61643600
C	3.32708200	3.82320800	1.41501900
C	1.60779700	4.54879800	-0.68742900
H	0.07015800	4.53693100	0.81072400
C	3.82773400	3.99659800	0.12308700
H	3.99794500	3.55582000	2.22640200
C	2.97538500	4.35366600	-0.92378700
H	4.88899800	3.86185200	-0.06722900
H	3.37476900	4.49757200	-1.92361800
C	2.81159300	0.49765900	-0.39211000
H	2.09377100	1.29400000	-0.28798200
H	3.86459900	0.75120000	-0.36356900
C	2.40406700	-0.77476800	-0.53589300
C	0.96624700	-1.14213100	-0.59708300
N	0.74065500	-1.24051300	-2.32504400
N	0.44778400	-0.84594000	-3.32053400
C	0.67520100	-2.53135200	-0.12945300
O	1.01882500	-2.89161400	0.97983900
O	-0.05479900	-3.26594200	-0.98088800
C	-0.43382900	-4.57903200	-0.51602400
H	0.45360900	-5.20337100	-0.38748200
H	-0.97671600	-4.50982500	0.42740100
H	-1.07559700	-4.98692300	-1.29588300
O	3.22751900	-1.84421200	-0.69750100
Si	4.88255000	-2.00353300	-0.30232300
C	5.17728000	-1.31273600	1.44253600
H	5.19189500	-0.22064800	1.31679500
C	5.14617700	-3.87037000	-0.46955900
H	6.22924000	-4.03781900	-0.37991300
C	5.90374400	-1.00642800	-1.56545500
H	6.06491100	-0.02270300	-1.10002700
C	5.15876700	-0.77411800	-2.89208700
H	4.21075000	-0.24800700	-2.74251600
H	5.76903000	-0.17061500	-3.57646300
H	4.93643500	-1.71834700	-3.40076300
C	7.28795500	-1.63184200	-1.81699800
H	7.20077700	-2.60813000	-2.30594700
H	7.89044900	-0.99136200	-2.47367100
H	7.85560200	-1.77706500	-0.89180000
C	4.07027300	-1.64096200	2.45861000
H	4.24089700	-1.09498800	3.39536000
H	3.07740900	-1.37477600	2.08992500
H	4.05188900	-2.70718300	2.70296100

C	6.56155900	-1.72954900	1.97422700
H	7.37373000	-1.41482800	1.31009300
H	6.75034300	-1.27880300	2.95695700
H	6.63474000	-2.81633700	2.09707300
C	4.44476700	-4.66862700	0.64309100
H	4.55928000	-5.74750400	0.47475700
H	4.85946000	-4.44469500	1.62987100
H	3.37168500	-4.45024700	0.67710600
C	4.70118700	-4.37472300	-1.85459400
H	5.22965800	-3.87252700	-2.67062900
H	4.88905400	-5.45169700	-1.95230200
H	3.62796400	-4.21233000	-2.00440800

16

Rh	-2.20342200	1.72331300	0.69755700
O	-2.76138500	0.26088100	2.01818600
O	-0.81996200	2.37239500	2.08330200
O	-1.57232700	3.10154000	-0.70296900
O	-3.47795800	0.94700600	-0.71686700
Rh	-0.49152200	0.21309700	-0.15113900
C	-3.05702100	0.05218600	-1.50996300
O	-1.87477200	-0.43336400	-1.51645600
C	-0.62886300	2.79122200	-1.49087600
O	0.01472600	1.68951200	-1.46540400
C	-2.12623000	-0.83701900	2.02088100
O	-1.15764600	-1.12967100	1.24242800
O	0.74803200	0.95326800	1.29094600
C	0.33346800	1.84467000	2.10413000
C	-2.50732000	-1.91732400	3.03810300
C	-4.00634500	-0.50684900	-2.57519600
C	-0.21006000	3.81555800	-2.55010500
C	1.31908000	2.32123500	3.17624600
C	-2.78460100	-3.25135800	2.27654500
H	-3.07507500	-3.99322800	3.02805900
H	-1.84517500	-3.58360500	1.82721000
C	-3.72521800	-1.48619200	3.86225700
H	-3.97539200	-2.27392000	4.58044500
H	-3.51464800	-0.56940300	4.41950500
H	-4.59780900	-1.30519800	3.23126100
C	-1.29273700	-2.12616400	3.96653600
H	-1.52135400	-2.90342600	4.70307000
H	-0.41127000	-2.43251000	3.39742500
H	-1.05295300	-1.20481300	4.50856000
C	-4.03659200	-2.06278500	-2.45400600

H	-4.72453700	-2.42991100	-3.22323100
H	-3.03871800	-2.43832900	-2.69610000
C	-3.42651200	-0.13436500	-3.95537400
H	-4.07418900	-0.52715800	-4.74602300
H	-3.36810400	0.95304400	-4.07394200
H	-2.42425600	-0.55036400	-4.08635400
C	-5.41029200	0.08748000	-2.42294400
H	-5.39023600	1.17313200	-2.55011000
H	-6.06970500	-0.33481600	-3.18821900
H	-5.83643800	-0.13069300	-1.44180600
C	0.81194400	3.21284200	-3.52225500
H	1.08743100	3.96456600	-4.26908300
H	1.71820800	2.88470500	-3.01051500
H	0.39012500	2.34921600	-4.04427200
C	-1.46468900	4.25840000	-3.32537000
H	-2.21613100	4.68080100	-2.65418500
H	-1.19149600	5.01729000	-4.06569300
H	-1.91233800	3.41137500	-3.85636300
C	0.38972400	5.05296200	-1.80978500
H	0.77564200	5.72971800	-2.57950100
H	-0.42683000	5.56942300	-1.29689500
C	1.63759600	3.82507300	2.90128300
H	0.74076400	4.40891200	3.12777600
H	2.41363900	4.12361700	3.61406200
C	0.63998200	2.19875000	4.55291000
H	0.40038900	1.15347900	4.77619700
H	1.31590400	2.56607300	5.33195300
H	-0.28424600	2.78023400	4.59072600
C	2.60113800	1.48039800	3.15467600
H	3.28632800	1.84335300	3.92785600
H	2.37921700	0.43012900	3.35710000
H	3.10630100	1.53680100	2.18936800
C	-3.84655500	-3.14913700	1.20653600
C	-3.49352700	-2.75914800	-0.09189800
C	-5.19650800	-3.39962100	1.48587100
C	-4.45381300	-2.57346500	-1.09458600
H	-2.44861400	-2.58713200	-0.32059100
C	-6.16352100	-3.24939000	0.49017700
H	-5.48765800	-3.72176600	2.48182400
C	-5.79742800	-2.83064000	-0.79003900
H	-7.20592400	-3.46027800	0.71254700
H	-6.55484300	-2.71056700	-1.55965400
C	2.07870600	4.11986600	1.48698000
C	1.12547900	4.47803500	0.52616300

C	3.41917100	4.01580900	1.09105500
C	1.47100200	4.71814300	-0.80947300
H	0.08637300	4.56823000	0.82551600
C	3.78387600	4.25953100	-0.23449800
H	4.17847800	3.76066100	1.82459700
C	2.81760500	4.60657700	-1.18098400
H	4.82751800	4.19120200	-0.52881300
H	3.11061600	4.80682100	-2.20757300
C	2.80754000	0.53833600	-0.78011000
H	2.13964000	1.35361900	-0.55510500
H	3.85999500	0.75764200	-0.91747600
C	2.32634700	-0.72917300	-0.91860900
C	0.92023500	-0.99296300	-0.85172200
C	0.49666100	-2.34809200	-1.27144500
O	0.35055100	-3.25999600	-0.47532100
O	0.25036700	-2.42735100	-2.58205100
C	-0.26126200	-3.69641400	-3.05090800
H	-0.46720400	-3.55119800	-4.11048900
H	0.48735700	-4.47990600	-2.91217100
H	-1.17551800	-3.95912200	-2.51514300
O	3.12993600	-1.80122500	-1.18611600
Si	4.51908400	-2.25475300	-0.29258900
C	4.19572300	-1.79171400	1.52182400
H	4.20390700	-0.69153400	1.52808900
C	4.68605600	-4.10465300	-0.65774700
H	5.64735300	-4.41354100	-0.22205800
C	6.01440800	-1.26783400	-0.94335000
H	6.04353100	-0.35275600	-0.33197700
C	5.88107100	-0.83936400	-2.41614600
H	4.95785000	-0.28580000	-2.61120900
H	6.72234900	-0.19731700	-2.70704300
H	5.88673400	-1.70459700	-3.08683200
C	7.34437800	-2.01463100	-0.72766200
H	7.39004300	-2.92163100	-1.34052900
H	8.19450400	-1.38364300	-1.01654300
H	7.49796000	-2.31322400	0.31415200
C	2.83333900	-2.23783400	2.07955200
H	2.68867100	-1.83410300	3.08952000
H	1.99419000	-1.89622400	1.46929100
H	2.76112200	-3.32639600	2.15247600
C	5.34108900	-2.26237400	2.43749900
H	6.30844000	-1.84550700	2.13983300
H	5.15711500	-1.95216500	3.47404600
H	5.43379600	-3.35485500	2.43807900

C	3.57801200	-4.95733500	-0.01631800
H	3.67750200	-6.00669900	-0.32376900
H	3.62373700	-4.93134500	1.07583300
H	2.58132400	-4.61690300	-0.31650900
C	4.75132500	-4.36393900	-2.17487700
H	5.59834200	-3.85871800	-2.64828300
H	4.85426800	-5.43784800	-2.37634400
H	3.83766100	-4.02151400	-2.67384800

17

Rh	-2.80794800	1.63054100	0.70736000
O	-3.61675700	-0.01477000	1.62575900
O	-1.83310200	2.08648600	2.47263900
O	-1.92594000	3.19118100	-0.28575000
O	-3.66348500	1.05311900	-1.06884300
Rh	-0.87207300	0.27460200	0.09615600
C	-3.01234400	0.31396800	-1.86646000
O	-1.83914400	-0.14728900	-1.65766100
C	-0.81603100	3.01547200	-0.87671400
O	-0.12687900	1.94009500	-0.84542700
C	-2.95275400	-1.09472700	1.61973600
O	-1.81048200	-1.25594300	1.07346100
O	-0.07085600	0.79683300	1.89767100
C	-0.70204000	1.55900000	2.70119700
C	-3.52137000	-2.32821900	2.32793100
C	-3.64546400	-0.06819400	-3.20870000
C	-0.25381100	4.20425100	-1.66498600
C	-0.01374300	1.87260000	4.03486000
C	-3.52703000	-3.52275100	1.32358600
H	-3.94856100	-4.38375000	1.85343600
H	-2.48813400	-3.75629100	1.07660900
C	-4.92778300	-2.05057400	2.86872200
H	-5.30977000	-2.94774000	3.36698800
H	-4.91201700	-1.23543900	3.59729400
H	-5.62218000	-1.77765100	2.07129000
C	-2.56909200	-2.67202800	3.49232400
H	-2.93609800	-3.55887500	4.01941000
H	-1.55978400	-2.87514900	3.12605600
H	-2.51840500	-1.84654300	4.21064000
C	-3.64127200	-1.62312600	-3.33888800
H	-4.10675400	-1.86556900	-4.30027400
H	-2.59978300	-1.95180900	-3.38237100
C	-2.76030300	0.52076600	-4.32631100
H	-3.18385000	0.26895700	-5.30418100

H	-2.70951100	1.61232200	-4.25003100
H	-1.74352800	0.12316400	-4.27367800
C	-5.06735700	0.49171800	-3.32217400
H	-5.06249100	1.58367000	-3.26741900
H	-5.49804200	0.19872900	-4.28529500
H	-5.71404800	0.11646300	-2.52652100
C	0.89826600	3.76869100	-2.57399700
H	1.26322400	4.63594500	-3.13507900
H	1.72504500	3.34401800	-2.00827100
H	0.56495600	3.01463000	-3.29252200
C	-1.37957100	4.82063700	-2.51419700
H	-2.22454100	5.12746800	-1.89402200
H	-0.99944800	5.69926400	-3.04572100
H	-1.74131900	4.10419100	-3.25981700
C	0.23437000	5.26990800	-0.62875300
H	0.78788400	6.03026900	-1.19006300
H	-0.64797100	5.75536000	-0.20145400
C	0.43005800	3.37099900	4.00712600
H	-0.46525200	3.99123400	4.10877400
H	1.04721200	3.53757600	4.89660300
C	-1.02518500	1.67483400	5.17762800
H	-1.34936200	0.63007700	5.23299400
H	-0.55957000	1.93684900	6.13333700
H	-1.90813000	2.30245700	5.03652500
C	1.19618900	0.95463200	4.25156100
H	1.66401400	1.19150300	5.21293600
H	0.88945500	-0.09396800	4.26733300
H	1.94198600	1.07157300	3.46410800
C	-4.29993700	-3.26612800	0.05061300
C	-3.66360600	-2.66319800	-1.04207300
C	-5.65915900	-3.58722900	-0.06257500
C	-4.35348100	-2.34545100	-2.21902400
H	-2.61094300	-2.42297600	-0.96652000
C	-6.35729100	-3.30008800	-1.23712100
H	-6.16740300	-4.07117100	0.76687100
C	-5.71199600	-2.67736800	-2.30712000
H	-7.40798100	-3.56430500	-1.31958700
H	-6.26160800	-2.45380700	-3.21738000
C	1.17388900	3.78648600	2.75940200
C	0.45947900	4.34494300	1.69351200
C	2.55689900	3.61025000	2.61439700
C	1.07865000	4.71659200	0.49437300
H	-0.61113100	4.49019300	1.79896500
C	3.19339600	3.98061800	1.42764700

H	3.13704400	3.19894500	3.43540600
C	2.46174800	4.52758100	0.37161400
H	4.26798300	3.85202500	1.32933400
H	2.96727500	4.82115800	-0.54362100
C	2.49351500	0.45244400	0.55785000
H	1.81537300	1.28385300	0.66073800
H	3.53188500	0.59762800	0.83084000
C	2.04885400	-0.74531500	0.08473600
C	0.68696400	-0.91704900	-0.31288900
C	0.33050100	-2.26777100	-0.81384300
O	0.11944800	-3.19070200	-0.04399400
O	0.19042400	-2.34609500	-2.13956700
C	-0.22953900	-3.62983300	-2.65235800
H	-0.31036700	-3.49718100	-3.73036400
H	0.51439200	-4.39500300	-2.41888300
H	-1.19478700	-3.91235200	-2.22817900
O	2.87618800	-1.82290000	-0.08397000
Si	3.91541600	-2.52610200	1.07583100
C	3.16200300	-2.23694600	2.79425200
H	3.18615200	-1.14263700	2.91076000
C	4.07375100	-4.32495300	0.50325200
H	4.93466800	-4.73732800	1.04898300
C	5.59778400	-1.63172200	0.98810600
H	5.52981700	-0.81844800	1.72723500
C	5.85569600	-0.99014400	-0.38441400
H	5.01120100	-0.37815200	-0.70295300
H	6.75166500	-0.35754000	-0.36536600
H	6.01223400	-1.74790700	-1.15913000
C	6.77809900	-2.53414300	1.39041600
H	6.92241500	-3.33965800	0.66175200
H	7.71249800	-1.95959200	1.42784900
H	6.63948000	-2.99905000	2.37189600
C	1.69881800	-2.67715000	2.96691100
H	1.31317400	-2.32978600	3.93379900
H	1.04482800	-2.28769800	2.18452900
H	1.60318400	-3.76678200	2.95360200
C	4.04899200	-2.83357300	3.90276800
H	5.06355800	-2.42279900	3.88921900
H	3.62342300	-2.62219800	4.89218700
H	4.12910400	-3.92346300	3.81179900
C	2.84634100	-5.19331800	0.82402000
H	2.97100700	-6.20188200	0.40750300
H	2.69454700	-5.30194700	1.90183600
H	1.93208800	-4.76653000	0.40017300

C	4.39766000	-4.38580000	-1.00185400
H	5.31775600	-3.84888700	-1.25271600
H	4.52404500	-5.42629700	-1.32735800
H	3.58670100	-3.94890300	-1.59521400
C	3.01770400	0.81241700	-2.73546900
C	3.77763500	-0.80627600	-4.26181800
C	1.87486200	0.22465400	-3.10635100
H	4.14503000	-0.63891300	-5.27626700
H	4.22158900	-1.72724600	-3.87339200
H	0.88794500	0.44994200	-2.73498700
C	2.21427400	-0.81851600	-4.16440900
H	1.85461900	-1.80992000	-3.87828900
H	1.76162600	-0.57697900	-5.13400100
O	3.38666600	1.77081400	-1.85298800
C	4.80119900	2.03158300	-2.05130100
H	4.92974300	3.03707800	-2.46571800
H	5.31942000	1.96018700	-1.09346600
C	5.28309400	0.96085100	-3.04371900
O	6.42903200	0.76233700	-3.42159100
N	4.14464800	0.31517400	-3.39477000

TS11

Rh	2.86701400	1.62317300	0.10645300
O	3.62713300	0.51576100	-1.43537700
O	2.02284000	2.86661700	-1.30695300
O	2.00691300	2.65441100	1.66162600
O	3.58326800	0.26733900	1.48096500
Rh	0.83391100	0.26333000	-0.02367800
C	2.88105800	-0.74017200	1.78933700
O	1.72484500	-1.00601700	1.31430400
C	0.86335700	2.29593200	2.08052700
O	0.15802100	1.35586200	1.58780300
C	2.90487100	-0.36814400	-1.98473600
O	1.72383600	-0.68864300	-1.62090300
O	0.12455600	1.64121200	-1.35121700
C	0.86146500	2.60176200	-1.74700600
C	3.47483400	-1.12354500	-3.19072800
C	3.42461500	-1.73994100	2.81538900
C	0.28797900	3.07792300	3.27050500
C	0.28372000	3.51995400	-2.83127200
C	3.53267100	-2.64404900	-2.84697800
H	4.00569500	-3.14668200	-3.69749500
H	2.50688100	-3.01000300	-2.78014200
C	4.86785000	-0.59650200	-3.55347100

H	5.25165000	-1.14939400	-4.41729700
H	4.82977800	0.46449700	-3.81560300
H	5.57196500	-0.71432200	-2.72747100
C	2.51152200	-0.92429100	-4.37733700
H	2.88528800	-1.46524600	-5.25305800
H	1.51159300	-1.29352200	-4.13733400
H	2.43325600	0.13601900	-4.64132600
C	3.45286600	-3.15717400	2.16147300
H	3.88268700	-3.84192600	2.90060400
H	2.41914600	-3.46862500	1.98613800
C	2.44957800	-1.76869400	4.00986800
H	2.80452000	-2.48336300	4.75974000
H	2.38513000	-0.78322900	4.48382100
H	1.44621400	-2.06458000	3.69327300
C	4.82090200	-1.32738900	3.29343200
H	4.79455100	-0.34612800	3.77502000
H	5.18710900	-2.05729500	4.02294300
H	5.53278600	-1.27822200	2.46709100
C	-1.01493700	2.44919500	3.77222700
H	-1.41529200	3.05152700	4.59466800
H	-1.76629900	2.38803300	2.98410200
H	-0.83339700	1.43725300	4.13473700
C	1.32903300	3.07367400	4.40570100
H	2.27461500	3.51188600	4.07794100
H	0.95220700	3.65211000	5.25587000
H	1.52297800	2.05202000	4.75040900
C	0.05173300	4.55210900	2.81358800
H	-0.44982100	5.06650700	3.64049700
H	1.02782100	5.02568000	2.67563200
C	0.01905800	4.91956500	-2.19048800
H	0.98624700	5.39549500	-2.00406800
H	-0.50527200	5.52222100	-2.93993300
C	1.32552000	3.67719300	-3.95375600
H	1.53814600	2.71132000	-4.42462600
H	0.93878700	4.35247800	-4.72413800
H	2.26265100	4.08693900	-3.56967200
C	-1.00857000	2.92975100	-3.40685400
H	-1.40758300	3.60294600	-4.17317600
H	-0.81567200	1.95858700	-3.86867000
H	-1.76844500	2.78522500	-2.63796800
C	4.26568500	-2.97924200	-1.56938000
C	3.57699300	-2.97561700	-0.34899000
C	5.63553600	-3.27344700	-1.56473400
C	4.22605700	-3.23428000	0.86517300

H	2.51598700	-2.75355500	-0.34121900
C	6.29402700	-3.55107300	-0.36534700
H	6.18303200	-3.29597100	-2.50294600
C	5.59592400	-3.52928100	0.84338900
H	7.35361000	-3.79136200	-0.37334000
H	6.11264200	-3.75089100	1.77310100
C	-0.76580400	4.87433600	-0.90140100
C	-0.07987100	4.78921400	0.31586700
C	-2.16673500	4.87479500	-0.87999600
C	-0.74904400	4.69246600	1.54090000
H	1.00523900	4.78844800	0.30892900
C	-2.85242500	4.78878100	0.33357300
H	-2.71939500	4.95655000	-1.81153300
C	-2.15082600	4.69747100	1.53741800
H	-3.93894700	4.80523600	0.34185800
H	-2.69187100	4.64621200	2.47791000
C	-2.52322500	0.84882900	0.23117200
H	-1.73413000	1.52424900	0.52047400
H	-3.54738800	1.20158400	0.27889300
C	-2.22830600	-0.40620500	-0.19109500
C	-0.85863900	-0.86854900	-0.27812100
C	-0.64843100	-2.01311200	-1.20956400
O	-1.00316500	-1.93725800	-2.37599100
O	0.04223800	-3.05060900	-0.71853000
C	0.23173800	-4.16300800	-1.61306100
H	0.96597300	-4.80646100	-1.12980500
H	-0.71160300	-4.70049000	-1.74433200
H	0.59312600	-3.82630800	-2.58418100
O	-3.19315400	-1.31180000	-0.54078900
Si	-4.64895500	-1.06693800	-1.39856500
C	-4.41856100	0.29451500	-2.70507300
H	-4.19134600	1.19500300	-2.11478400
C	-5.05187600	-2.79452700	-2.06687800
H	-6.09165000	-2.74052100	-2.41934300
C	-6.00538400	-0.46969400	-0.19276700
H	-6.02065200	0.62499600	-0.30752600
C	-5.69723800	-0.77576400	1.27957000
H	-4.72987700	-0.36858200	1.58121600
H	-6.46223300	-0.34669200	1.93922800
H	-5.67593100	-1.85313400	1.47037300
C	-7.40432800	-0.99498400	-0.56486300
H	-7.46834500	-2.07934600	-0.42233300
H	-8.17203700	-0.53801200	0.07275500
H	-7.67333400	-0.78373700	-1.60464100

C	-3.26158200	0.09646500	-3.69590400
H	-3.12207400	1.00262300	-4.29832600
H	-2.32084100	-0.13431800	-3.19387500
H	-3.46960900	-0.72312400	-4.39037200
C	-5.73898800	0.55628400	-3.45388800
H	-6.55221300	0.84431900	-2.78047700
H	-5.61444800	1.36872300	-4.18142300
H	-6.06539300	-0.32922000	-4.01279700
C	-4.17265700	-3.23628300	-3.24858600
H	-4.38620900	-4.27984200	-3.51669600
H	-4.35341200	-2.62786500	-4.13886900
H	-3.10714500	-3.16257600	-3.00843100
C	-4.99204400	-3.83996800	-0.93849900
H	-5.61955100	-3.56960200	-0.08326900
H	-5.32774100	-4.82089900	-1.29884400
H	-3.96557400	-3.95583000	-0.57597500
C	-1.87498500	-1.73557800	2.63009200
C	-3.05989100	-3.74375900	2.34826400
C	-1.03865600	-2.43787200	1.82817200
H	-3.07594400	-4.47925700	3.15692300
H	-3.94157300	-3.88515100	1.72300300
H	0.00143700	-2.21137600	1.65947300
C	-1.72659200	-3.76866600	1.53264400
H	-1.94155400	-3.88193400	0.46781300
H	-1.10353900	-4.61974100	1.82547800
O	-1.84665900	-0.53455900	3.21511400
C	-3.05196800	-0.40002700	4.01851100
H	-2.77132800	-0.27934500	5.06838000
H	-3.61386600	0.47327300	3.68210600
C	-3.83237200	-1.70109700	3.79794400
O	-4.89110000	-2.03506800	4.30099100
N	-3.05728600	-2.39391700	2.91426000

18

Rh	3.10805000	0.29067600	0.69627000
O	2.41609300	1.74913100	1.97107100
O	2.69850900	-1.06813900	2.16480700
O	3.61935000	-1.20341100	-0.64614600
O	3.44039400	1.67778600	-0.76259800
Rh	0.80465200	0.06923200	-0.11609400
C	2.49685700	1.97650500	-1.55644200
O	1.32101800	1.48912200	-1.52681900
C	2.71988700	-1.71718900	-1.38227300
O	1.49409800	-1.37620500	-1.40149800

C	1.17334600	2.01306200	2.00313200
O	0.28225200	1.49536000	1.25642100
O	0.59614700	-1.35884700	1.39089700
C	1.53671600	-1.58080900	2.21546600
C	0.67532600	3.04692800	3.02202800
C	2.78731100	3.00747100	-2.65516500
C	3.14864800	-2.83763400	-2.34083500
C	1.28443600	-2.54701800	3.38217700
C	0.05443900	4.24574100	2.23701100
H	-0.23622000	5.00011000	2.97671200
H	-0.85589900	3.88960500	1.75033900
C	1.81699800	3.51697400	3.92977600
H	1.43810000	4.25618400	4.64386700
H	2.23561600	2.67934500	4.49514100
H	2.62694700	3.97297300	3.35731000
C	-0.43284900	2.39163700	3.86861900
H	-0.83791600	3.11809200	4.58149900
H	-1.24612400	2.03075500	3.23509600
H	-0.03676700	1.54285700	4.43761000
C	1.82412300	4.21996300	-2.46760800
H	2.09607400	4.96810600	-3.22054100
H	0.81211200	3.87925500	-2.69136800
C	2.49592800	2.34736600	-4.01658500
H	2.63989700	3.07300300	-4.82436700
H	3.17646700	1.50655900	-4.19114900
H	1.47142000	1.97320100	-4.05736000
C	4.24959600	3.46510200	-2.60480200
H	4.92857500	2.62101000	-2.75454700
H	4.43051000	4.19550800	-3.40087500
H	4.49657400	3.92912900	-1.64797500
C	1.94457500	-3.39413500	-3.11044600
H	2.27727600	-4.19231900	-3.78268300
H	1.19098300	-3.80402900	-2.43490900
H	1.47272300	-2.61420200	-3.71432300
C	4.16891800	-2.24433000	-3.33243700
H	5.03729800	-1.83889800	-2.80672000
H	4.51182000	-3.02039000	-4.02485500
H	3.71501100	-1.43964000	-3.92104900
C	3.84764300	-3.96668200	-1.52399600
H	4.12614700	-4.75211200	-2.23500800
H	4.77262000	-3.55739700	-1.10821800
C	2.28793600	-3.73636600	3.25722900
H	3.29383600	-3.34682400	3.43719600
H	2.05860600	-4.44114700	4.06378900

C	1.57023500	-1.79257600	4.69517400
H	0.88900000	-0.94211100	4.80925600
H	1.42297400	-2.46237200	5.54907200
H	2.59565100	-1.41646300	4.71854800
C	-0.15762100	-3.05812200	3.39356300
H	-0.30139400	-3.73111600	4.24537100
H	-0.86929600	-2.23376700	3.48421100
H	-0.38789800	-3.60766300	2.48210500
C	0.96836200	4.85178400	1.19915400
C	0.96105000	4.34687800	-0.10768000
C	1.85560600	5.88977400	1.51386200
C	1.83600500	4.83384500	-1.08777500
H	0.26202000	3.55757400	-0.36631600
C	2.72065300	6.39819800	0.54323100
H	1.85991400	6.30651900	2.51734700
C	2.71615800	5.87044000	-0.74933800
H	3.39552000	7.21253500	0.79278200
H	3.38782000	6.27294800	-1.50271000
C	2.26052400	-4.44593200	1.92262600
C	3.03580000	-3.96059000	0.86153200
C	1.46595400	-5.57901300	1.70429900
C	3.01650300	-4.55448900	-0.40598600
H	3.66617700	-3.09432000	1.02470000
C	1.45189100	-6.20033700	0.45282200
H	0.87489200	-5.98621400	2.52016400
C	2.21384100	-5.68738700	-0.59934400
H	0.85354300	-7.09488000	0.30053000
H	2.20324200	-6.17940700	-1.56814200
C	-2.32449400	-0.61218300	1.30438800
H	-1.35668900	-0.88452600	1.69130200
H	-3.19115900	-0.72449600	1.94715400
C	-2.43844800	-0.13296200	0.05738100
C	-1.32167800	-0.05256600	-0.96252900
C	-1.40656600	1.22076800	-1.71620700
O	-1.70883700	2.31054300	-1.24867100
O	-1.11807100	1.08061600	-3.04300600
C	-1.33610000	2.23774100	-3.85599000
H	-0.97340400	1.97782500	-4.85132800
H	-2.40400400	2.47521500	-3.90300200
H	-0.79856000	3.10512500	-3.47382100
O	-3.66108000	0.22461700	-0.47156900
Si	-5.06068000	0.76990500	0.32893500
C	-4.60480100	2.01734000	1.68875100
H	-4.09661100	1.40525200	2.44737800

C	-6.08213400	1.46963300	-1.10567600
H	-7.07275000	1.71144300	-0.69518600
C	-5.96664100	-0.68566100	1.18118600
H	-5.63599900	-0.64106400	2.22996100
C	-5.58586600	-2.07279200	0.64034300
H	-4.50390400	-2.22843300	0.64811000
H	-6.04185100	-2.86751100	1.24523400
H	-5.94117200	-2.21121300	-0.38622200
C	-7.49705200	-0.51219100	1.17195400
H	-7.89608500	-0.57567900	0.15374900
H	-7.98165800	-1.30146700	1.76127000
H	-7.81445300	0.44878200	1.58867700
C	-3.62736700	3.12804800	1.27456000
H	-3.27688300	3.67154600	2.16176700
H	-2.76031500	2.74017000	0.73650200
H	-4.11162400	3.86177200	0.62126000
C	-5.86432500	2.61097000	2.34764400
H	-6.51187500	1.84249800	2.78227100
H	-5.58706900	3.29895700	3.15693100
H	-6.46308900	3.18446300	1.62943300
C	-5.48162700	2.75644400	-1.69778000
H	-6.03612100	3.06703300	-2.59350800
H	-5.51662100	3.58648000	-0.98668200
H	-4.43405200	2.61434000	-1.98504100
C	-6.27461400	0.41336600	-2.20970000
H	-6.72480100	-0.51061000	-1.83224800
H	-6.92654000	0.79636100	-3.00559400
H	-5.31539200	0.15265000	-2.66919400
C	-1.59016800	-2.53432400	-1.21786000
C	-3.59628800	-2.39042800	-2.42816800
C	-1.39468300	-1.26375500	-1.94909800
H	-3.95497200	-3.08088200	-3.19200400
H	-4.43816200	-1.95787400	-1.89149600
H	-0.44489700	-1.31699500	-2.48272300
C	-2.60952200	-1.32350900	-2.95288200
H	-3.10029000	-0.35864400	-3.03313400
H	-2.24149300	-1.60877800	-3.94047400
O	-0.83713700	-3.18144800	-0.38509900
C	-1.57588300	-4.37250200	0.04686900
H	-0.97491200	-5.24906700	-0.19598100
H	-1.73661900	-4.29872000	1.12305800
C	-2.88744400	-4.30884200	-0.72108200
O	-3.82943700	-5.05787300	-0.71735000
N	-2.75527100	-3.12120800	-1.46786500

TS12

Rh	2.32614100	2.02630100	0.66042200
O	0.94682700	2.90929400	1.87576100
O	2.70710200	0.69777400	2.17386200
O	3.62123700	1.04468100	-0.61203500
O	1.80921700	3.32549200	-0.83678500
Rh	0.56309400	0.52114400	-0.11303500
C	0.86243000	3.00802000	-1.62077500
O	0.20978800	1.91645900	-1.58487500
C	3.18785900	0.06520000	-1.29783700
O	1.98450300	-0.34271900	-1.31789300
C	-0.23538500	2.44721000	1.92512700
O	-0.68408900	1.47639200	1.23093000
O	1.10069400	-0.71692800	1.45327200
C	2.02089900	-0.36937700	2.25788000
C	-1.20575400	3.10264300	2.91597600
C	0.46704900	4.00004100	-2.72175500
C	4.19866800	-0.67293400	-2.18738700
C	2.33865200	-1.28870700	3.44531600
C	-2.50187900	3.50163200	2.14614400
H	-3.19063500	3.94539400	2.87331400
H	-2.96466000	2.59080700	1.76054900
C	-0.56797000	4.32754000	3.58400400
H	-1.28629600	4.77809400	4.27756400
H	0.32119000	4.04171400	4.15188500
H	-0.27391700	5.08367200	2.85408400
C	-1.53734600	2.05708900	3.99920400
H	-2.28727700	2.45738800	4.69012800
H	-1.92344400	1.13787100	3.55958900
H	-0.64046100	1.81199100	4.57871900
C	-1.06333900	4.28140600	-2.61769600
H	-1.32036100	4.96588300	-3.43372700
H	-1.58617300	3.33968700	-2.79134400
C	0.75424500	3.32238500	-4.07735200
H	0.44994400	3.98187000	-4.89713400
H	1.82463500	3.11603900	-4.18750700
H	0.21154700	2.37908500	-4.16538400
C	1.27382200	5.29846800	-2.61241900
H	2.34496400	5.10292900	-2.71206600
H	0.97493700	5.98246200	-3.41411300
H	1.10987500	5.79846600	-1.65563300
C	3.55841200	-1.90099900	-2.84626500
H	4.30582800	-2.42116600	-3.45475500

H	3.17016700	-2.59834800	-2.10155300
H	2.73253900	-1.60710100	-3.49974500
C	4.66681600	0.31630300	-3.27398900
H	5.13679000	1.19720500	-2.82831800
H	5.39378800	-0.17013300	-3.93285900
H	3.82145100	0.64870500	-3.88637600
C	5.43177600	-1.08890000	-1.32964900
H	6.14109600	-1.57954400	-2.00469100
H	5.90836800	-0.17597200	-0.96186900
C	3.86234600	-1.62146000	3.43005300
H	4.41096400	-0.69237400	3.60885900
H	4.05602400	-2.28569100	4.27912200
C	2.01365500	-0.50847400	4.73510600
H	0.95049500	-0.24726100	4.77157500
H	2.24260500	-1.12517100	5.61066300
H	2.59766100	0.41335000	4.79540300
C	1.50571400	-2.57239100	3.39928900
H	1.75962500	-3.20406900	4.25697200
H	0.43649200	-2.34983000	3.44214400
H	1.69894600	-3.13664800	2.48722700
C	-2.24750400	4.46676900	1.00985600
C	-1.86857900	3.98333000	-0.25013500
C	-2.32264800	5.85316600	1.20114200
C	-1.52303400	4.85035600	-1.29569500
H	-1.83904800	2.91303400	-0.42241700
C	-2.00752400	6.72953600	0.16127300
H	-2.63201800	6.24537800	2.16622500
C	-1.60020200	6.23260900	-1.07800000
H	-2.07942300	7.80255500	0.31740000
H	-1.35301400	6.91863400	-1.88378100
C	4.36157200	-2.25959600	2.15290800
C	4.69298300	-1.45615700	1.05383700
C	4.50414900	-3.64785100	2.03025100
C	5.12317600	-1.99948800	-0.16232400
H	4.60967900	-0.38051000	1.14676300
C	4.96135400	-4.20750900	0.83443800
H	4.27390200	-4.28877600	2.87718900
C	5.25656700	-3.39156500	-0.26011700
H	5.08973000	-5.28383800	0.75615400
H	5.61038300	-3.83370000	-1.18758900
C	-1.27820500	-2.48414600	0.78257900
H	-0.33784800	-2.19650200	1.22732100
H	-1.87179300	-3.23271000	1.29795200
C	-1.88288100	-1.60494700	-0.09588800

C	-1.04436000	-0.87075400	-1.07470800
C	-1.79461900	0.08283000	-1.92038500
O	-2.66101400	0.86410600	-1.55605000
O	-1.41383000	0.00872100	-3.22904600
C	-2.18773500	0.78057800	-4.15361600
H	-1.78554600	0.54932400	-5.14117000
H	-3.24341800	0.49759800	-4.10462500
H	-2.09765600	1.84945400	-3.95854800
O	-3.19288300	-1.59638800	-0.32703100
Si	-4.58919700	-2.16011700	0.49977300
C	-4.58622500	-1.40671000	2.23683800
H	-3.89333700	-2.03035100	2.82097700
C	-5.96129500	-1.52581800	-0.64024100
H	-6.90475000	-1.92076500	-0.23657400
C	-4.56755800	-4.06124200	0.60910100
H	-4.07857500	-4.29133300	1.56728700
C	-3.75509200	-4.74609900	-0.50218700
H	-2.71321200	-4.42199500	-0.49714200
H	-3.76394900	-5.83580500	-0.37082700
H	-4.16753200	-4.53456700	-1.49389700
C	-5.99691700	-4.63372600	0.66540800
H	-6.52812400	-4.46622800	-0.27790500
H	-5.97123400	-5.71703300	0.83763200
H	-6.59771000	-4.18931700	1.46560300
C	-4.05269500	0.03274000	2.27108100
H	-4.03280000	0.40368500	3.30267900
H	-3.03931200	0.10439200	1.86827100
H	-4.68259800	0.71554800	1.69409900
C	-5.97406900	-1.50217700	2.89729900
H	-6.33101900	-2.53486800	2.97125400
H	-5.94497200	-1.09319600	3.91517700
H	-6.72333300	-0.92954600	2.33882600
C	-6.04985100	0.01063500	-0.66293300
H	-6.81281000	0.33895400	-1.38119100
H	-6.32441400	0.41866700	0.31389000
H	-5.09494200	0.45629900	-0.96096400
C	-5.79173200	-2.06839300	-2.07128800
H	-5.80982900	-3.16175700	-2.10865500
H	-6.59831100	-1.70268500	-2.71952500
H	-4.84372400	-1.73224700	-2.50549200
C	0.13782000	-3.09246900	-0.94303300
C	-0.95427400	-4.28820600	-2.68404300
C	-0.33904200	-1.99026400	-1.86312400
H	-0.31281400	-4.64896700	-3.49253400

H	-1.82905700	-4.93454900	-2.60951500
H	0.53830100	-1.63025600	-2.40426100
C	-1.30020100	-2.79117700	-2.81815500
H	-2.33477700	-2.62533600	-2.51318700
H	-1.19536100	-2.45152700	-3.84610700
O	1.26507300	-3.13929700	-0.23754700
C	1.56788900	-4.53441500	0.02337400
H	2.63147100	-4.69328600	-0.14825300
H	1.31284300	-4.77360100	1.06066600
C	0.68463300	-5.29886100	-0.95011600
O	0.70956000	-6.46943900	-1.26030200
N	-0.17378400	-4.32430900	-1.44249500

19

Rh	1.71356100	-2.28427900	1.01857100
O	2.84290300	-0.92283000	2.02751600
O	0.28737800	-2.18914200	2.48961200
O	0.57050600	-3.59128000	-0.05826300
O	3.07336800	-2.29412600	-0.50576000
Rh	0.58948300	-0.48172900	-0.06359700
C	2.92119200	-1.47546000	-1.46855800
O	2.00539600	-0.59347200	-1.53516100
C	-0.30159800	-3.13031200	-0.86557600
O	-0.50004500	-1.89357700	-1.07784200
C	2.65320200	0.31908900	1.82145800
O	1.77224000	0.79930100	1.03444800
O	-0.78600200	-0.49927900	1.45042900
C	-0.66731900	-1.34945000	2.38890500
C	3.53864500	1.31121600	2.58481100
C	3.89035900	-1.55218200	-2.65129100
C	-1.13369800	-4.15407300	-1.64475800
C	-1.71938100	-1.35673900	3.50410100
C	4.24056300	2.25852700	1.56286400
H	4.85183900	2.95618300	2.14549100
H	3.46830300	2.84246000	1.05638300
C	4.57029200	0.57369900	3.44614800
H	5.19257200	1.30612700	3.97083700
H	4.07742300	-0.05377300	4.19362200
H	5.22184200	-0.06330900	2.84502000
C	2.62228000	2.16119100	3.48488200
H	3.22490800	2.87400400	4.05732400
H	1.90198500	2.71698300	2.88565700
H	2.07373500	1.53201700	4.19399900
C	4.56619000	-0.15872600	-2.83913000

H	5.28506600	-0.25944000	-3.65912200
H	3.79825400	0.54799900	-3.16073100
C	3.05730900	-1.87107200	-3.91000100
H	3.71306300	-1.91229200	-4.78591800
H	2.56068700	-2.84246400	-3.81116800
H	2.29199700	-1.10940900	-4.07822500
C	4.94327000	-2.64377600	-2.42984800
H	4.47332800	-3.62511600	-2.32268900
H	5.61654100	-2.67835400	-3.29259900
H	5.54000000	-2.45452700	-1.53511500
C	-2.25569600	-3.47113100	-2.43563600
H	-2.85161200	-4.23356300	-2.94802800
H	-2.91407800	-2.89192900	-1.78517600
H	-1.84451600	-2.79847900	-3.19263500
C	-0.17181200	-4.87166400	-2.61545400
H	0.63130700	-5.37906200	-2.07392600
H	-0.72357300	-5.61681000	-3.19790000
H	0.27722500	-4.15835700	-3.31480800
C	-1.71890000	-5.20472900	-0.65261000
H	-2.26822100	-5.93686100	-1.25354600
H	-0.88301700	-5.72942800	-0.18150900
C	-2.20342800	-2.81708400	3.75332500
H	-1.34319900	-3.41153800	4.07344200
H	-2.90712100	-2.77876200	4.59153200
C	-1.02548800	-0.83868200	4.78205100
H	-0.63477500	0.17283700	4.62990300
H	-1.74656000	-0.80441000	5.60531900
H	-0.19643500	-1.48937700	5.07403900
C	-2.90416300	-0.45079800	3.14944300
H	-3.66246800	-0.52236800	3.93620000
H	-2.58885200	0.59151400	3.07774700
H	-3.35444800	-0.73723300	2.19800100
C	5.09318700	1.55187600	0.53641200
C	4.51644000	1.09900400	-0.65635700
C	6.45412800	1.30171600	0.75906200
C	5.25196400	0.37550000	-1.60440500
H	3.46810100	1.30140900	-0.84515400
C	7.20794400	0.60448600	-0.18624600
H	6.92399500	1.66180200	1.67003800
C	6.61031600	0.13696700	-1.35813000
H	8.26538500	0.42711200	-0.01060600
H	7.20108500	-0.40625200	-2.09057300
C	-2.85937400	-3.47031000	2.55827000
C	-2.06943700	-4.07673600	1.57448700

C	-4.24990500	-3.46595200	2.38803400
C	-2.62319600	-4.62857700	0.41306300
H	-0.99616100	-4.11057900	1.71148400
C	-4.82302000	-4.04432100	1.25365100
H	-4.88339200	-3.01782000	3.14868200
C	-4.01596300	-4.61003800	0.26438900
H	-5.90341100	-4.05272900	1.13912200
H	-4.46821400	-5.04883400	-0.62080900
O	-3.78149300	-0.78142700	-0.35098400
C	-3.44104500	0.41146700	-1.05829900
C	-5.19815100	-0.81387000	-0.18684600
N	-4.68345400	0.82882400	-1.71528100
C	-2.41867900	0.20204300	-2.21380800
C	-5.73618700	0.05460700	-1.31839000
H	-5.50424000	-0.42158600	0.79395100
H	-5.55386400	-1.84055300	-0.28422900
C	-4.45039000	1.24665800	-3.09810100
C	-1.63435400	1.99211200	-0.85197100
C	-3.24659200	0.38526800	-3.51210400
H	-1.99656500	-0.79675800	-2.15130400
O	-6.86523200	0.04709500	-1.78952700
H	-5.35609300	1.06328300	-3.67959200
H	-4.22202200	2.31556200	-3.13581800
H	-3.60434300	-0.59274800	-3.85045500
H	-2.65852200	0.82976500	-4.31535100
O	-0.93783300	3.02833900	-0.39757200
Si	-1.46494400	4.42725200	0.45295400
C	-1.97337100	3.92000600	2.21213500
H	-2.94743600	3.42573900	2.08434500
C	-2.97213500	5.16269700	-0.45093100
C	0.06595300	5.53156000	0.33416500
H	-0.19001600	6.47947300	0.82870500
C	1.28169200	4.92402200	1.05453900
H	1.50535400	3.92339200	0.67128300
H	2.17358000	5.54470000	0.89756800
H	1.12506200	4.84200200	2.13331400
C	0.41594100	5.83197000	-1.13577500
H	-0.38158700	6.37742100	-1.64846500
H	1.32471400	6.44462400	-1.19532900
H	0.59879100	4.90594200	-1.69067900
C	-1.02552500	2.91564300	2.88589400
H	-1.46397500	2.54859000	3.82246400
H	-0.80852700	2.04889700	2.25626500
H	-0.07426800	3.38714500	3.14269800

C	-2.19253400	5.14736900	3.11567900
H	-2.50552600	4.83515300	4.12014900
H	-1.27118300	5.73038200	3.22998300
H	-2.96576900	5.81788800	2.72813200
C	-3.09135300	6.68202600	-0.22197800
H	-2.25843500	7.21975700	-0.68725100
H	-4.01683000	7.06560300	-0.66950800
H	-3.10590700	6.95146200	0.83860600
H	-3.84931500	4.68782800	0.01281900
C	-3.01334400	4.84533000	-1.95548200
H	-2.17157300	5.30023900	-2.48729200
H	-2.97984200	3.77168200	-2.15297100
H	-3.93520000	5.23580300	-2.40493600
C	-2.85427100	1.49162000	-0.12728700
H	-3.57776700	2.28646500	0.07631000
H	-2.55017500	1.04262000	0.82140700
C	-1.35713400	1.25280300	-1.96720200
C	-0.26273300	1.41781600	-2.92314100
O	-0.15643000	0.75485400	-3.94923200
O	0.62506500	2.38221000	-2.58858700
C	1.69319300	2.59607500	-3.52306100
H	2.42347000	3.21673000	-3.00364100
H	2.14040600	1.64935500	-3.82651500
H	1.32356800	3.11841600	-4.41142300

TS13

Rh	-2.67379900	1.51439500	-0.72440500
O	-3.68148600	0.57404200	0.79683500
O	-2.11649700	2.97564500	0.59790600
O	-1.53989900	2.32993200	-2.23539800
O	-3.16930500	-0.02037100	-1.98237100
Rh	-0.67387900	0.28338800	-0.04359800
C	-2.37555500	-1.00557900	-2.06194300
O	-1.28886100	-1.13374900	-1.40545300
C	-0.30636000	2.04181400	-2.32654100
O	0.32417000	1.25014300	-1.55146000
C	-3.06504100	-0.24595000	1.54032800
O	-1.82641700	-0.54623500	1.44172700
O	-0.23927600	1.86989100	1.19689300
C	-1.04113400	2.86024700	1.26197200
C	-3.84410600	-0.93209300	2.66944000
C	-2.71697100	-2.14348800	-3.03190600
C	0.47850600	2.69370300	-3.47323200
C	-0.70606700	4.00757000	2.22440200

C	-3.62279600	-2.47253300	2.57702800
H	-4.16901100	-2.92656600	3.41077800
H	-2.55888700	-2.67161200	2.73136100
C	-5.33602000	-0.58761800	2.59078600
H	-5.86830000	-1.09461800	3.40245200
H	-5.49485300	0.48859900	2.69702600
H	-5.77547700	-0.90239300	1.64213800
C	-3.26840800	-0.42525300	4.00718200
H	-3.80642300	-0.88920500	4.84042200
H	-2.20855600	-0.67010100	4.09949600
H	-3.38124700	0.66094400	4.09249500
C	-2.66296800	-3.49707400	-2.26118000
H	-2.89121200	-4.28808600	-2.98361600
H	-1.63513100	-3.64247900	-1.92106300
C	-1.63327000	-2.16143600	-4.12868200
H	-1.85338600	-2.95394600	-4.85165900
H	-1.60595000	-1.20830700	-4.66787500
H	-0.64593200	-2.34428200	-3.70050200
C	-4.09483300	-1.92469500	-3.66669000
H	-4.11853100	-0.99357500	-4.23901000
H	-4.31590900	-2.75191000	-4.34940600
H	-4.88462300	-1.87927300	-2.91398100
C	1.96003000	2.30517800	-3.42859000
H	2.49010600	2.80056200	-4.24889600
H	2.42938500	2.59956500	-2.48795600
H	2.08132100	1.22756100	-3.54467500
C	-0.14310700	2.20413000	-4.79689700
H	-1.20171800	2.46924900	-4.85822900
H	0.38124900	2.66121200	-5.64255800
H	-0.05230500	1.11643200	-4.88954300
C	0.31006400	4.24126900	-3.37979100
H	0.87818400	4.67683600	-4.20866800
H	-0.74474800	4.47977000	-3.54168200
C	-0.69979800	5.34655600	1.42494800
H	-1.71225700	5.52745100	1.05373600
H	-0.46127400	6.14335300	2.13747600
C	-1.82826900	4.06393900	3.28125200
H	-1.86992700	3.13103700	3.85387200
H	-1.63494200	4.88337100	3.98134400
H	-2.80290400	4.22708200	2.81413700
C	0.64009100	3.78247900	2.91589400
H	0.84285000	4.61466000	3.59854600
H	0.63009200	2.85444800	3.48748800
H	1.45507700	3.72803400	2.19212200

C	-4.07052600	-3.08751900	1.27059900
C	-3.21312300	-3.07987400	0.16351000
C	-5.34781400	-3.64363100	1.12052400
C	-3.60473900	-3.58453900	-1.08290800
H	-2.22138000	-2.66176600	0.26965400
C	-5.74987500	-4.16766100	-0.10961600
H	-6.02483700	-3.67159400	1.97001800
C	-4.88719000	-4.13476100	-1.20694100
H	-6.73897600	-4.60535500	-0.21298900
H	-5.20624900	-4.54370300	-2.16174200
C	0.27525300	5.37048800	0.27128600
C	-0.12018700	4.89611100	-0.98526500
C	1.59256200	5.82197100	0.43046400
C	0.76701300	4.83304000	-2.06689500
H	-1.14032100	4.55643500	-1.12118400
C	2.48509700	5.78794200	-0.64265800
H	1.91427200	6.21082200	1.39261700
C	2.07854900	5.29107500	-1.88258400
H	3.49969700	6.15490300	-0.51376200
H	2.77745500	5.26849700	-2.71421700
C	2.67942200	0.84953700	0.43203600
H	1.91896200	1.61604200	0.46517800
H	3.72200000	1.14246800	0.40004500
C	2.31733300	-0.46980200	0.32889000
C	0.95561100	-0.84478900	0.40648000
C	0.68807700	-2.24472400	0.81190100
O	0.62238800	-2.54071400	1.99533000
O	0.47401500	-3.11275400	-0.18194400
C	0.13553300	-4.45954900	0.22338600
H	-0.01499400	-5.01107400	-0.70307800
H	0.95019100	-4.90199600	0.79911100
H	-0.78022200	-4.45808700	0.81607900
O	3.28276800	-1.45231700	0.27787200
Si	4.16209400	-1.98124500	-1.09825000
C	5.95124200	-1.33879800	-0.95387200
H	5.90789800	-0.28440700	-1.26798400
C	4.17080300	-3.88138200	-0.97773200
H	5.16730300	-4.18395800	-1.32660600
C	3.33977000	-1.15436300	-2.60013600
H	3.26039100	-0.11031200	-2.26092300
C	1.91698200	-1.62873700	-2.93586300
H	1.25518900	-1.66662800	-2.06986000
H	1.45797200	-0.94947500	-3.66427400
H	1.93058100	-2.62564600	-3.38542400

C	4.20592900	-1.14379700	-3.87130000
H	4.41219700	-2.15811600	-4.23288100
H	3.68359700	-0.61466400	-4.67899300
H	5.16377100	-0.63924100	-3.71822200
C	6.50771800	-1.38471600	0.47632600
H	7.52186200	-0.96614700	0.51611100
H	5.88770400	-0.81927700	1.17126800
H	6.56836200	-2.41450500	0.84674800
C	6.92019900	-2.07770000	-1.89840600
H	6.55900600	-2.14599800	-2.92792600
H	7.89250800	-1.56961300	-1.92457100
H	7.10157700	-3.09917800	-1.54600100
C	4.04033100	-4.33742200	0.48846400
H	4.07560400	-5.43258200	0.55425600
H	4.84714900	-3.94410300	1.11565200
H	3.09808200	-4.00308300	0.93066200
C	3.14435200	-4.59361900	-1.87287100
H	3.32654200	-4.39500400	-2.93377900
H	3.19703900	-5.68079800	-1.72738500
H	2.12372200	-4.27802000	-1.64785700
C	2.39578600	0.52896500	3.60625500
C	4.31165600	-0.81407100	3.45287200
C	3.30913500	1.37886800	3.09227500
H	4.93443500	-1.26107200	4.22881800
H	4.35144000	-1.42972300	2.55074800
H	3.15915700	2.42264100	2.86965100
C	4.66002400	0.67892200	3.15570400
H	5.23132100	0.77337700	2.22846600
H	5.28359100	1.09655600	3.95692500
O	1.09098400	0.57961300	3.91672900
C	0.71050700	-0.72005500	4.45497200
H	0.33665000	-0.58583400	5.47347300
H	-0.05042700	-1.15847000	3.80977000
C	1.98685200	-1.56618000	4.42150300
O	2.13479000	-2.71480100	4.80100400
N	2.91785900	-0.72255800	3.89057300

TS14

Rh	1.76527500	0.07729600	-2.57748900
O	1.08706400	2.01356500	-2.58782300
O	3.35990000	0.69171600	-1.42909500
O	2.39095300	-1.87111500	-2.41880400
O	0.02857000	-0.51257900	-3.53774500
Rh	0.51583900	-0.26025500	-0.45729500

C	-1.01434700	-0.60390500	-2.84373300
O	-1.15509700	-0.49336100	-1.59330900
C	1.88359800	-2.55831600	-1.49813400
O	1.00250000	-2.23949900	-0.65295100
C	0.47364500	2.41038500	-1.56950800
O	0.17438500	1.77881400	-0.51638400
O	2.30282600	0.05752100	0.48592400
C	3.23468100	0.57976300	-0.18089800
C	-3.49738000	-1.35051400	-2.77825000
C	4.27461800	2.80171300	0.46522400
C	-2.32085800	-0.82012400	-3.63356200
F	-2.68518500	0.38051400	-4.16296200
F	-2.09729300	-1.68628700	-4.65079800
F	-3.08165500	-2.42826000	-2.07174600
F	-3.89328200	-0.37302700	-1.92887100
C	-4.74279100	-1.78960800	-3.58700200
F	-5.74144600	-2.06663800	-2.73467200
F	-5.13810900	-0.81021000	-4.40997500
F	-4.47792200	-2.88625500	-4.30357000
C	2.45750400	-3.97624000	-1.31331700
F	1.48079300	-4.82416900	-0.89757200
F	2.96414500	-4.43938300	-2.47639700
C	3.59449100	-3.96373400	-0.25631600
C	4.04836800	-5.36081200	0.23022300
F	3.19027500	-3.26598100	0.83435600
F	4.65885500	-3.32880200	-0.79962000
F	3.09767700	-5.91465900	0.99344900
F	5.16418100	-5.23199700	0.95694400
F	4.29688500	-6.16358200	-0.81125900
C	4.34527800	1.25270100	0.64507200
C	-0.01440300	3.87330700	-1.58721200
F	4.20594700	0.95054100	1.95814000
F	5.56380100	0.82796100	0.23444700
F	5.00508000	3.14755600	-0.61483300
F	2.98480100	3.17330500	0.24616200
C	4.78847100	3.60879500	1.68024200
F	3.93273700	3.51025300	2.70586800
F	5.98749800	3.14852900	2.06147700
F	4.90525900	4.89704600	1.34067400
F	0.39627700	4.49198500	-2.71582200
F	0.50559800	4.53691600	-0.52075300
C	-1.56412300	3.94681000	-1.50989600
F	-2.08234700	2.91695500	-2.22896500
F	-1.94829700	3.81187800	-0.21907400

C	-2.17343800	5.26306900	-2.04917100
F	-3.46439000	5.32728800	-1.70584000
F	-2.07565500	5.31417400	-3.38032300
F	-1.52964300	6.31147700	-1.51685000
C	-1.94627500	1.24598700	1.57038300
H	-1.38661400	1.75764700	0.80656000
H	-2.75806800	1.77180800	2.05673700
C	-1.64251900	-0.04006200	1.88805200
C	-0.55745700	-0.73605700	1.25427800
C	-0.54037500	-2.20513600	1.50940000
O	-1.38548300	-2.88714700	0.95376000
O	0.44996900	-2.68688100	2.25498100
C	0.52051300	-4.12839600	2.35574600
H	1.39270100	-4.32837900	2.97596900
H	-0.38181900	-4.51843700	2.82992300
H	0.64346100	-4.56714700	1.36679000
O	-2.31805900	-0.72134000	2.86232300
Si	-4.01336400	-1.01230800	2.91744800
C	-4.57665800	-1.40461600	1.13239400
H	-3.76885400	-0.99618600	0.51172900
C	-4.12743900	-2.45903100	4.14296100
H	-5.12667700	-2.89540400	3.99335600
C	-4.87270600	0.57164700	3.53885300
H	-4.92109900	1.22497000	2.65535400
C	-4.10307700	1.34392200	4.62367400
H	-3.09790700	1.61129500	4.29045700
H	-4.62525400	2.27564200	4.87635200
H	-4.00502900	0.76610100	5.54699400
C	-6.32361000	0.30600900	3.98536800
H	-6.35579200	-0.27865000	4.91063200
H	-6.84493200	1.25118100	4.18261400
H	-6.90478800	-0.23628000	3.23445300
C	-4.67818600	-2.90571700	0.80727100
H	-5.00682900	-3.04184500	-0.23010900
H	-3.71669900	-3.40921300	0.91191000
H	-5.40958500	-3.41035100	1.44981100
C	-5.87203800	-0.69702500	0.69322100
H	-5.84820700	0.38327600	0.86456900
H	-6.03345800	-0.85477800	-0.37905600
H	-6.74850200	-1.09925200	1.21335500
C	-3.07927700	-3.55227300	3.86190300
H	-3.21931600	-4.39763900	4.54779700
H	-3.12600800	-3.93513700	2.84177400
H	-2.06832500	-3.16228200	4.01799700

C	-4.01768200	-2.02583200	5.61669800
H	-4.81409900	-1.34100800	5.91708000
H	-4.07222000	-2.90198100	6.27570600
H	-3.05952300	-1.53203800	5.81641700
C	0.88985000	1.17205000	3.08755900
C	-0.33694800	0.69614100	5.03402000
C	1.20856800	-0.12428900	3.32431600
H	0.03461400	1.10002800	5.97903000
H	-1.40620400	0.51342300	5.11289200
H	1.91898500	-0.71260600	2.77169800
C	0.45026500	-0.56803200	4.56478200
H	-0.23511700	-1.38625200	4.33423600
H	1.12638600	-0.92010500	5.35096100
O	1.23398000	2.09475900	2.18416300
C	0.56529900	3.33670000	2.53736400
H	1.32041800	4.07887700	2.81061600
H	-0.01008200	3.69142100	1.68400700
C	-0.32087700	2.98872400	3.73852900
O	-1.06571200	3.72144100	4.36241300
N	-0.05604600	1.66077600	3.96214700

TS15

Rh	1.24768600	0.50967100	-2.67392700
O	2.97610800	1.09551100	-1.70800200
O	1.93709600	-1.43648800	-2.67045900
O	-0.57737000	-0.10024100	-3.41861600
O	0.54042600	2.42790600	-2.48541100
Rh	0.30828500	0.06475400	-0.41436000
C	0.06458600	2.75501600	-1.37094600
O	-0.08218000	2.06653000	-0.32194500
C	-1.48596300	-0.36336600	-2.59454800
O	-1.48422400	-0.28533200	-1.33176600
C	3.01811100	0.97137800	-0.46240000
O	2.17364400	0.45529000	0.32951300
O	0.82109900	-1.89959000	-0.73894100
C	1.61161700	-2.14829100	-1.69010200
C	-2.01093000	4.19016100	-1.05909500
C	3.83144000	-3.20912900	-1.09051200
C	-0.46691900	4.19449000	-1.22707200
F	0.08341300	4.77622700	-0.13053200
F	-0.14591100	4.93071500	-2.31409700
F	-2.52846000	3.22477400	-1.86592900
F	-2.31848400	3.90034800	0.22342600
C	-2.70528800	5.52419200	-1.41885700

F	-3.98328000	5.47809500	-1.02079000
F	-2.09418200	6.53991300	-0.79165900
F	-2.67287900	5.73552000	-2.73725800
C	-2.80398800	-0.93046100	-3.16057700
F	-3.85829600	-0.19974300	-2.71499600
F	-2.79843700	-0.90142700	-4.51101300
C	-2.99732300	-2.39986500	-2.69651300
C	-3.99651700	-3.22409300	-3.54093200
F	-3.43652700	-2.41507200	-1.41675800
F	-1.79198300	-3.03218400	-2.74594800
F	-5.14627700	-2.54969200	-3.67308000
F	-4.24478600	-4.38449700	-2.91708500
F	-3.49335600	-3.48617800	-4.74922800
C	2.37006200	-3.48279300	-1.56740100
C	4.21733100	1.60368900	0.26596700
F	1.75793200	-4.29512300	-0.65960100
F	2.41726800	-4.13185600	-2.74862800
F	4.60867200	-2.99075800	-2.16568500
F	3.84993900	-2.08825200	-0.31160300
C	4.46362000	-4.34435900	-0.25239500
F	3.89353800	-4.40188200	0.96379200
F	4.30424500	-5.52163600	-0.86671700
F	5.76947400	-4.10639700	-0.09424700
F	5.21914100	1.87903200	-0.59478800
F	4.68487700	0.75048000	1.21896100
C	3.76581600	2.91676400	0.96326500
F	2.95652500	3.59902400	0.11011100
F	3.05967500	2.60357300	2.07198300
C	4.91753200	3.86104600	1.37864400
F	4.43098200	4.83473900	2.15719700
F	5.48603000	4.41121600	0.30252600
F	5.84267700	3.17662600	2.06681300
C	-1.57650700	-2.46054000	1.01811700
H	-1.35214700	-2.34217500	-0.03407200
H	-2.53055600	-2.96395000	1.17986700
C	-1.39370100	-1.22301000	1.81471300
C	-0.56761200	-0.22694000	1.46345000
C	-0.24085900	0.84673400	2.41712600
O	0.69815600	0.75516700	3.20142300
O	-0.97955600	1.96081800	2.30233400
C	-0.49484600	3.12346500	2.99845000
H	-1.07425100	3.95551000	2.60197900
H	-0.65326100	3.01993300	4.07460800
H	0.56817500	3.26229900	2.79658500

O	-2.17698800	-1.16218400	2.96680000
Si	-3.80788800	-0.61725200	2.92347800
C	-4.81762200	-2.10072400	3.56936800
H	-4.75455800	-2.87190100	2.78544300
C	-3.94361100	0.77900700	4.21870000
H	-4.84597100	0.52943200	4.79616500
C	-4.19151600	-0.27430300	1.08409900
H	-3.51702200	-0.98048800	0.58355800
C	-3.80130900	1.11704500	0.55689000
H	-2.79333700	1.40890600	0.84809000
H	-3.84076100	1.11732700	-0.53593000
H	-4.49121600	1.88704600	0.91353700
C	-5.61019800	-0.63740100	0.61344300
H	-6.36849600	0.02707300	1.04322200
H	-5.66755100	-0.53423200	-0.47663200
H	-5.88618900	-1.66773600	0.85791900
C	-4.22469300	-2.68805300	4.86251100
H	-4.76696700	-3.59059700	5.17094300
H	-3.16969800	-2.95048000	4.75304800
H	-4.29830200	-1.97134000	5.68811600
C	-6.30518100	-1.77213400	3.79708300
H	-6.79631900	-1.38205100	2.90326400
H	-6.85638300	-2.66614300	4.11400200
H	-6.42432200	-1.02616100	4.59094400
C	-2.75382500	0.73679300	5.19870700
H	-2.88371600	1.48794800	5.98769600
H	-2.65212100	-0.23852700	5.68530100
H	-1.80927700	0.94167000	4.69003900
C	-4.14307700	2.19912900	3.66504200
H	-5.05880700	2.27932700	3.07181600
H	-4.21931100	2.92137400	4.48787200
H	-3.30886900	2.50098600	3.02908400
C	0.87955400	-2.85958500	2.39319300
C	-0.29217700	-3.06493400	4.40581900
C	-0.28171200	-3.66077600	2.00096900
H	0.04158000	-3.50233900	5.34726900
H	-0.99816600	-2.25352200	4.58477300
H	-0.05957500	-4.44920700	1.28533100
C	-0.83145800	-4.10416600	3.38103400
H	-1.92055100	-4.13813900	3.38887800
H	-0.45664600	-5.10184100	3.62964300
O	1.88777800	-2.39079900	1.72979000
C	2.67320200	-1.54296900	2.64096300
H	3.69437300	-1.92412600	2.64033500

H	2.61579300	-0.52242500	2.26037600
C	1.97291000	-1.68521800	3.98815900
O	2.27194100	-1.28080500	5.07442500
N	0.86017300	-2.51861700	3.67361400

2s

Cu	0.36952500	0.94459800	0.18229300
N	-0.54314400	1.50665100	-1.47840300
N	0.55093700	-1.18876200	-0.18199800
N	-1.05986900	0.96317300	1.56931400
C	-1.35443600	1.55285100	-2.30324900
C	0.06950500	-2.23029600	-0.35190000
C	-2.04777700	0.78086300	2.14508200
C	-0.52736600	-3.53742700	-0.56129000
H	-0.50618700	-4.10038500	0.37612900
H	-1.56697600	-3.41728300	-0.87755300
H	0.03649200	-4.08272900	-1.32330300
C	-2.41066900	1.56145500	-3.29775000
H	-3.13584500	0.79252400	-3.01750700
H	-2.89954200	2.53940200	-3.31701900
H	-2.00061900	1.34125900	-4.28719800
C	-3.30343900	0.54067100	2.83171000
H	-3.14728400	-0.17375400	3.64487800
H	-3.68757300	1.47799700	3.24354400
H	-4.01720200	0.12118800	2.11715300
B	-3.46226500	-1.53678500	-0.16295400
F	-2.90533000	-0.57824800	-1.03376500
F	-2.57926700	-1.77373300	0.91069900
F	-4.68516400	-1.06032100	0.34271400
F	-3.66345500	-2.74005600	-0.86501700
N	-0.17839600	4.12153000	0.64323500
N	-1.26692300	4.11161800	0.45524300
C	3.73659300	-2.03304400	1.15887600
C	4.60618900	-2.28265300	-0.11002600
C	4.16697400	-1.21561800	-1.15170300
H	2.84912500	-2.67495800	1.19525100
H	4.28053400	-2.15218100	2.09824500
H	5.65944100	-2.13561900	0.13858800
H	4.48273400	-3.29445000	-0.49635300
H	4.99883100	-0.78119700	-1.70672300
H	3.41940200	-1.58933200	-1.85699600
N	3.53863400	-0.20562200	-0.29639400
C	3.03731400	1.14221200	-0.46139700
O	3.21511400	1.81246700	-1.47203000

C	2.31435800	1.35285000	0.77596200
H	2.37253600	2.29048200	1.31713100
C	3.29984300	-0.63332500	0.92553900
O	2.67800800	0.23121900	1.66105800

3s

Cu	1.92603000	-0.30972800	0.37193500
N	2.00958600	-1.88510600	-0.84372900
N	3.26854600	1.03001500	-0.61834400
N	2.96118000	-0.86128900	1.97009700
C	2.47399900	-2.73829300	-1.47374400
C	4.31451200	1.32619200	-1.02203400
C	3.83770400	-1.19438600	2.65019100
C	5.62649200	1.68973300	-1.52678000
H	6.08537900	2.42154400	-0.85590500
H	6.25719500	0.79736700	-1.56330500
H	5.53176300	2.12450600	-2.52573200
C	3.12216700	-3.78871300	-2.23639900
H	4.19694300	-3.72396100	-2.04502300
H	2.75007900	-4.76713100	-1.92015800
H	2.92771500	-3.65481500	-3.30408100
C	4.96013600	-1.62055400	3.46517900
H	5.38649200	-0.75640900	3.98262100
H	4.62720600	-2.35515700	4.20355800
H	5.71986800	-2.05955200	2.81208300
B	6.29861200	-1.46978700	0.06512200
F	5.15644700	-2.05348000	-0.51829200
F	5.92590200	-0.31809000	0.78821100
F	6.90163600	-2.38992300	0.94215900
F	7.20412100	-1.10138100	-0.94788600
C	1.37273500	4.28307700	-0.45745000
C	0.72796900	4.53637100	-1.85312400
C	0.36087900	3.13435600	-2.41444700
H	2.46462900	4.19996400	-0.51102300
H	1.12508300	5.03605100	0.29199300
H	-0.18430600	5.12373600	-1.72693700
H	1.39747300	5.07701200	-2.52205300
H	-0.60213200	3.10884200	-2.92528200
H	1.13063200	2.72057700	-3.07172000
N	0.30230500	2.33416500	-1.18918000
C	-0.18976400	1.02630100	-0.82060900
O	-0.79137400	0.29528400	-1.59958000
C	0.25950000	0.90160100	0.55163300
H	-0.39009000	0.51845200	1.32930700

C	0.81288400	2.94467500	-0.14008700
O	0.76192600	2.23390200	0.93931800
C	-3.03762800	0.13648100	2.37719800
H	-2.67775500	0.82550600	3.12660400
H	-3.26796700	-0.88214100	2.66532400
C	-3.21146600	0.54127800	1.10721500
C	-2.92032900	1.90220600	0.62181600
N	-3.12322300	2.12367600	-0.66039800
N	-3.30144900	2.31508100	-1.76386000
C	-2.36664800	3.00955800	1.39937600
O	-2.17231000	2.98664700	2.60160700
O	-2.08751500	4.07811700	0.61397600
C	-1.63473500	5.25317100	1.31506400
H	-1.45328800	6.00063100	0.54357600
H	-2.40493300	5.60501000	2.00581100
H	-0.71874200	5.04299900	1.87063800
O	-3.66874700	-0.22435300	0.09076600
Si	-4.19220200	-1.84784500	0.03323400
C	-5.68395200	-2.04736400	1.19876900
H	-5.25309400	-2.30619200	2.17697800
C	-4.63490300	-2.00130900	-1.80071800
H	-5.01253500	-3.02332500	-1.94764400
C	-2.80278200	-3.03324900	0.57222900
H	-2.94712400	-3.17996500	1.65265100
C	-1.38383100	-2.47480900	0.36379300
H	-1.20026900	-1.61096700	1.00624400
H	-0.63233000	-3.23657500	0.61143100
H	-1.20771400	-2.14936900	-0.66385700
C	-2.95849300	-4.41245700	-0.09808800
H	-2.79639400	-4.35309100	-1.17946700
H	-2.22061200	-5.11892500	0.30294100
H	-3.94985300	-4.84960300	0.06377600
C	-6.50427200	-0.75958000	1.38583000
H	-7.32593500	-0.92835300	2.09424400
H	-5.89205000	0.05783600	1.77769100
H	-6.95208400	-0.41987500	0.44634400
C	-6.58712300	-3.21881100	0.76953100
H	-6.03710500	-4.16285600	0.69234600
H	-7.39604100	-3.37075200	1.49552900
H	-7.05500900	-3.02834800	-0.20282300
C	-5.74823800	-1.01782200	-2.20274800
H	-5.97924400	-1.11040000	-3.27192900
H	-6.67576900	-1.19258200	-1.64942700
H	-5.44178500	0.01885000	-2.02269000

C	-3.40101700	-1.80508100	-2.70084500
H	-2.63461800	-2.56519200	-2.52223700
H	-3.68416700	-1.86470300	-3.76011200
H	-2.93479700	-0.82988700	-2.53031100

TS2's

Cu	2.30813800	-0.45886400	0.39423800
N	3.28417700	-1.95965400	-0.50205700
N	3.08299100	1.16212300	-0.65737900
N	3.40319900	-0.30092200	2.09480500
C	4.14293600	-2.61431700	-0.91929400
C	3.96880300	1.72203100	-1.15328800
C	4.37520000	-0.24811800	2.72314100
C	5.08782900	2.39636900	-1.78399700
H	5.61531600	3.00189600	-1.04316900
H	5.76775100	1.63139900	-2.16580300
H	4.73431600	3.03332800	-2.59918000
C	5.24153300	-3.42099900	-1.41642300
H	5.53166600	-3.07230400	-2.41057200
H	6.08459400	-3.29683900	-0.73334300
H	4.94468000	-4.47187400	-1.46776700
C	5.61199100	-0.20010900	3.47995200
H	5.44717800	-0.56689800	4.49656500
H	6.34419700	-0.82500500	2.96369000
H	5.98006800	0.82825500	3.51607500
B	6.72343600	-0.33216500	-0.03463700
F	6.48495100	-1.48823500	0.74651700
F	6.15265500	0.78574400	0.60760000
F	8.09933600	-0.14141600	-0.18931400
F	6.11824100	-0.50226800	-1.30048100
C	0.04466400	2.90785600	-0.73873400
C	0.00672600	2.78492300	-2.27687700
C	0.08188100	1.27215000	-2.55017100
H	1.07291000	2.90860600	-0.36942100
H	-0.44821400	3.80684000	-0.36975400
H	-0.92555400	3.20025700	-2.66936100
H	0.83304200	3.31939200	-2.74951300
H	-0.47102400	0.96794900	-3.43934800
H	1.11812500	0.93035400	-2.63988700
N	-0.50408200	0.68474000	-1.33025100
C	-0.14199600	-0.60380300	-0.82063800
O	-0.11653800	-1.61889800	-1.51863700
C	0.24221700	-0.36596500	0.55133200
H	-0.04389500	-1.04121800	1.35068000

C	-0.57126300	1.59073400	-0.25877300
O	-0.05012900	1.00564000	0.86476200
C	-2.89685300	0.49687300	2.27183700
H	-2.60095000	1.32509100	2.89834700
H	-3.21982100	-0.41889400	2.75178700
C	-2.82104500	0.57517500	0.93917800
C	-2.28438500	1.80636900	0.22041300
N	-2.99379600	1.89727100	-1.02369800
N	-2.96129000	1.57627800	-2.11221600
C	-2.38325100	3.10553300	0.99833200
O	-1.77363300	3.30140300	2.02551000
O	-3.17417400	3.98725700	0.38413500
C	-3.28660200	5.28330500	1.02399000
H	-3.95521600	5.85867400	0.38582600
H	-3.70944500	5.16999900	2.02387300
H	-2.30566800	5.75854500	1.08486100
O	-3.15131300	-0.39303700	0.05940500
Si	-4.41085600	-1.55834500	0.20849100
C	-5.92970100	-0.64447300	0.89395100
H	-5.74158000	-0.53804700	1.97165800
C	-4.62016100	-2.21764600	-1.55024200
H	-5.33690900	-3.04689300	-1.45447500
C	-3.84833000	-2.91799000	1.41411400
H	-4.19838100	-2.59589400	2.40633100
C	-2.31708300	-3.06153300	1.48486400
H	-1.84220900	-2.14038200	1.83035500
H	-2.03931600	-3.86181800	2.18280500
H	-1.88120100	-3.30736000	0.51169100
C	-4.51028700	-4.27534100	1.11024700
H	-4.17729800	-4.67402200	0.14619100
H	-4.24203200	-5.01273300	1.87713900
H	-5.60338900	-4.21496300	1.08350400
C	-6.13905900	0.77011300	0.32557900
H	-7.01036900	1.24279100	0.79680300
H	-5.28031800	1.42235200	0.51114600
H	-6.32125900	0.75912700	-0.75300500
C	-7.20123600	-1.49881100	0.73035900
H	-7.10650000	-2.47823500	1.21100300
H	-8.06559100	-0.99594800	1.18195400
H	-7.43876000	-1.66861600	-0.32575300
C	-5.22244300	-1.19647400	-2.52905300
H	-5.31276600	-1.63489100	-3.53111300
H	-6.21997000	-0.86978300	-2.22208700
H	-4.59187100	-0.30613600	-2.62252400

C	-3.30347600	-2.79149500	-2.10541000
H	-2.92147200	-3.61293000	-1.49177500
H	-3.45636700	-3.18324500	-3.11951700
H	-2.51611200	-2.03356600	-2.15457600

3_Rh

Rh	-0.94860100	0.44303800	0.02435400
O	0.01549400	1.90753000	1.11697900
O	-1.91608700	-0.12008100	1.73962300
O	-2.02662300	-0.89684400	-1.10829600
O	-0.09206700	1.14853700	-1.70292400
Rh	-2.76772600	2.01648000	-0.33719700
C	-0.69013600	2.04477300	-2.37693400
O	-1.80182500	2.58297800	-2.06810400
C	-3.17757700	-0.57494100	-1.55900300
O	-3.73673800	0.55137800	-1.40396800
C	-0.55934900	3.03364100	1.26963000
O	-1.69441800	3.35371200	0.79265400
O	-3.63836000	1.30225500	1.38960500
C	-3.03658200	0.39943400	2.04972600
C	0.14622700	4.11333600	2.10291000
C	-0.03264100	2.51511700	-3.68167300
C	-3.91197800	-1.64843700	-2.37113800
C	-3.67208300	-0.11767600	3.34644200
C	0.29498200	5.39969500	1.23308200
H	0.81608900	6.14234500	1.84698600
H	-0.70678100	5.78755900	1.02800700
C	1.51256600	3.63666700	2.59836600
H	1.98919200	4.43268200	3.18040000
H	1.41154800	2.75855700	3.23856200
H	2.17048200	3.37682600	1.76890600
C	-0.75717500	4.43592000	3.31031000
H	-0.29229200	5.21538200	3.92326300
H	-1.73978200	4.78747600	2.98569800
H	-0.89623400	3.54891700	3.93789400
C	0.16326900	4.06144400	-3.61830800
H	0.65064900	4.36197600	-4.55215200
H	-0.82656400	4.52667800	-3.60043400
C	-0.99900000	2.18616400	-4.83699100
H	-0.57061800	2.52187400	-5.78730600
H	-1.16968100	1.10601200	-4.90450100
H	-1.96436200	2.67918500	-4.69645400
C	1.30743600	1.80790200	-3.91293600
H	1.17290700	0.72450500	-3.97330000

H	1.74305200	2.15395700	-4.85650000
H	2.01561700	2.01322400	-3.10959900
C	-5.34207900	-1.20774700	-2.70185700
H	-5.84269200	-1.99339700	-3.27773500
H	-5.92594100	-1.01750800	-1.79902100
H	-5.33904000	-0.29367900	-3.30094100
C	-3.12056600	-1.85463600	-3.67871600
H	-2.08391000	-2.13033200	-3.47254300
H	-3.58316200	-2.64815300	-4.27488500
H	-3.11590700	-0.93794600	-4.27785400
C	-3.90756800	-2.97994200	-1.56119900
H	-4.39800800	-3.73901700	-2.18006800
H	-2.86698400	-3.28227700	-1.42835000
C	-3.70588800	-1.67737300	3.30689200
H	-2.67273700	-2.03211200	3.26605500
H	-4.13794800	-2.01341600	4.25571900
C	-2.75802100	0.32223900	4.50937200
H	-2.68979000	1.41448900	4.55779700
H	-3.16850900	-0.03451300	5.46004100
H	-1.74968000	-0.08222800	4.38953200
C	-5.07647200	0.46252900	3.54316200
H	-5.50572000	0.07580400	4.47360500
H	-5.04114200	1.55305300	3.61045800
H	-5.74368600	0.19696000	2.72024700
C	1.03074800	5.19862500	-0.07204200
C	0.32677800	4.79235900	-1.21220000
C	2.41505600	5.39125700	-0.17663700
C	0.96663000	4.54932100	-2.43408500
H	-0.74576300	4.65296600	-1.14459900
C	3.06723800	5.17732500	-1.39236200
H	2.97911000	5.72124400	0.69154000
C	2.35065400	4.75297400	-2.51355600
H	4.13871300	5.34184100	-1.46676800
H	2.86515000	4.58734700	-3.45620400
C	-4.48942400	-2.25568300	2.15099300
C	-3.87431700	-2.43769200	0.90515200
C	-5.84579200	-2.58391200	2.27855700
C	-4.58573700	-2.89190900	-0.21315400
H	-2.82416200	-2.19686100	0.79949700
C	-6.56280800	-3.06841300	1.18304400
H	-6.33823600	-2.46506100	3.23983600
C	-5.94055100	-3.21394600	-0.05797100
H	-7.61101900	-3.33105200	1.29638800
H	-6.50588900	-3.58207800	-0.90973500

C	-0.00117100	-3.96312000	-1.94738000
C	-0.66697600	-5.04588400	-1.04184400
C	-0.54076200	-4.55009400	0.43020000
H	0.96301400	-4.28216700	-2.35502100
H	-0.62867000	-3.65035800	-2.78467500
H	-1.71872100	-5.15624200	-1.30711000
H	-0.18380300	-6.01438200	-1.16871300
H	-1.48205000	-4.58944300	0.97939800
H	0.23233200	-5.07958100	0.99194100
N	-0.11977100	-3.15705100	0.25353200
C	0.28261400	-2.09018300	1.13813800
O	0.22573900	-2.16449500	2.35213400
C	0.66693600	-1.02394700	0.21194900
H	1.59382800	-0.49553700	0.38660400
C	0.21413700	-2.85479700	-0.98509000
O	0.74624800	-1.68506300	-1.11027600
C	3.95271000	-3.15727400	2.07431300
H	3.85387500	-4.21371300	2.27604700
H	4.16803600	-2.48493000	2.89473400
C	3.79080700	-2.68724000	0.82825600
C	3.47616100	-3.53017200	-0.34072900
N	3.56139100	-2.94342500	-1.51733500
N	3.61583600	-2.42376700	-2.52441300
C	3.13269000	-4.95257700	-0.33156100
O	2.97231700	-5.62122900	0.67515300
O	3.00467000	-5.44231900	-1.58594000
C	2.69469800	-6.84769100	-1.67737800
H	2.52111500	-7.03751800	-2.73597000
H	3.53730600	-7.44344500	-1.31798200
H	1.80472400	-7.08790400	-1.09278400
O	3.89527800	-1.38352300	0.45506100
Si	4.92198100	-0.16568500	1.08425400
C	6.66495400	-0.90866700	1.23792600
H	6.64286800	-1.50269600	2.16280200
C	4.74969700	1.20264200	-0.21287700
H	5.21523200	2.09428700	0.23146100
C	4.29414500	0.38393700	2.79558700
H	4.81733900	-0.26328600	3.51544100
C	2.78308400	0.17083900	2.99256400
H	2.48720500	-0.86978000	2.84557300
H	2.48703500	0.45376300	4.01172800
H	2.18771100	0.77856200	2.30711600
C	4.69278700	1.83831100	3.10891700
H	4.22667200	2.54012100	2.41090000

H	4.36839000	2.11909900	4.11899800
H	5.77571100	1.99340400	3.05898500
C	7.03798400	-1.86321100	0.09087200
H	8.03800500	-2.28544300	0.25473100
H	6.33959900	-2.70157800	0.01367500
H	7.05578900	-1.35362700	-0.87705900
C	7.73204900	0.18754900	1.41665200
H	7.53593100	0.81835400	2.28987200
H	8.72581800	-0.25775700	1.55271900
H	7.78720200	0.84318900	0.54045600
C	5.47528600	0.89768500	-1.53405800
H	5.30959500	1.70669300	-2.25757500
H	6.55550000	0.78960100	-1.40128000
H	5.09855500	-0.02570600	-1.98916200
C	3.27006600	1.52282300	-0.49363700
H	2.68522900	1.70446500	0.41086100
H	3.17935500	2.41672800	-1.11880200
H	2.79338200	0.69980400	-1.03326200

4_Rh

Rh	-1.06324000	0.05991900	0.01221900
O	-1.40421500	1.17914300	1.67624500
O	-1.44300100	-1.64123100	1.11703300
O	-0.84267200	-1.04397300	-1.70722800
O	-0.83362200	1.78586700	-1.05753400
Rh	-3.40277700	0.16585700	-0.45615200
C	-1.85038600	2.33567200	-1.58872000
O	-3.03986200	1.88212900	-1.52667300
C	-1.86827400	-1.30506900	-2.41861300
O	-3.05247000	-0.92825000	-2.15223400
C	-2.59263600	1.51331000	1.98223400
O	-3.62574400	1.22659100	1.29529400
O	-3.64381200	-1.54866400	0.62165300
C	-2.64095400	-2.07487800	1.19670400
C	-2.80091800	2.30236200	3.27808000
C	-1.63938500	3.62926700	-2.38350500
C	-1.63132900	-2.12820100	-3.68908100
C	-2.88750300	-3.31873100	2.05782200
C	-3.60621200	3.59869500	2.95649100
H	-3.74807000	4.13068600	3.90324400
H	-4.59495900	3.30496400	2.59257100
C	-1.45607500	2.63852600	3.93421900
H	-1.63611000	3.17360300	4.87285300
H	-0.88232100	1.73392500	4.14777800

H	-0.84580400	3.27697000	3.29121100
C	-3.63664700	1.41774800	4.22592700
H	-3.82114300	1.95293000	5.16309700
H	-4.59979700	1.15819900	3.77825500
H	-3.10253700	0.49157600	4.46357100
C	-2.62509600	4.71753500	-1.85833300
H	-2.46183500	5.61438600	-2.46548000
H	-3.64539200	4.37288700	-2.04794700
C	-1.97624100	3.32431000	-3.85779100
H	-1.84154000	4.22776100	-4.46144900
H	-1.31365300	2.54850000	-4.25639700
H	-3.00981700	2.98460600	-3.96508800
C	-0.18807900	4.11008900	-2.27588000
H	0.49893500	3.36174400	-2.67186500
H	-0.06592700	5.03083100	-2.85592700
H	0.09668600	4.31456400	-1.24189200
C	-2.94763800	-2.37938100	-4.43286500
H	-2.75027300	-2.97438300	-5.33063400
H	-3.66692700	-2.91846500	-3.81318400
H	-3.40731600	-1.43660600	-4.74165700
C	-0.66418000	-1.33504700	-4.59106500
H	0.29102700	-1.16496400	-4.08989600
H	-0.47990900	-1.89375600	-5.51454800
H	-1.09025400	-0.36304400	-4.86159900
C	-0.94593900	-3.47422700	-3.29572100
H	-0.80551000	-4.04111600	-4.22227100
H	0.04693500	-3.24259300	-2.89975800
C	-2.01298200	-4.49178500	1.51625700
H	-0.96224500	-4.24389200	1.68335500
H	-2.24260300	-5.37040600	2.12816900
C	-2.45986600	-2.98815800	3.50181100
H	-3.07548600	-2.17918900	3.90946800
H	-2.59327400	-3.86955700	4.13761400
H	-1.41480100	-2.67596900	3.55175100
C	-4.37160900	-3.70587700	2.04247600
H	-4.51919600	-4.59576400	2.66322300
H	-4.98987600	-2.90011100	2.44701700
H	-4.72302100	-3.92684900	1.03280500
C	-2.93951300	4.50478600	1.94716000
C	-3.12460800	4.28462000	0.57623900
C	-2.09276400	5.54699600	2.34758700
C	-2.46127400	5.04762400	-0.39286400
H	-3.78930200	3.49115700	0.25563300
C	-1.44392400	6.33551800	1.39568400

H	-1.94869800	5.74416900	3.40627800
C	-1.61970000	6.08383500	0.03389700
H	-0.80025500	7.15006900	1.71625500
H	-1.10933400	6.69838800	-0.70259400
C	-2.22586500	-4.80442400	0.05331100
C	-1.50709900	-4.09877000	-0.91925900
C	-3.15311100	-5.76542400	-0.37003700
C	-1.70817300	-4.30470000	-2.28934600
H	-0.78072600	-3.36301500	-0.59950800
C	-3.35403500	-5.99915900	-1.73197700
H	-3.70997600	-6.33668400	0.36751600
C	-2.64150500	-5.27142600	-2.68698400
H	-4.06596300	-6.75548300	-2.05059100
H	-2.80136200	-5.46129600	-3.74469900
C	1.86784700	-2.22520400	-0.08742300
C	1.91575800	-3.36356300	0.96302900
C	1.46810000	-2.73461700	2.30455400
H	2.62774300	-2.32804900	-0.86287300
H	0.89458400	-2.16655600	-0.57487900
H	1.27078300	-4.19817700	0.67998400
H	2.93426900	-3.75093100	1.05373800
H	0.40701400	-2.89778100	2.50013600
H	2.04787100	-3.10822100	3.15333500
N	1.70282500	-1.31403700	2.09054500
C	1.29257300	-0.19103100	2.73826600
O	0.84823900	-0.07994100	3.87030800
C	1.54580800	0.90037500	1.66342200
H	0.93788100	1.79245000	1.76483100
C	2.06342700	-0.96687800	0.72578600
O	1.19532100	0.16048900	0.44669400
C	3.05690500	1.09147100	1.45121200
H	3.58618900	1.28706400	2.37994000
H	3.21451800	1.91477000	0.75670300
C	3.46422800	-0.25388000	0.76692700
C	4.46342000	-1.09886700	1.55727800
N	5.10834400	-1.99489300	0.85383100
N	5.66435200	-2.75400400	0.21608800
C	4.68010200	-1.12521700	3.00139200
O	4.20565500	-0.33072800	3.79712300
O	5.49008500	-2.14570300	3.35875100
C	5.79796100	-2.23180900	4.76338200
H	6.46064000	-3.09132700	4.86192700
H	6.30091700	-1.32346200	5.10381100
H	4.88731900	-2.38535800	5.34729000

O	3.94651500	-0.15807800	-0.54140400
Si	4.54502600	1.04218900	-1.57237800
C	5.57057800	2.34652400	-0.62501300
H	4.83373100	3.05566800	-0.21860100
C	5.59743700	0.03929100	-2.80050200
H	5.78606600	0.70970800	-3.65275200
C	3.03039900	1.87216100	-2.36706100
H	2.49300300	2.31803100	-1.51614600
C	2.07242100	0.86948600	-3.03270400
H	1.86870300	0.00748900	-2.39320700
H	1.11008200	1.34447400	-3.25297000
H	2.47999300	0.50655600	-3.98211400
C	3.38346800	3.00793000	-3.34296800
H	4.03125200	2.65574200	-4.15493100
H	2.47734600	3.41498300	-3.80911800
H	3.89250800	3.83818700	-2.84495200
C	6.37876300	1.78522500	0.55902300
H	6.91783900	2.59376400	1.06973400
H	5.75176900	1.29151500	1.30504600
H	7.12560300	1.05660800	0.22863700
C	6.49835800	3.14890100	-1.55981100
H	5.96618700	3.60361500	-2.39929800
H	6.98823600	3.95916800	-1.00496900
H	7.29125200	2.51999900	-1.97625100
C	6.96061600	-0.38720400	-2.22391000
H	7.52465500	-0.96572800	-2.96711600
H	7.58234500	0.46164500	-1.93101300
H	6.83697800	-1.02876900	-1.34514500
C	4.86357100	-1.20979500	-3.32495800
H	3.93239900	-0.96953700	-3.84260400
H	5.50122600	-1.76044400	-4.02861200
H	4.61981800	-1.89074200	-2.50207200

12s

Rh	-0.03365900	-0.01805600	0.33315500
O	-1.44485000	-1.07693100	1.37749900
O	1.40598300	-0.97312300	1.43798000
O	1.35269700	0.94043400	-0.83814400
O	-1.47105800	0.82011900	-0.86799500
Rh	0.08027700	-1.86386800	-1.23161600
C	-1.81978300	0.22152300	-1.93748200
O	-1.37304700	-0.90140900	-2.33210300
C	1.81940400	0.36168400	-1.87319300
O	1.50070000	-0.80035600	-2.27209500

C	-1.78614200	-2.23380300	0.97084100
O	-1.33443000	-2.81197100	-0.06875800
O	1.54939000	-2.67362800	-0.04528200
C	1.89163800	-2.07685200	1.02186300
C	-2.82800800	-2.99787900	1.79761800
C	-2.86523800	0.89941600	-2.83133900
C	2.84190600	1.16482900	-2.68454500
C	2.96848300	-2.71409000	1.90769800
C	-4.06000600	-3.29457600	0.88673900
H	-4.80668900	-3.79774600	1.51058600
H	-3.74543300	-4.00283800	0.11513600
C	-3.24608600	-2.19448700	3.03510600
H	-3.98792900	-2.76352300	3.60550600
H	-2.38737400	-2.00506900	3.68532200
H	-3.68356400	-1.23139500	2.76521300
C	-2.20472000	-4.33689500	2.23697900
H	-2.93653800	-4.91658000	2.80936100
H	-1.89048600	-4.92803600	1.37331500
H	-1.33113300	-4.16832600	2.87625200
C	-4.09376900	-0.05466800	-2.96359800
H	-4.84789400	0.47248100	-3.55795700
H	-3.77926100	-0.93284100	-3.53453500
C	-2.24209500	1.10075200	-4.22640400
H	-2.97425400	1.56194600	-4.89746500
H	-1.36916500	1.76057100	-4.17142000
H	-1.92631700	0.14765800	-4.65760500
C	-3.28507700	2.25496300	-2.25501000
H	-2.42622000	2.92843700	-2.19215100
H	-4.03413300	2.71556400	-2.90751900
H	-3.71176000	2.15274400	-1.25579500
C	3.35477100	0.35498600	-3.87997800
H	4.08098700	0.95185500	-4.44192300
H	3.84070400	-0.56975100	-3.56301500
H	2.53453900	0.09138000	-4.55341300
C	2.14422400	2.44579500	-3.18406600
H	1.77452900	3.04183700	-2.34574100
H	2.85019100	3.05357300	-3.75978200
H	1.29747400	2.20204400	-3.83511400
C	4.01190500	1.57340200	-1.73569700
H	4.73816800	2.12745600	-2.34050200
H	3.60970000	2.25787000	-0.98389500
C	4.12485200	-1.68422800	2.10393800
H	3.73051200	-0.84046900	2.67700300
H	4.88878100	-2.17259900	2.71869200

C	2.33424300	-3.00888500	3.28209000
H	1.50342300	-3.71614800	3.18394200
H	3.08110300	-3.45346300	3.94820000
H	1.95617600	-2.09376900	3.74544300
C	3.48903700	-4.01588000	1.28851400
H	4.25948000	-4.44626400	1.93690300
H	2.68277800	-4.74695500	1.18336300
H	3.92312100	-3.84798600	0.30103300
C	-4.66384500	-2.07502600	0.23014300
C	-4.19282100	-1.65232600	-1.01906600
C	-5.67463800	-1.32783200	0.84988900
C	-4.68289500	-0.49959600	-1.64520700
H	-3.41716500	-2.22795100	-1.51165800
C	-6.18802200	-0.18560900	0.23254400
H	-6.06883900	-1.64916600	1.80997300
C	-5.69382600	0.23000100	-1.00539000
H	-6.98262600	0.37776600	0.71406100
H	-6.10232600	1.11540600	-1.48459900
C	4.73720000	-1.17539500	0.81940100
C	4.18925300	-0.05534700	0.18031300
C	5.83217000	-1.81751600	0.22562700
C	4.68548600	0.41035300	-1.04453500
H	3.35484000	0.46241500	0.64047300
C	6.35488400	-1.35075700	-0.98163700
H	6.28184800	-2.67672000	0.71580500
C	5.78235900	-0.24757700	-1.61715100
H	7.21324700	-1.84633400	-1.42692800
H	6.19400700	0.11090600	-2.55667700
C	-2.05246700	4.41011600	0.43211100
C	-1.03251700	5.15494200	-0.47693300
C	0.37275500	4.74778900	0.04014300
H	-2.35906500	5.01518800	1.29182300
H	-2.94007500	4.05427900	-0.09105800
H	-1.15157500	4.81506600	-1.50871000
H	-1.17271300	6.23551200	-0.44917900
H	1.10493300	4.60693600	-0.75486800
H	0.76684300	5.43837500	0.78890800
N	0.07857900	3.47066900	0.69710600
C	0.82945200	2.51046500	1.44393200
O	2.04990100	2.55412100	1.59636500
C	-0.18624400	1.56562200	1.85253900
H	-0.16286300	1.07244300	2.81492400
C	-1.20755200	3.31014500	0.95129300
O	-1.46232400	2.25678800	1.65775000

O	-0.54083500	4.88088800	3.21478000
H	-0.70963800	4.15593000	3.84663200
H	0.43100400	4.98590100	3.21604900
O	2.27728900	4.95500600	3.00293100
H	2.62078800	5.66000100	2.43561800
H	2.39952200	4.13420300	2.48608300
O	-0.96298100	2.71911900	4.99741100
H	-0.15144200	2.19132600	5.03813700
H	-1.63114900	2.11099300	4.64749400

TS8s

Rh	-0.04814300	-0.03285100	-0.34411000
O	1.23252200	-1.28035900	-1.34566900
O	-1.55878400	-0.73221000	-1.55001000
O	-1.33446000	1.10307200	0.78247200
O	1.43042600	0.55036900	0.94739700
Rh	-0.53559300	-1.87303300	1.17944500
C	1.61187800	-0.09713000	2.02842200
O	0.97429700	-1.13829000	2.38411100
C	-1.94095900	0.58862600	1.77754200
O	-1.83220200	-0.61400200	2.16674400
C	1.38004700	-2.47806300	-0.94132300
O	0.79387700	-2.99852400	0.05953900
O	-2.03544400	-2.42295200	-0.12084300
C	-2.22687000	-1.75671200	-1.18378400
C	2.34815500	-3.37369800	-1.72667100
C	2.69711000	0.41525000	2.98402900
C	-2.86818100	1.53347500	2.55165100
C	-3.34557900	-2.20239000	-2.13436700
C	3.46759500	-3.86270700	-0.75531800
H	4.16654700	-4.46391300	-1.34697200
H	3.00777800	-4.52589700	-0.01714100
C	2.95295600	-2.62041700	-2.91734900
H	3.63961700	-3.28082700	-3.45766800
H	2.17170100	-2.29831800	-3.61168200
H	3.50530100	-1.73528800	-2.59628100
C	1.56383100	-4.59935200	-2.23322100
H	2.23395200	-5.27140700	-2.77984400
H	1.11775900	-5.15257500	-1.40292900
H	0.76199200	-4.29355600	-2.91426900
C	3.76765600	-0.70677300	3.15733500
H	4.55937900	-0.30152900	3.79681100
H	3.30193500	-1.53616500	3.69717600
C	2.04276500	0.69157700	4.35091400

H	2.79922100	1.03640700	5.06387500
H	1.27751200	1.47098600	4.26469000
H	1.57143000	-0.20937200	4.75131700
C	3.33631200	1.70134600	2.44799000
H	2.58904400	2.49264100	2.34656500
H	4.10790900	2.04558800	3.14509400
H	3.79570500	1.54661500	1.47069300
C	-3.57125200	0.79833800	3.69788400
H	-4.23287700	1.49217100	4.22734500
H	-4.16921700	-0.03946700	3.33402700
H	-2.84344400	0.40628000	4.41363500
C	-2.00498200	2.67841000	3.11862700
H	-1.49561500	3.21817300	2.31608600
H	-2.63640700	3.38456600	3.66839600
H	-1.24807900	2.29061500	3.80937000
C	-3.90122500	2.13891500	1.55117600
H	-4.56557800	2.79204200	2.12766200
H	-3.35235400	2.76435700	0.84207100
C	-4.30887800	-0.99792500	-2.37243500
H	-3.75301400	-0.22213300	-2.90639100
H	-5.10480600	-1.35052000	-3.03743700
C	-2.69645700	-2.58546800	-3.47943000
H	-2.00049400	-3.42181600	-3.35184900
H	-3.46903100	-2.89329000	-4.19209900
H	-2.14711100	-1.74158400	-3.90491900
C	-4.10312000	-3.40709800	-1.56569100
H	-4.89830400	-3.70098300	-2.25921700
H	-3.43315900	-4.26086600	-1.43236300
H	-4.55555200	-3.18043300	-0.59825500
C	4.20830800	-2.75565500	-0.04065300
C	3.73095000	-2.27541100	1.18531600
C	5.35908200	-2.16875000	-0.58431700
C	4.35436700	-1.21968800	1.86259100
H	2.84466400	-2.72714500	1.61714000
C	6.00196000	-1.12436900	0.08288200
H	5.75890800	-2.53924300	-1.52419400
C	5.50221600	-0.64879300	1.29670500
H	6.90159600	-0.68572800	-0.34028100
H	6.01264400	0.15852800	1.81481600
C	-4.90586400	-0.41263400	-1.11310500
C	-4.22107600	0.58827800	-0.41135500
C	-6.12792000	-0.87151700	-0.60280900
C	-4.71004200	1.11180000	0.79295100
H	-3.28012900	0.96005100	-0.80123300

C	-6.64008300	-0.34560500	0.58444300
H	-6.68259000	-1.63479000	-1.14180200
C	-5.93404600	0.63594100	1.28205300
H	-7.59450600	-0.69898100	0.96516600
H	-6.33839200	1.04194500	2.20531100
C	2.88002300	3.96356200	-0.54043100
C	2.19397700	4.95047700	0.42100000
C	0.67374600	4.76470000	0.12556000
H	2.60316300	4.58977000	-1.98109900
H	3.93571700	3.72464200	-0.48051000
H	2.40641900	4.69642800	1.46605400
H	2.50077900	5.98661800	0.25997400
H	0.05291300	4.77340500	1.02189500
H	0.29289000	5.51314200	-0.57597700
N	0.64817500	3.43730500	-0.50668900
C	-0.28065400	2.73877200	-1.28055100
O	-1.43154200	3.12788900	-1.51103600
C	0.44010800	1.54044100	-1.71365400
H	0.29204200	1.20170900	-2.73646200
C	1.90840900	3.01355200	-0.81756900
O	1.87458400	1.90784700	-1.54334900
O	-0.29878600	5.26568300	-2.99687500
H	-0.85719800	4.60812400	-2.52881100
H	-0.67939900	5.35588800	-3.88399200
O	2.72727500	2.65333000	-4.18638300
H	2.69945900	2.05785600	-3.41651400
H	2.02770000	2.33504400	-4.77896000
O	2.28270200	4.91614900	-3.01027500
H	1.27636200	5.06850600	-3.00396900
H	2.45480700	4.09351500	-3.58213200

13s

Rh	-0.04734700	-0.02908700	-0.33206700
O	1.21577600	-1.30162100	-1.32593000
O	-1.56242500	-0.70898600	-1.54888600
O	-1.32571700	1.12686100	0.78417000
O	1.42319700	0.53245200	0.97713200
Rh	-0.57741100	-1.86356800	1.19343800
C	1.58048300	-0.11204800	2.06314000
O	0.93177900	-1.14878300	2.41211700
C	-1.94607800	0.62344300	1.77634000
O	-1.86202200	-0.58025000	2.16867700
C	1.34148600	-2.50023000	-0.91734200
O	0.74586100	-3.00813000	0.08409700

O	-2.07530600	-2.38920600	-0.11913800
C	-2.25007700	-1.72074000	-1.18319500
C	2.29970900	-3.41264700	-1.69624100
C	2.65544500	0.39572000	3.03323400
C	-2.86051700	1.58666100	2.54382800
C	-3.37383600	-2.14880800	-2.13673000
C	3.43554800	-3.87227500	-0.72881300
H	4.13862700	-4.46986800	-1.31942500
H	2.99261200	-4.53361100	0.02137300
C	2.88465300	-2.68698800	-2.91373300
H	3.56061700	-3.36061200	-3.45137800
H	2.09153300	-2.37905400	-3.60126700
H	3.44396400	-1.79593100	-2.62292100
C	1.51576300	-4.65439000	-2.16123800
H	2.18273000	-5.33846900	-2.69669900
H	1.08097400	-5.18646500	-1.31154700
H	0.70506800	-4.37069900	-2.84135800
C	3.74283600	-0.71456600	3.17857400
H	4.53948000	-0.30675000	3.81040600
H	3.29548900	-1.55529400	3.71652400
C	1.99964400	0.63064200	4.40663800
H	2.75290600	0.96609700	5.12755000
H	1.22617200	1.40385300	4.33997200
H	1.53794700	-0.28460900	4.78498300
C	3.27472500	1.70358500	2.52731200
H	2.51299600	2.48265400	2.43774200
H	4.03596800	2.04729600	3.23614500
H	3.74117800	1.57839500	1.54958400
C	-3.58417200	0.86703800	3.68691300
H	-4.23696100	1.57361400	4.21062500
H	-4.19439700	0.03898600	3.32095000
H	-2.86827100	0.46367300	4.40840900
C	-1.97915300	2.71627400	3.11356800
H	-1.45533000	3.24403000	2.31243700
H	-2.59978300	3.43548800	3.65875200
H	-1.23312200	2.31552200	3.80876300
C	-3.87595500	2.20959100	1.53625800
H	-4.53149700	2.87658200	2.10707100
H	-3.31030400	2.82246000	0.82925700
C	-4.31597200	-0.92917600	-2.38147200
H	-3.74439500	-0.16350600	-2.91353200
H	-5.11393100	-1.26946000	-3.05050300
C	-2.72755600	-2.54693200	-3.47867800
H	-2.04649100	-3.39473100	-3.34631400

H	-3.50289800	-2.84367500	-4.19310300
H	-2.16223900	-1.71396600	-3.90483500
C	-4.15463500	-3.33857800	-1.56779100
H	-4.95294300	-3.61973500	-2.26306500
H	-3.50055300	-4.20390000	-1.43033300
H	-4.60578900	-3.10162700	-0.60223300
C	4.16424200	-2.74618700	-0.03191200
C	3.70216700	-2.27844600	1.20444900
C	5.28703500	-2.12952600	-0.60066700
C	4.31410100	-1.20855600	1.86978800
H	2.83623400	-2.75188300	1.65448600
C	5.91679000	-1.06854200	0.05264900
H	5.67616100	-2.48994100	-1.54887900
C	5.43303900	-0.60722600	1.27845100
H	6.79477900	-0.60621300	-0.39034900
H	5.93431200	0.21261500	1.78566100
C	-4.91070600	-0.33109300	-1.12696300
C	-4.21222000	0.65857000	-0.42303400
C	-6.14479500	-0.76506100	-0.62398200
C	-4.69946300	1.19606700	0.77566100
H	-3.26070000	1.00903300	-0.80619600
C	-6.65532000	-0.22516800	0.55779200
H	-6.70975500	-1.51987600	-1.16418400
C	-5.93608900	0.74563700	1.25705100
H	-7.61892500	-0.55915400	0.93287700
H	-6.33941000	1.16291500	2.17574000
C	3.08539500	3.79786100	-0.55009000
C	2.47585700	4.89095700	0.33274600
C	0.94014200	4.77734700	0.06935400
H	2.57867300	4.52249200	-2.31678500
H	4.14127900	3.57734000	-0.62377700
H	2.69178900	4.70743100	1.39265300
H	2.84095200	5.89322900	0.09339000
H	0.34065800	4.84944100	0.97736400
H	0.58745400	5.53022900	-0.64354100
N	0.82466500	3.43829800	-0.52208800
C	-0.14580600	2.77751700	-1.24509500
O	-1.28734100	3.21712800	-1.46700400
C	0.48886900	1.52682200	-1.68180800
H	0.29049100	1.21949900	-2.70803600
C	2.07455900	2.94150600	-0.85195800
O	1.95126900	1.80859000	-1.55456500
O	-0.25648200	5.18854200	-3.04644200
H	-0.78655800	4.55467700	-2.49961200

H	-0.70830300	5.26502600	-3.90182900
O	2.67282200	2.38329800	-4.17553700
H	2.61814500	1.86886000	-3.34513100
H	2.01880700	1.98883700	-4.77515800
O	2.18986100	4.67589300	-3.23966400
H	1.15850700	4.88149900	-3.16469300
H	2.34654600	3.77398200	-3.73336100

12_Cu

Cu	-0.07640900	-1.16730500	0.39030800
N	-1.39812500	-1.85996700	1.72707100
N	-0.20946700	0.92370600	0.72069500
N	-1.03553500	-1.40919700	-1.32425200
C	-2.43464900	-1.94173400	2.23805800
C	-0.75148700	1.94713700	0.66695500
C	-1.80360500	-1.31176600	-2.18510600
C	-1.42581800	3.23113000	0.60128100
H	-1.12025100	3.75657700	-0.30798600
H	-2.50693000	3.07103900	0.57213600
H	-1.15854300	3.83329300	1.47418500
C	-3.75641900	-1.99903700	2.83338100
H	-4.38709600	-1.27375600	2.31185400
H	-4.17580500	-3.00248300	2.71905600
H	-3.70262000	-1.74706000	3.89606700
C	-2.79251400	-1.16879300	-3.23698000
H	-2.42591800	-0.46552100	-3.99006800
H	-2.97951800	-2.13763200	-3.70820300
H	-3.71405500	-0.77689900	-2.79760200
B	-3.97383700	1.00550300	-0.54571600
F	-3.64184200	0.14185000	0.51831500
F	-2.82435200	1.26812800	-1.31966900
F	-4.94947400	0.39945800	-1.35728300
F	-4.46204100	2.21794900	-0.02367900
C	3.19172300	1.95027400	1.53375100
C	3.19207700	2.73187900	0.18579400
C	3.24366000	1.65822700	-0.93641900
H	4.19833400	1.83854300	1.95100600
H	2.54078300	2.38226300	2.29616900
H	2.26484000	3.30246600	0.09870000
H	4.03128200	3.42404300	0.11618000
H	2.60264300	1.89129200	-1.78731500
H	4.25635500	1.45284200	-1.29015300
N	2.73756300	0.47714200	-0.23140600
C	2.44061200	-0.88313100	-0.57410500

O	2.57554900	-1.34548800	-1.71713900
C	1.98625100	-1.42535500	0.67413900
H	2.18973600	-2.43888900	0.99688500
C	2.73416500	0.61678500	1.07796200
O	2.36128300	-0.45553400	1.70149700
O	5.23821900	-0.72855800	-2.07814900
H	4.29501500	-0.99558900	-2.13969000
H	5.74066700	-1.50143600	-2.37385300
O	5.42168500	-0.41516200	0.68771700
H	5.44628200	-0.53890000	-0.28607600
H	5.21030100	-1.29389000	1.03077300

13_Cu

H	-2.91502600	2.68588400	-0.92859400
C	-2.35523800	-2.27980900	0.57083700
C	-2.97219200	-2.62430500	-0.80248100
C	-3.16742300	-1.23993600	-1.48724300
H	-2.33288400	-3.01408100	1.36957500
H	-2.34538100	-3.27705800	-1.41341800
H	-3.94920500	-3.11247900	-0.68261100
H	-2.28675900	-0.94805700	-2.06609200
H	-4.05424500	-1.18708500	-2.11934300
N	-3.29814900	-0.36076800	-0.31880800
C	-3.25418600	1.01265700	-0.09035700
O	-3.48429300	1.86320800	-1.08141900
C	-2.95483300	1.17975400	1.22536700
H	-2.98583800	2.01967500	1.89702600
C	-2.80288200	-0.97797900	0.79298300
O	-2.74065600	-0.10455400	1.80571800
O	-1.78649100	3.76170300	-0.68707600
H	-2.08334900	4.60001200	-0.30401400
H	-1.11323800	3.39059700	-0.05475200
O	-0.10227800	2.55597500	1.00480600
H	0.75217600	2.25246500	0.64275000
H	-0.62037500	1.74585300	1.13548600
Cu	-0.35965700	-1.51935700	0.31423500
N	-0.21486900	0.01822000	-1.02344300
N	0.46995600	-0.60806400	1.95074100
N	1.20672600	-2.60056400	-0.34328400
C	0.07237700	0.89833500	-1.71838000
C	1.21713700	0.05462000	2.53815500
C	2.29237700	-2.67485400	-0.74338300
C	2.16550700	0.90629500	3.23117300
H	3.16439300	0.69241800	2.84478800

H	1.91675100	1.95178200	3.03169300
H	2.12872200	0.71883100	4.30741300
C	0.44503000	2.01835400	-2.56168900
H	1.51845800	2.18546500	-2.45327600
H	0.21216000	1.79112800	-3.60577700
H	-0.11004600	2.90871900	-2.25157900
C	3.64939100	-2.71582000	-1.25507900
H	4.35210500	-2.82353800	-0.42492300
H	3.76771800	-3.55368500	-1.94731600
H	3.84312200	-1.77016800	-1.76743900
B	3.36660100	0.86309400	-0.31438500
F	2.35984200	1.77246500	0.14092600
F	3.43191200	-0.22233100	0.57505800
F	3.00955900	0.40646300	-1.59657800
F	4.58663200	1.53150500	-0.35746900

TS9_Cu

H	-2.39644900	2.99260000	-0.87253400
C	-2.39150900	-2.26023300	0.55258800
C	-3.05908400	-2.55361500	-0.80525100
C	-3.22948800	-1.14763100	-1.45463800
H	-2.33589400	-3.01207400	1.33232700
H	-2.47251400	-3.21375800	-1.44803800
H	-4.04563600	-3.01609600	-0.66564400
H	-2.38271400	-0.89116300	-2.09633500
H	-4.15621800	-1.04021300	-2.01951500
N	-3.22957900	-0.27383200	-0.27677200
C	-3.09999100	1.08739500	-0.06185200
O	-3.28263700	1.95113900	-0.97794900
C	-2.65514600	1.23326900	1.28039700
H	-3.09863500	1.95279200	1.96027100
C	-2.74157100	-0.94351300	0.82104100
O	-2.61607700	-0.11364700	1.84922400
O	-1.56550300	3.68670600	-0.77873900
H	-1.89907800	4.55289200	-0.49362100
H	-0.85808200	3.22176200	0.04489200
O	-0.28249900	2.58613400	0.93772700
H	0.52085000	2.11978800	0.62325700
H	-1.03566400	1.90278200	1.14568500
Cu	-0.36318700	-1.54859200	0.25505200
N	-0.21901300	-0.05270900	-1.12496100
N	0.43581600	-0.66032300	1.90848700
N	1.20779700	-2.63677500	-0.37400900
C	0.10317600	0.77990700	-1.86166500

C	1.12831700	0.02601500	2.53327000
C	2.31394400	-2.69750800	-0.71661200
C	2.01035800	0.90779400	3.27504000
H	3.03069900	0.75178600	2.91787500
H	1.71912300	1.94596600	3.09452500
H	1.94954200	0.69299600	4.34513000
C	0.53122900	1.83252500	-2.76365200
H	1.62297000	1.83030000	-2.79281400
H	0.13046600	1.65184000	-3.76494700
H	0.16780100	2.79731200	-2.39927100
C	3.69740500	-2.71754400	-1.15314500
H	4.35438400	-2.83226900	-0.28711700
H	3.86244400	-3.54337100	-1.85026200
H	3.90946600	-1.76234700	-1.63987700
B	3.26132300	0.89603900	-0.23619400
F	2.12489200	1.67331700	0.16519000
F	3.41454300	-0.17649100	0.65491500
F	3.02952700	0.40427700	-1.53485500
F	4.38677800	1.71324200	-0.21791200

14_Cu

H	-2.56657100	3.05772500	-1.04803800
C	-2.28159700	-2.39597900	0.69446600
C	-2.75288000	-2.85816900	-0.68608700
C	-3.15258600	-1.54126600	-1.42627300
H	-1.96751100	-3.05473400	1.49234900
H	-1.97916400	-3.39604400	-1.23969300
H	-3.61893100	-3.52525500	-0.59929200
H	-2.38882000	-1.22109300	-2.13843800
H	-4.11517000	-1.60942700	-1.93408200
N	-3.21868100	-0.56785800	-0.32863800
C	-3.28641600	0.77941800	-0.24439600
O	-3.55476000	1.57817400	-1.14205200
C	-2.93206100	1.09666400	1.20805900
H	-3.75205300	1.59228700	1.73262700
C	-2.68250400	-1.11172500	0.84205000
O	-2.68719200	-0.20087400	1.82769600
O	-1.86522300	3.74168800	-0.98087600
H	-2.32336300	4.56191500	-0.74898400
H	-0.69452900	3.22053300	0.30585400
O	-0.17150100	2.82987600	1.03666200
H	0.58509100	2.39591500	0.61324800
H	-2.01394000	1.69563300	1.26160800
Cu	-0.12792100	-1.35126100	0.30082900

N	-0.32419300	0.03389000	-1.11107700
N	0.44284300	-0.45986600	1.97682500
N	1.29385200	-2.61058800	-0.27523300
C	-0.02154400	0.93025600	-1.77890800
C	1.05098100	0.34362700	2.54780400
C	2.40330100	-2.72383300	-0.59395000
C	1.82705400	1.37197200	3.21201400
H	2.85509800	1.31588500	2.84611100
H	1.39957000	2.34741800	2.96402000
H	1.80877500	1.22318400	4.29489400
C	0.38353200	2.07179300	-2.57440400
H	1.32366000	2.44537800	-2.16154000
H	0.52885300	1.77303000	-3.61587300
H	-0.38174400	2.85085800	-2.50476800
C	3.79257900	-2.80333300	-1.00010000
H	4.43310600	-2.83303300	-0.11478600
H	3.96189200	-3.69697800	-1.60657600
H	4.01941400	-1.90423100	-1.57848600
B	3.26737300	0.83903600	-0.34139900
F	2.25483700	1.77873400	0.01316400
F	3.40309100	-0.09826200	0.69756200
F	2.87874200	0.18274300	-1.52634900
F	4.46829500	1.51855200	-0.54031400

TS8_N

Rh	0.01792900	-0.01593800	0.62826000
O	-1.26287800	-1.57507700	0.99149400
O	1.56067400	-1.21336500	1.27624200
O	1.29275800	1.50298300	0.09121200
O	-1.49690700	1.12824500	-0.15948900
Rh	0.37212600	-0.94435700	-1.59919900
C	-1.74607600	1.05411400	-1.40735300
O	-1.16807900	0.27972100	-2.23179900
C	1.83058900	1.50285600	-1.06476900
O	1.66609500	0.61568100	-1.95765400
C	-1.45656300	-2.45365300	0.09196500
O	-0.93475500	-2.45169500	-1.06774100
O	1.90954600	-2.04791900	-0.79763100
C	2.17461900	-1.95630700	0.43940300
C	-2.40826900	-3.61030100	0.42455400
C	-2.84302800	1.96753100	-1.96954200
C	2.74736300	2.69435700	-1.36972800
C	3.32185200	-2.80652000	1.00091300
C	-3.62032100	-3.54349000	-0.55694500

H	-4.31903800	-4.33306600	-0.25945200
H	-3.25604700	-3.78786100	-1.55889600
C	-2.88215000	-3.53307800	1.88049000
H	-3.56187500	-4.36670400	2.08755000
H	-2.03567000	-3.60276800	2.56958500
H	-3.40669600	-2.59861700	2.08728000
C	-1.66035000	-4.93682100	0.19223600
H	-2.32862200	-5.78104300	0.39241200
H	-1.30289700	-5.01215500	-0.83760600
H	-0.79832800	-5.02025600	0.86312700
C	-3.98440600	1.06614600	-2.53681100
H	-4.79330900	1.73202200	-2.85673700
H	-3.60288300	0.56015600	-3.42821700
C	-2.24294900	2.79352100	-3.12282500
H	-3.01342400	3.43754300	-3.56000600
H	-1.43088700	3.43447700	-2.76168900
H	-1.84481300	2.14470800	-3.90641500
C	-3.38018600	2.91146100	-0.88900500
H	-2.58185900	3.55504000	-0.51108600
H	-4.16272700	3.54886200	-1.31422800
H	-3.79841500	2.36467100	-0.04278500
C	3.33925500	2.58872600	-2.77896800
H	3.99068900	3.44862900	-2.96803000
H	3.92707400	1.67711500	-2.90299900
H	2.54907900	2.58557500	-3.53498600
C	1.90486500	3.98016300	-1.25186600
H	1.48194100	4.07772100	-0.24876700
H	2.53105900	4.85587800	-1.45312600
H	1.08355300	3.97692400	-1.97716300
C	3.87344300	2.74125800	-0.29004600
H	4.53231500	3.57760000	-0.54800100
H	3.40539600	2.97026200	0.67101800
C	4.35436200	-1.86240300	1.69164900
H	3.86913500	-1.40956800	2.56094800
H	5.16983800	-2.49409700	2.06065100
C	2.73256600	-3.75502900	2.06383000
H	1.98978100	-4.42512100	1.61736600
H	3.52875000	-4.37117600	2.49483400
H	2.25182800	-3.19392600	2.86931200
C	3.98864400	-3.62737100	-0.10887100
H	4.80868400	-4.21683600	0.31490300
H	3.27397800	-4.31588200	-0.56803000
H	4.39422600	-2.98927500	-0.89636300
C	-4.32694200	-2.20848900	-0.59777800

C	-3.91258500	-1.23210600	-1.51166300
C	-5.38196400	-1.90317100	0.27268100
C	-4.50707500	0.03477100	-1.56449100
H	-3.09834200	-1.45969300	-2.19105700
C	-5.99469400	-0.64946600	0.22687900
H	-5.73245000	-2.65360800	0.97565600
C	-5.55984400	0.31584200	-0.68359400
H	-6.82227300	-0.42802000	0.89536900
H	-6.04883500	1.28535700	-0.72286500
C	4.90457300	-0.77299800	0.80035200
C	4.23139600	0.45072000	0.69498900
C	6.06856800	-0.96363600	0.04332100
C	4.67262900	1.46523200	-0.16443400
H	3.33622600	0.61467700	1.28434100
C	6.53399700	0.04437600	-0.80291800
H	6.61563500	-1.89885300	0.12561400
C	5.83856200	1.25010400	-0.91139900
H	7.44430200	-0.10839600	-1.37624100
H	6.20687900	2.03214500	-1.56977500
C	-3.15635800	2.97572000	2.69222800
C	-2.65769400	4.38032000	2.35276600
C	-1.11791700	4.20536500	2.13275200
H	-1.86163800	2.91796800	3.73246100
H	-4.18885900	2.69162300	2.83684000
H	-3.13285900	4.74541700	1.43973200
H	-2.88225300	5.09271000	3.15305100
H	-0.86852000	4.12192400	1.07237800
H	-0.51646500	4.97993700	2.60449000
N	-0.87168800	2.89641800	2.77720300
C	0.23536500	1.96873600	2.82014600
O	1.39301400	2.31962400	2.94326800
C	-0.36276100	0.64340600	2.63362100
H	-0.06247200	-0.13941100	3.32628400
C	-2.09721900	2.10834900	2.66830100
O	-1.84801100	0.83509000	2.78343800

TS8_O

Rh	-0.03147900	0.09492800	0.69638900
O	1.20242100	1.70971400	0.91018600
O	-1.57909400	1.29624100	1.13812400
O	-1.24927000	-1.51025200	0.29735200
O	1.62656700	-1.18685400	-0.03928000
Rh	-0.31440700	0.76125400	-1.64627200
C	1.84484000	-1.25949000	-1.34583300

O	1.21413700	-0.53350000	-2.13087600
C	-1.77245900	-1.62935000	-0.86149400
O	-1.60548800	-0.82948100	-1.83286200
C	1.45618800	2.46262900	-0.08481100
O	0.99798700	2.31337200	-1.26233600
O	-1.84887800	1.95355100	-1.00921800
C	-2.15707400	1.97391900	0.21807200
C	2.41064800	3.63732500	0.16231100
C	2.89202600	-2.19942100	-1.94099200
C	-2.67025600	-2.85372900	-1.07184800
C	-3.30366500	2.87756500	0.68061300
C	3.70355400	3.40116600	-0.68259400
H	4.42196500	4.17436400	-0.38930500
H	3.45547800	3.56718400	-1.73470700
C	2.75101300	3.75896900	1.65303200
H	3.43573100	4.60049300	1.80237400
H	1.84966700	3.94228400	2.24484100
H	3.22349300	2.85342200	2.03679200
C	1.73542500	4.93336400	-0.32252100
H	2.41758300	5.77946600	-0.18857200
H	1.46658300	4.86712700	-1.37948900
H	0.82606400	5.13744200	0.25307500
C	4.10085600	-1.30395800	-2.38417700
H	4.92603800	-1.98543300	-2.61382400
H	3.82033700	-0.79962800	-3.31283700
C	2.27732200	-2.86008800	-3.19157500
H	3.03964300	-3.47373200	-3.68052200
H	1.44061900	-3.51064600	-2.91661500
H	1.91938900	-2.11343900	-3.90225400
C	3.35114200	-3.29753500	-0.98146900
H	2.50144200	-3.87826000	-0.61268700
H	4.01230600	-3.97880400	-1.52433900
H	3.90563500	-2.90454200	-0.13133300
C	-3.19926700	-2.90525500	-2.50941600
H	-3.83672300	-3.78718100	-2.63180500
H	-3.78543400	-2.01852400	-2.75721700
H	-2.37630200	-2.97627300	-3.22617500
C	-1.83246000	-4.11397100	-0.77941900
H	-1.45387600	-4.10199200	0.24539700
H	-2.44910000	-5.00898300	-0.91237800
H	-0.98042300	-4.18583800	-1.46495400
C	-3.84336300	-2.78597700	-0.04398500
H	-4.49728100	-3.64107700	-0.24633600
H	-3.42196000	-2.91822500	0.95591400

C	-4.36327600	2.00242000	1.42078300
H	-3.91271000	1.63693700	2.34766100
H	-5.18896800	2.66757400	1.69563100
C	-2.72660200	3.90200700	1.67868900
H	-1.96369500	4.52508600	1.19972900
H	-3.52651300	4.55883600	2.03565000
H	-2.27569800	3.40277200	2.54016600
C	-3.92869000	3.61158400	-0.51122400
H	-4.74935500	4.24437000	-0.15777500
H	-3.19231800	4.25101700	-1.00575300
H	-4.32392700	2.91557100	-1.25355500
C	4.31976300	2.02912600	-0.53713600
C	4.00203400	1.03016300	-1.46484400
C	5.19669100	1.70967000	0.50854300
C	4.52414900	-0.26586700	-1.37125600
H	3.32960300	1.26977700	-2.28264900
C	5.73016900	0.42370900	0.61593100
H	5.47653600	2.47251600	1.22898300
C	5.39825500	-0.56125800	-0.31672900
H	6.41993700	0.19212000	1.42268700
H	5.83399800	-1.55304800	-0.23738000
C	-4.88149600	0.83112400	0.61895800
C	-4.22454300	-0.40437400	0.68351800
C	-5.99556900	0.95412800	-0.22254700
C	-4.63284500	-1.49861700	-0.09008200
H	-3.37065600	-0.51689400	1.34268000
C	-6.42922700	-0.13280900	-0.98346200
H	-6.52984900	1.89885700	-0.27193000
C	-5.74991700	-1.35091800	-0.92307700
H	-7.30235700	-0.03161500	-1.62221600
H	-6.09260900	-2.19400300	-1.51659600
C	2.88020400	-2.41469000	2.07923000
C	2.49830800	-3.88461900	2.31077900
C	0.96672500	-3.82559700	2.58940400
H	3.90658900	-2.07224300	2.00965400
H	2.21501000	-1.78495900	0.72125500
H	2.72252300	-4.53369300	1.46267400
H	3.02164300	-4.29044500	3.18507800
H	0.37987700	-3.96814800	1.67576800
H	0.63277700	-4.53993700	3.34226400
N	0.79408100	-2.43905900	3.05156900
C	-0.32325500	-1.58011500	3.12162300
O	-1.47691000	-1.93149400	3.32544800
C	0.23490700	-0.25012500	2.80519100

H	-0.09299500	0.60719200	3.38661200
C	1.90491100	-1.70084800	2.74877700
O	1.70071900	-0.40794200	2.92500300

12_O

Rh	-0.01812500	0.11581800	0.67132000
O	1.18715700	1.74469400	0.93824800
O	-1.58429100	1.25590800	1.18790900
O	-1.19255900	-1.50210100	0.20158900
O	1.63476600	-1.06171900	-0.14746600
Rh	-0.34735600	0.86688900	-1.65791300
C	1.83124600	-1.15768400	-1.48068500
O	1.18283100	-0.42831800	-2.22841100
C	-1.74627500	-1.57995700	-0.94614400
O	-1.62809600	-0.73277800	-1.88455300
C	1.43517800	2.52050900	-0.04173100
O	0.96956400	2.40160800	-1.21954400
O	-1.87754200	2.00545100	-0.92797400
C	-2.17972400	1.96166600	0.30076400
C	2.40013200	3.68295800	0.22093800
C	2.87374700	-2.11863800	-2.02613900
C	-2.61945200	-2.81833700	-1.17672900
C	-3.34234500	2.81999900	0.80767400
C	3.69948700	3.42995500	-0.61095300
H	4.42657100	4.18973500	-0.30413100
H	3.46562500	3.60745900	-1.66439500
C	2.72171000	3.79862200	1.71617000
H	3.41859900	4.62824000	1.87554400
H	1.81467100	3.99863300	2.29395600
H	3.17142500	2.88529400	2.10816100
C	1.75160100	4.98963200	-0.27135200
H	2.44462600	5.82507200	-0.12673900
H	1.49658800	4.92888200	-1.33196600
H	0.83743100	5.20675300	0.29161000
C	4.12725500	-1.24691700	-2.39455400
H	4.94510300	-1.94862100	-2.58478700
H	3.90814600	-0.72981700	-3.33288400
C	2.31092800	-2.76209300	-3.30667500
H	3.08618200	-3.38706400	-3.75863800
H	1.44885900	-3.39640900	-3.07767600
H	2.00527400	-2.00533100	-4.03139400
C	3.24348600	-3.21638700	-1.02275000
H	2.36107600	-3.78178200	-0.70770500
H	3.93268000	-3.91317400	-1.50654700

H	3.74546000	-2.82512900	-0.13605300
C	-3.19314900	-2.83068700	-2.59746700
H	-3.81378100	-3.72268100	-2.73283900
H	-3.80717400	-1.94981500	-2.79355500
H	-2.39237600	-2.85571000	-3.34211000
C	-1.74158300	-4.06608800	-0.95580500
H	-1.33412800	-4.08213100	0.05815800
H	-2.33902300	-4.97156100	-1.10477200
H	-0.90831300	-4.09095400	-1.66741200
C	-3.75742800	-2.81816000	-0.10705000
H	-4.39278800	-3.68610100	-0.31405100
H	-3.29468600	-2.96632300	0.87221200
C	-4.36372600	1.89813600	1.54442100
H	-3.88394300	1.51562600	2.44943700
H	-5.19805000	2.53516100	1.85731600
C	-2.77212200	3.83457300	1.81991600
H	-2.03436700	4.48812900	1.34212400
H	-3.58127900	4.46202300	2.20749400
H	-2.29242400	3.32659400	2.66054700
C	-4.01002500	3.56662900	-0.35282600
H	-4.84452100	4.16234100	0.03133500
H	-3.30274400	4.24295000	-0.84049300
H	-4.39537700	2.87925500	-1.10837000
C	4.29478600	2.04800000	-0.47130500
C	4.00990500	1.07332000	-1.43510000
C	5.12224200	1.69572600	0.60408200
C	4.51604800	-0.23019100	-1.34644000
H	3.38103300	1.33995200	-2.27944500
C	5.63684400	0.40227700	0.70777500
H	5.37939600	2.43966200	1.35183500
C	5.33681100	-0.55897300	-0.25971300
H	6.28684800	0.14590600	1.53949500
H	5.75752700	-1.55733200	-0.18303300
C	-4.87359300	0.74064700	0.71744800
C	-4.18254400	-0.47801800	0.71910400
C	-6.01527500	0.86255900	-0.08632300
C	-4.58375100	-1.55379900	-0.08366400
H	-3.30746000	-0.59205700	1.34991900
C	-6.44206300	-0.20781800	-0.87416100
H	-6.57576200	1.79333300	-0.08530000
C	-5.72820700	-1.40749000	-0.87880500
H	-7.33632400	-0.10816800	-1.48325600
H	-6.06490500	-2.23761700	-1.49364900
C	3.00717100	-2.64690600	2.31043000

C	2.54424300	-4.09831700	2.40689300
C	0.99017100	-3.99734800	2.55896600
H	4.02806900	-2.31829800	2.18002400
H	2.19343000	-1.64900700	0.42767600
H	2.81366000	-4.69276100	1.52857400
H	2.98078600	-4.59874300	3.28075400
H	0.47531100	-4.19516300	1.61192600
H	0.59055400	-4.66778900	3.32121400
N	0.79714300	-2.59114900	2.92918400
C	-0.28785900	-1.72963700	2.97448900
O	-1.46165200	-2.04467700	3.14471400
C	0.30109100	-0.38493400	2.70555100
H	-0.02093000	0.43417500	3.34649500
C	1.96936900	-1.87939100	2.70448700
O	1.75558600	-0.56482200	2.85315800

13_O

Rh	-0.09415400	-0.06019100	0.65735500
O	-1.59062100	-1.35058600	1.18890700
O	1.26342200	-1.49624900	1.16236800
O	1.35429500	1.22279700	-0.01614300
O	-1.47467500	1.32209400	-0.00131800
Rh	-0.14711700	-1.01646900	-1.58112100
C	-1.88312700	1.33817900	-1.23188300
O	-1.51635500	0.48455400	-2.07412000
C	1.78052200	1.12688700	-1.21700400
O	1.37412600	0.28645200	-2.07515500
C	-2.03830400	-2.17069900	0.32119100
O	-1.64656400	-2.25456000	-0.88511600
O	1.22166600	-2.38521300	-0.92052900
C	1.63116200	-2.34380700	0.28052300
C	-3.14400700	-3.13793900	0.76109300
C	-2.86243700	2.42941500	-1.65590300
C	2.86624300	2.13236400	-1.61513600
C	2.64855700	-3.39400100	0.74065300
C	-4.40051100	-2.88801400	-0.13119400
H	-5.18862700	-3.55673000	0.23105700
H	-4.15467100	-3.19159800	-1.15268100
C	-3.48048800	-2.95375500	2.24525400
H	-4.27418400	-3.65311900	2.52847500
H	-2.60668000	-3.15706600	2.87052900
H	-3.82060500	-1.93924700	2.46164000
C	-2.64618800	-4.57604300	0.51728900
H	-3.42538200	-5.29067700	0.80226500

H	-2.39698700	-4.73389500	-0.53491000
H	-1.75569700	-4.78705000	1.11919600
C	-4.17869900	1.72999100	-2.12333900
H	-4.88730800	2.52589500	-2.37432100
H	-3.95907200	1.18123000	-3.04343800
C	-2.24386100	3.18356100	-2.84923200
H	-2.93892300	3.95502100	-3.19498700
H	-1.30866200	3.67317000	-2.55733400
H	-2.03545200	2.50433500	-3.67917500
C	-3.13925400	3.41178400	-0.51198700
H	-2.22607400	3.93910800	-0.22107700
H	-3.86173900	4.16149900	-0.84748500
H	-3.55538800	2.91469400	0.36738800
C	3.30572800	1.92128300	-3.06742300
H	4.08772200	2.64463500	-3.32116900
H	3.69955400	0.91604500	-3.22884700
H	2.46725500	2.06953500	-3.75366700
C	2.28118700	3.54879700	-1.44553200
H	1.95009500	3.71619200	-0.41838100
H	3.04072500	4.29703800	-1.69527500
H	1.42517700	3.69972700	-2.11245100
C	4.06971200	1.97252900	-0.63350000
H	4.84225800	2.67919500	-0.95525500
H	3.73428700	2.27822700	0.36145200
C	3.89120900	-2.65988900	1.33470400
H	3.57208800	-2.13758400	2.24046000
H	4.60703900	-3.43367100	1.63249700
C	1.98940800	-4.22883600	1.85713700
H	1.09645600	-4.74209400	1.48389200
H	2.69189100	-4.98831100	2.21617800
H	1.69825700	-3.59770400	2.70073200
C	3.05243000	-4.30884100	-0.42103100
H	3.78741900	-5.04090900	-0.07039200
H	2.18700500	-4.85229800	-0.80965100
H	3.49369100	-3.74484400	-1.24515400
C	-4.89047000	-1.45891200	-0.13876500
C	-4.39915400	-0.55908000	-1.09277300
C	-5.81218600	-0.99032200	0.80726900
C	-4.78150600	0.78837800	-1.10668500
H	-3.69758600	-0.91627700	-1.83899500
C	-6.21665800	0.34575900	0.79881500
H	-6.22317500	-1.67654500	1.54227300
C	-5.70220700	1.23298400	-0.14840400
H	-6.94225500	0.69515700	1.52806900

H	-6.02773800	2.26942500	-0.15512800
C	4.54723300	-1.67835900	0.39144500
C	4.10272600	-0.35043500	0.34447100
C	5.57806600	-2.07049100	-0.47315800
C	4.63591200	0.57379300	-0.56315200
H	3.32023000	-0.03357400	1.02524900
C	6.13823500	-1.15510900	-1.36582800
H	5.94881500	-3.09115500	-0.43827000
C	5.66665600	0.15769300	-1.41657600
H	6.94720300	-1.46482000	-2.02177100
H	6.10605900	0.86589900	-2.11368400
C	1.27761500	5.17649800	2.07262100
C	2.07245500	3.97303100	2.69033800
H	1.77682200	5.55284400	1.17392100
H	1.21498000	6.00866600	2.78160100
H	2.92193300	3.67323800	2.07202700
H	2.42837700	4.17963200	3.70171200
N	1.07486600	2.89596400	2.71137800
C	1.10770100	1.55229400	2.96802400
O	2.04725400	0.93063600	3.45616900
C	-0.18402800	0.96221700	2.50530000
H	-0.78674000	0.50528800	3.29019100
C	-0.10063400	3.34657000	2.14672600
O	-1.02311900	2.29854700	2.14127400
H	-1.39675300	2.09747100	1.16347500
C	-0.10495000	4.61580600	1.75208000
H	-0.92248700	5.16449100	1.30977300

TS9_O

Rh	0.00896600	-0.03105600	0.64238800
O	-1.21524900	-1.59320400	1.01216700
O	1.56000300	-1.18194600	1.34154100
O	1.25527200	1.48549300	0.02244500
O	-1.50645900	1.03393800	-0.19360400
Rh	0.47386000	-0.95928300	-1.53534800
C	-1.70636300	0.96044800	-1.44968500
O	-1.06620500	0.20247400	-2.24697800
C	1.84208000	1.48692000	-1.10738000
O	1.74514900	0.56819600	-1.97960300
C	-1.36612800	-2.49633900	0.12299800
O	-0.80810700	-2.47626000	-1.01828700
O	2.00161800	-2.03099400	-0.70413000
C	2.22349500	-1.92440400	0.54121200
C	-2.28595200	-3.67261100	0.44772100

C	-2.80631000	1.84530100	-2.03929100
C	2.71797400	2.70778300	-1.39279500
C	3.36613700	-2.73753300	1.15403600
C	-3.46846900	-3.65900700	-0.57357600
H	-4.14709300	-4.46669400	-0.28005600
H	-3.06690800	-3.90932200	-1.55971100
C	-2.80158100	-3.58101100	1.88868400
H	-3.46083600	-4.43135500	2.09044500
H	-1.97334300	-3.61362100	2.60213800
H	-3.36033800	-2.65982900	2.06226000
C	-1.48386900	-4.97519800	0.25933200
H	-2.13092500	-5.83510000	0.45951000
H	-1.09910100	-5.05914300	-0.76005000
H	-0.63833300	-5.01728700	0.95420900
C	-3.91362300	0.91238400	-2.62530400
H	-4.72830800	1.55978200	-2.96646000
H	-3.50216500	0.40979000	-3.50551400
C	-2.19632400	2.67860700	-3.18243900
H	-2.97192300	3.30556800	-3.63399500
H	-1.40532100	3.33619500	-2.80584300
H	-1.77155800	2.03713900	-3.95822000
C	-3.38403000	2.77972600	-0.96828600
H	-2.60878300	3.44379900	-0.57647100
H	-4.17113600	3.39623300	-1.41431600
H	-3.80626900	2.22568400	-0.12921100
C	3.34440400	2.61798600	-2.78788500
H	3.96771100	3.50083900	-2.96226400
H	3.96825200	1.72852700	-2.89649700
H	2.57200400	2.58691000	-3.56166900
C	1.82406600	3.96059000	-1.28976200
H	1.37974000	4.03815500	-0.29461600
H	2.42596700	4.85564400	-1.47762500
H	1.02094000	3.92939400	-2.03423700
C	3.81123900	2.79099200	-0.28005900
H	4.45733700	3.63803600	-0.53370700
H	3.30784200	3.02442200	0.66182500
C	4.36673700	-1.74719800	1.82967800
H	3.85969600	-1.28116500	2.67931700
H	5.18966500	-2.35038700	2.22708500
C	2.76780300	-3.65613500	2.23819600
H	2.04900800	-4.35743800	1.80097800
H	3.56727700	-4.23861100	2.70711000
H	2.25968100	-3.07570900	3.01232300
C	4.06687500	-3.58406700	0.08535600

H	4.88151200	-4.14935800	0.54922500
H	3.37093000	-4.29568500	-0.36735100
H	4.48543900	-2.96646100	-0.71143900
C	-4.21405100	-2.34744900	-0.65487600
C	-3.81049900	-1.37501900	-1.57785900
C	-5.29106400	-2.05711200	0.19302900
C	-4.43250500	-0.12257700	-1.65488800
H	-2.98607400	-1.59537300	-2.24797400
C	-5.93347900	-0.82015700	0.11923200
H	-5.63342700	-2.80552300	0.90185600
C	-5.50553900	0.14425000	-0.79494900
H	-6.77585500	-0.60935000	0.77209700
H	-6.01407000	1.10250200	-0.85152700
C	4.90230600	-0.67284300	0.91169500
C	4.20735800	0.53469900	0.76839200
C	6.07432500	-0.86163800	0.16712000
C	4.63361100	1.53454600	-0.11541400
H	3.30970700	0.69902400	1.35395400
C	6.52602100	0.13251500	-0.70257300
H	6.63913900	-1.78294000	0.27891700
C	5.80869900	1.32117300	-0.84850600
H	7.44372100	-0.01739800	-1.26449800
H	6.16798300	2.09272500	-1.52370300
C	-3.14609400	4.29958200	2.50318400
C	-1.60577500	4.29462500	2.36193500
H	-3.62001300	4.63254300	1.56935600
H	-3.48420500	4.98938800	3.28548100
H	-1.25186900	4.75882000	1.43900700
H	-1.10575200	4.78984100	3.20083500
N	-1.25141700	2.87304300	2.36372300
C	0.06523100	2.45385600	2.40864800
O	0.99590800	3.27062300	2.43877000
C	0.20272000	0.98942800	2.41521300
H	1.07917400	0.63597000	2.95951900
C	-2.37632200	2.07653800	2.66729300
O	-2.26493000	0.78804100	2.76773500
H	-1.05527400	0.56135600	2.58945600
C	-3.47711400	2.87727600	2.82375700
H	-4.45305700	2.50901000	3.10959900

16'

Rh	2.17830400	1.71120900	0.72726800
O	3.47791400	0.99844800	-0.69452500
O	1.54349000	3.13013900	-0.62815300

O	0.77624400	2.29937500	2.11657800
O	2.74014200	0.20998800	2.00398000
Rh	0.48762000	0.22465000	-0.20494800
C	2.11347600	-0.89156200	1.95192700
O	1.15298000	-1.15775400	1.15412600
C	-0.38133100	1.78100700	2.09101100
O	-0.78077000	0.91833000	1.24035200
C	3.07459900	0.13524700	-1.53012000
O	1.89457900	-0.35426200	-1.57474800
O	-0.03148100	1.74513200	-1.46338100
C	0.59849500	2.85522900	-1.42728200
C	4.04584800	-0.37236300	-2.60100900
C	2.49338100	-2.01519400	2.92186600
C	-1.38291200	2.22684600	3.16157300
C	0.17636100	3.93472500	-2.42874700
C	4.07614600	-1.93194000	-2.55671000
H	4.77720500	-2.26009600	-3.33152200
H	3.08326900	-2.29641800	-2.83337100
C	5.44653600	0.21187100	-2.38839900
H	6.12097800	-0.16954000	-3.16200300
H	5.42977800	1.30285000	-2.45651300
H	5.85294400	-0.06026400	-1.41220300
C	3.49441400	0.07100800	-3.97187700
H	4.15784500	-0.28149300	-4.76840100
H	2.49501400	-0.33673000	-4.14393200
H	3.43938400	1.16328200	-4.03444800
C	2.76173200	-3.31668100	2.10346100
H	3.03447800	-4.09628200	2.82274400
H	1.82229400	-3.61392500	1.63005600
C	1.27990200	-2.25707200	3.84396100
H	1.50727900	-3.06418200	4.54806800
H	1.04458500	-1.35743300	4.42296800
H	0.39564400	-2.53688400	3.26523500
C	3.71569800	-1.62600200	3.75982800
H	3.51121900	-0.73377000	4.35757600
H	3.96494200	-2.44546000	4.44193800
H	4.58687000	-1.42177200	3.13388300
C	-2.71477800	1.48147200	3.01477400
H	-3.41305400	1.83051500	3.78259900
H	-3.16595200	1.64746900	2.03507500
H	-2.57418100	0.40589500	3.14227000
C	-0.76815300	1.92516200	4.54217500
H	0.18362800	2.44597500	4.67292800
H	-1.45461800	2.24914200	5.33116400

H	-0.59400400	0.85049700	4.66330100
C	-1.58770400	3.76786300	3.02544600
H	-2.33776900	4.05816800	3.76869400
H	-0.64894600	4.25940200	3.29564200
C	-0.29224000	5.18851400	-1.62565600
H	0.57899400	5.60656500	-1.11338100
H	-0.63131300	5.92893800	-2.35773300
C	1.41319600	4.31464500	-3.26643300
H	1.77719500	3.45205600	-3.83478400
H	1.14786900	5.10326800	-3.97797200
H	2.22476900	4.67742500	-2.63081500
C	-0.93676600	3.42615300	-3.35251200
H	-1.21459600	4.21916400	-4.05439300
H	-0.60027800	2.56005200	-3.92888000
H	-1.82715600	3.13201900	-2.79378200
C	4.47409200	-2.50979700	-1.21825200
C	3.50333900	-2.71944200	-0.23049000
C	5.80892700	-2.81152100	-0.91699100
C	3.83575000	-3.18178600	1.04925100
H	2.46669100	-2.50420800	-0.45628400
C	6.15537400	-3.29840100	0.34472800
H	6.57494800	-2.67217800	-1.67478400
C	5.17754300	-3.47582800	1.32535700
H	7.19125500	-3.54187500	0.56419100
H	5.45408400	-3.85217900	2.30636300
C	-1.38189400	4.91116100	-0.61627800
C	-1.04132600	4.54189300	0.69112000
C	-2.73915500	4.97889300	-0.95909000
C	-2.01243400	4.21899600	1.64740600
H	0.00612800	4.49467600	0.96833000
C	-3.72160900	4.67530200	-0.01456600
H	-3.02539800	5.28126700	-1.96246400
C	-3.36267700	4.29356100	1.27953100
H	-4.77142700	4.74540700	-0.28561900
H	-4.13220000	4.06618700	2.01180900
C	-2.81916600	0.49822700	-0.83595000
H	-2.15764300	1.32407700	-0.63208900
H	-3.88155800	0.69725100	-0.91617200
C	-2.31295200	-0.75458300	-1.00539800
C	-0.90118300	-0.99518300	-0.93370900
C	-0.45206700	-2.30115900	-1.46642600
O	-0.23038700	-2.44148600	-2.65766800
O	-0.27090300	-3.23896900	-0.53395300
C	0.23682000	-4.51045500	-0.99985700

H	0.21719800	-5.16487200	-0.12963700
H	-0.39888300	-4.90988400	-1.79225600
H	1.25933200	-4.39512500	-1.36494100
O	-3.09282400	-1.84533000	-1.26773900
Si	-4.51368000	-2.29320500	-0.42466000
C	-5.97972200	-1.29187200	-1.11777200
H	-6.02121000	-0.37636100	-0.50795100
C	-4.67739100	-4.14007600	-0.80705000
H	-5.65283200	-4.44900200	-0.40456000
C	-4.23829300	-1.85875600	1.40562200
H	-4.27928200	-0.76010000	1.44009200
C	-2.87011700	-2.27826000	1.97063000
H	-2.03634500	-1.86778900	1.39623000
H	-2.76054600	-1.92006900	3.00225600
H	-2.75212200	-3.36508500	1.99060900
C	-5.38293200	-2.38951000	2.28865800
H	-5.43632500	-3.48421800	2.26388900
H	-5.23096600	-2.09543000	3.33497400
H	-6.35880100	-2.00131800	1.97992900
C	-5.79350700	-0.86399500	-2.58524000
H	-6.62298800	-0.22054900	-2.90527600
H	-4.86330400	-0.31119900	-2.74597200
H	-5.77585400	-1.72870700	-3.25612200
C	-7.32201200	-2.02733400	-0.94559300
H	-7.51241400	-2.32212000	0.09120700
H	-8.15650900	-1.38967400	-1.26376100
H	-7.35526300	-2.93519200	-1.55804100
C	-4.69142400	-4.39059600	-2.32677700
H	-4.78590900	-5.46337500	-2.53811500
H	-5.52351900	-3.88385100	-2.82432500
H	-3.76295100	-4.04292800	-2.79350700
C	-3.59344300	-4.99718400	-0.13170500
H	-3.68303100	-4.98578300	0.95806400
H	-3.67201400	-6.04253600	-0.45758800
H	-2.58825300	-4.64670700	-0.38721500

20

Rh	-0.89061500	-0.55750000	-2.26734100
O	-1.34411700	-2.49037600	-1.72962500
O	-2.80380000	0.00982100	-1.83450800
O	-0.39083400	1.39057900	-2.64877900
O	1.03741000	-1.14334600	-2.58372700
Rh	-0.31136200	-0.13621200	0.03815500
C	1.79626500	-1.19838100	-1.57642000

O	1.55218900	-0.86612300	-0.38768900
C	-0.01000700	2.10423000	-1.67898700
O	0.21299900	1.76338600	-0.48991300
C	-1.21259900	-2.78589200	-0.51325300
O	-0.90109900	-2.03466900	0.45084700
O	-2.22659900	0.54521400	0.29647900
C	-3.03182700	0.41366600	-0.66235900
C	4.07597900	-0.59580800	-2.51751200
C	-5.15523400	-0.48674300	0.38852600
C	3.21909200	-1.71500600	-1.87284000
F	3.81055900	-2.13571100	-0.73242300
F	3.15160400	-2.75592700	-2.73626400
F	3.62214200	-0.38379500	-3.77279000
F	3.90278300	0.54271400	-1.79758300
C	5.59247900	-0.88595300	-2.59872500
F	6.18661500	0.08926200	-3.29543200
F	6.13182700	-0.93424300	-1.37644300
F	5.80047800	-2.05452300	-3.21878800
C	0.09728000	3.60677800	-1.99366200
F	0.80020200	4.24591200	-1.03173500
F	0.71180000	3.79397700	-3.18408500
C	-1.33024100	4.21789000	-2.06766700
C	-1.37977800	5.75790800	-1.92520000
F	-2.08292000	3.68097200	-1.06891400
F	-1.88400100	3.87781400	-3.25066400
F	-1.12848100	6.11614400	-0.66241300
F	-2.59630900	6.19571200	-2.26697100
F	-0.47095200	6.32218200	-2.73214800
C	-4.50335000	0.72406200	-0.32956600
C	-1.37181700	-4.26490800	-0.11879700
F	-4.57256900	1.81002500	0.47747300
F	-5.19810200	0.97471700	-1.46036200
F	-5.19859300	-1.51269200	-0.49518500
F	-4.38126600	-0.85395000	1.43853000
C	-6.58424100	-0.24261400	0.92781500
F	-6.55570900	0.66369900	1.91346200
F	-7.38813600	0.19576500	-0.04698800
F	-7.06967900	-1.39140000	1.41049400
F	-1.88754600	-4.97768200	-1.14478100
F	-2.19584300	-4.36973400	0.94963800
C	0.01633600	-4.85113900	0.25962700
F	0.92310800	-4.41049900	-0.65546500
F	0.37220700	-4.39023700	1.47717300
C	0.08063400	-6.39669000	0.28854600

F	1.23826200	-6.78131900	0.83617200
F	0.00234800	-6.89029200	-0.95085900
F	-0.93091600	-6.88097600	1.02150700
C	2.12385200	-1.09513700	4.06449600
H	1.59932300	-1.83846700	4.65367700
H	3.20544100	-1.11477100	4.08001300
C	1.44430900	-0.18452400	3.34443100
C	-0.03335200	-0.22127300	3.23657400
N	-0.61136900	-1.40399400	3.34898800
N	-1.09944800	-2.42279600	3.42940800
C	-0.93759700	0.94193800	3.21771400
O	-0.58146800	2.09904600	3.10683300
O	-2.22364200	0.55147700	3.34459100
C	-3.20451600	1.60614000	3.29395400
H	-4.16850400	1.10606700	3.22780700
H	-3.15102100	2.21082800	4.20298300
H	-3.04105700	2.23528100	2.42006800
O	1.98945400	0.82200500	2.63081700
Si	3.38137700	1.74209500	3.03215500
C	4.93109200	0.66696400	2.75981200
H	5.06515700	0.11226600	3.70034100
C	3.29699200	3.20650400	1.83785200
H	4.17270000	3.82812500	2.07738600
C	3.28673300	2.26041200	4.86352800
H	3.73415900	1.42735400	5.42442300
C	1.86389000	2.47157700	5.40806600
H	1.26768600	1.55741300	5.35664900
H	1.90577500	2.78158800	6.46081100
H	1.32340500	3.24522400	4.85644200
C	4.15182300	3.50957200	5.12450300
H	3.74869600	4.38823400	4.60917100
H	4.17475700	3.74349800	6.19650600
H	5.18853900	3.38167700	4.79687900
C	4.76694500	-0.36325600	1.62988800
H	5.65464400	-1.00534500	1.56117800
H	3.89958900	-1.00916000	1.78708000
H	4.64129100	0.11932800	0.65887700
C	6.20134800	1.51099900	2.54558100
H	6.38910800	2.20330400	3.37253600
H	7.08319200	0.86351500	2.45640200
H	6.14056200	2.10255400	1.62559600
C	3.41877900	2.76755900	0.36793000
H	3.34619600	3.63433800	-0.30116900
H	4.37227000	2.27347100	0.16566300

H	2.61521200	2.07895300	0.09612600
C	2.03265400	4.05605900	2.05587000
H	1.99667300	4.47845800	3.06487500
H	2.00241900	4.89319900	1.34676900
H	1.12750100	3.45939900	1.91897700

TS16

Rh	0.77101600	0.90561700	-2.13338300
O	1.09799800	2.82343100	-1.48032600
O	2.74170500	0.40531300	-1.81001400
O	0.42727500	-1.02791600	-2.66533600
O	-1.20804700	1.37604000	-2.26216700
Rh	0.32713200	0.25622300	0.20252300
C	-1.91726600	1.29586800	-1.22513400
O	-1.60431800	0.89906800	-0.06758100
C	0.13944900	-1.83535200	-1.74334800
O	-0.12171100	-1.60356900	-0.53164900
C	0.99065600	3.01941900	-0.24896500
O	0.83277000	2.17188300	0.68100800
O	2.28646600	-0.30108300	0.30678000
C	3.03662900	-0.05950400	-0.68468200
C	-4.13803000	0.68364600	-2.29556400
C	5.05038100	0.70475500	0.63916000
C	-3.38280600	1.72972000	-1.43653200
F	-4.01635200	1.87098400	-0.25007100
F	-3.40663400	2.91909500	-2.08270800
F	-3.69153300	0.75752100	-3.56574000
F	-3.85256900	-0.55367700	-1.80372600
C	-5.67619200	0.84509500	-2.32543500
F	-6.18657400	0.00899800	-3.23700800
F	-6.21173900	0.55951700	-1.13358800
F	-5.99564400	2.10219300	-2.65904200
C	0.23469700	-3.31981000	-2.14295600
F	-0.37706600	-4.10631100	-1.22974500
F	-0.33757300	-3.52407800	-3.34967900
C	1.73569200	-3.72097400	-2.22713900
C	2.00321700	-5.24063600	-2.12444100
F	2.40582900	-3.11464000	-1.20653000
F	2.24222500	-3.27571200	-3.39408300
F	1.78357600	-5.67314500	-0.87969600
F	3.27835600	-5.48691500	-2.44859700
F	1.20374200	-5.90340600	-2.97129900
C	4.52538700	-0.32804500	-0.39432900
C	0.94028100	4.47690000	0.24232300

F	4.67771200	-1.57518500	0.12198800
F	5.25611200	-0.23290000	-1.52365200
F	4.54940900	1.92558500	0.31101100
F	4.59833300	0.36948200	1.86910300
C	6.59013800	0.82413800	0.71621600
F	7.13112600	-0.39368400	0.86296000
F	7.07579600	1.39397500	-0.38856800
F	6.92014000	1.57547000	1.77359400
F	1.34038900	5.32214200	-0.73045000
F	1.74151300	4.63426800	1.32296800
C	-0.51970700	4.82088100	0.65024600
F	-1.35810300	4.30783200	-0.29159400
F	-0.79325200	4.23499700	1.83657300
C	-0.81891400	6.33246200	0.77895100
F	-2.02087500	6.49719300	1.34290600
F	-0.82014900	6.91384600	-0.42287700
F	0.10812900	6.91415600	1.55259400
C	-1.91262800	0.29887800	3.64647200
H	-1.37690500	1.09294300	4.14554800
H	-2.95074800	0.15426400	3.91890800
C	-1.35013500	-0.47977300	2.71194400
C	0.03546900	-0.38991100	2.14776400
N	0.76489500	1.05700900	3.17993100
N	1.28686700	2.02234700	3.31935100
C	0.99928800	-1.48952900	2.50448600
O	0.79401200	-2.61386500	2.10372400
O	2.07907200	-1.09402300	3.18413100
C	3.13223900	-2.07812500	3.29016700
H	3.88428400	-1.61981000	3.93027000
H	2.74666800	-2.99791800	3.73283300
H	3.53819400	-2.27494900	2.29703200
O	-1.94731600	-1.49263900	2.05804100
Si	-3.17402100	-2.56320300	2.60645000
C	-4.83215800	-1.62597500	2.60510400
H	-4.92932700	-1.19103500	3.61283600
C	-3.11547100	-3.94478500	1.32141500
H	-3.97442700	-4.59869300	1.53765400
C	-2.77125800	-3.11657700	4.38283600
H	-3.14955300	-2.31659500	5.03635400
C	-1.27156900	-3.28025600	4.68386700
H	-0.75234300	-2.31863000	4.63118800
H	-1.12778800	-3.67683100	5.69810400
H	-0.77857100	-3.96059300	3.98448200
C	-3.55331000	-4.39836300	4.73455200

H	-3.24066600	-5.24467400	4.11286500
H	-3.38000700	-4.68031000	5.78109300
H	-4.63423000	-4.27370600	4.60467900
C	-4.86853300	-0.47209100	1.58956700
H	-5.82077100	0.07028700	1.65428900
H	-4.06061800	0.24618000	1.74734900
H	-4.77491500	-0.83805100	0.56454900
C	-6.03210300	-2.56997100	2.39514500
H	-6.06529100	-3.38179300	3.13068000
H	-6.97631200	-2.01593400	2.47394700
H	-6.00590300	-3.02720000	1.39942400
C	-3.29332700	-3.37764500	-0.10092500
H	-3.24536800	-4.18382100	-0.84414700
H	-4.25387800	-2.86802600	-0.22539600
H	-2.49950500	-2.66312500	-0.33342100
C	-1.83090200	-4.78886900	1.41742700
H	-1.75581500	-5.30983000	2.37781900
H	-1.81642500	-5.55091000	0.62770500
H	-0.93994500	-4.16763100	1.29935200

21

Rh	1.50464100	0.79034900	-2.14842700
O	1.29491700	2.71280600	-1.44270600
O	3.25848200	0.60211600	-1.09211000
O	1.65219100	-1.18353600	-2.68446900
O	-0.35644000	0.90554900	-3.03732300
Rh	0.32962000	0.04940200	-0.09828100
C	-1.36035700	0.68996400	-2.32021400
O	-1.41661400	0.37882200	-1.09322100
C	1.14163900	-2.02499000	-1.90196700
O	0.43502100	-1.83692200	-0.87349300
C	0.73555700	2.87562500	-0.33379000
O	0.31844900	2.00742900	0.48878500
O	2.17285500	-0.21594900	0.73741600
C	3.18156100	0.18006400	0.08976900
C	-3.65906900	-0.38446000	-2.64900100
C	4.70144100	1.70709000	1.39499200
C	-2.74997300	0.83053000	-2.97266900
F	-3.34118500	1.95429000	-2.48646800
F	-2.63217500	0.95109200	-4.31289700
F	-2.91222900	-1.51617200	-2.73108200
F	-4.13273300	-0.25678700	-1.38938500
C	-4.87584900	-0.55073000	-3.59007300
F	-5.70762100	-1.46444100	-3.07568400

F	-5.52725700	0.61518300	-3.70331600
F	-4.48320800	-0.95540500	-4.80118900
C	1.51825200	-3.49301900	-2.17148200
F	0.63226600	-4.32847400	-1.58152100
F	1.54075700	-3.74439000	-3.49971000
C	2.93547700	-3.76525200	-1.59237200
C	3.28047300	-5.26128300	-1.40462700
F	3.03442800	-3.15941000	-0.37862600
F	3.84967800	-3.21334500	-2.41938200
F	2.58363500	-5.77311800	-0.38534600
F	4.58632900	-5.38628900	-1.14313100
F	2.99329900	-5.94252300	-2.52209200
C	4.48509100	0.24829100	0.90557500
C	0.42659900	4.32513500	0.08639800
F	4.41506600	-0.57414600	1.97987800
F	5.54222800	-0.11469300	0.14548400
F	5.12338100	2.44979600	0.34871600
F	3.50958900	2.20260900	1.82260600
C	5.72092000	1.86127200	2.54703200
F	5.22180900	1.35820800	3.68098400
F	6.85650900	1.21929200	2.24229700
F	5.98950300	3.15842900	2.72986000
F	1.13460900	5.19618200	-0.66708000
F	0.74521700	4.51080100	1.38903100
C	-1.08793600	4.61172000	-0.10178000
F	-1.48392200	4.06774800	-1.28335400
F	-1.77138100	4.01043000	0.89808400
C	-1.46759500	6.11142700	-0.11278500
F	-2.79721600	6.23113500	-0.02891800
F	-1.04989700	6.69020500	-1.24216500
F	-0.90767900	6.73086900	0.93505700
C	-2.49472200	0.88261600	1.64829100
H	-2.08412400	1.45562100	0.83298400
H	-3.40330600	1.24049700	2.11990700
C	-1.86079500	-0.24254100	2.09267900
C	-0.57568100	-0.58124000	1.57635500
C	0.16887900	-1.62698800	2.32138400
O	0.07498500	-2.79966500	2.00786800
O	0.95337700	-1.12365400	3.26697400
C	1.85815000	-2.05677500	3.91017800
H	2.47839100	-1.44776100	4.56557200
H	1.29237700	-2.78984100	4.48873200
H	2.46889500	-2.56073400	3.15900200
O	-2.33531200	-1.02758800	3.09079700

Si	-3.91930100	-1.69659600	3.19005900
C	-4.47507300	-2.02513900	1.40487200
H	-4.55955200	-1.02129600	0.96335500
C	-3.67602200	-3.20892300	4.29727700
H	-4.68602500	-3.58688700	4.51349100
C	-5.06027300	-0.39780600	3.98970900
H	-5.46750400	0.18582400	3.14987100
C	-4.32675900	0.58151300	4.92409000
H	-3.49160400	1.08839000	4.43132600
H	-5.01658900	1.35405100	5.28688500
H	-3.92185600	0.07031100	5.80333500
C	-6.24771300	-1.04773600	4.72529900
H	-5.90644800	-1.61917700	5.59535700
H	-6.94289800	-0.28151400	5.09062700
H	-6.81816300	-1.72919600	4.08604100
C	-3.48432000	-2.82123700	0.53839800
H	-3.79554400	-2.79533200	-0.51178600
H	-2.46357400	-2.43147200	0.58480000
H	-3.44210700	-3.87094000	0.84152800
C	-5.87778100	-2.65837700	1.35141300
H	-6.63036900	-2.03934700	1.84995500
H	-6.19888400	-2.78935300	0.31020900
H	-5.89082500	-3.64770700	1.82357600
C	-2.87670300	-4.33925600	3.62635300
H	-2.70573700	-5.15768600	4.33760200
H	-3.40483900	-4.75877800	2.76615000
H	-1.89736900	-3.99141200	3.28087600
C	-3.02332900	-2.81320100	5.63594400
H	-3.62512700	-2.09179700	6.19608500
H	-2.89142400	-3.69694900	6.27279400
H	-2.03336100	-2.37065600	5.47730300

21'

Rh	-1.59249100	0.43376500	-2.06472000
O	-3.27879900	-0.27621700	-1.11291900
O	-2.03985500	2.34934600	-1.47943700
O	0.20137200	1.10730300	-2.83214800
O	-1.08447400	-1.51455000	-2.48845300
Rh	-0.42997000	0.17599800	0.10807000
C	-0.50397500	-2.15466100	-1.58010400
O	-0.14249700	-1.76876700	-0.43241700
C	1.18795300	1.13203000	-2.05949900
O	1.27688500	0.73768800	-0.86088400
C	-3.18759600	-0.56087200	0.10561400

O	-2.22341900	-0.37604400	0.90475600
O	-0.87937900	2.13906500	0.46919000
C	-1.62408800	2.73747600	-0.36024200
C	1.40769500	-3.80009800	-1.88924400
C	-3.58705600	3.90510100	0.71508400
C	-0.13471200	-3.62387300	-1.86178200
F	-0.64361800	-4.41048400	-0.88080500
F	-0.64947600	-4.02045800	-3.04704200
F	1.95010600	-2.70670200	-2.49130300
F	1.86452500	-3.87282600	-0.62194600
C	1.89976300	-5.05537100	-2.64758900
F	3.20060700	-5.24233800	-2.39668100
F	1.21805900	-6.13259900	-2.23252600
F	1.73029500	-4.90645500	-3.96455200
C	2.47834700	1.79500900	-2.58154700
F	3.54546300	0.99169600	-2.35456100
F	2.38402600	2.02823200	-3.90952400
C	2.71161700	3.14468100	-1.84668000
C	3.63735700	4.13475800	-2.59274600
F	3.25649800	2.89912200	-0.63386600
F	1.50593200	3.74856600	-1.66524300
F	4.75556000	3.50492200	-2.97867700
F	3.96547800	5.13832200	-1.77165900
F	3.02009100	4.63649000	-3.66576800
C	-2.16941400	4.09795000	0.11346300
C	-4.36191700	-1.33459000	0.73340000
F	-1.35925300	4.62838700	1.05997500
F	-2.25168600	4.95785800	-0.92646400
F	-4.44263000	3.62167500	-0.29208700
F	-3.55205900	2.84631000	1.56528200
C	-4.13761500	5.12252900	1.49466300
F	-3.45759000	5.29071600	2.63338800
F	-4.03309600	6.23231900	0.75228400
F	-5.42611200	4.91314000	1.78529800
F	-5.44796600	-1.28653900	-0.07094000
F	-4.68437000	-0.80907800	1.93757200
C	-3.94300300	-2.81875600	0.93422900
F	-3.22781300	-3.21528700	-0.15442000
F	-3.14907400	-2.90368800	2.02322100
C	-5.11970100	-3.80703600	1.11041900
F	-4.64633900	-4.98804800	1.52340900
F	-5.76017200	-3.97849300	-0.04994600
F	-5.97989200	-3.33822800	2.02429200
C	1.92269900	1.88969900	1.87097800

H	1.19967900	2.36723500	1.22713400
H	2.74060200	2.48806000	2.25554800
C	1.77293400	0.58154500	2.22451900
C	0.62136100	-0.14238800	1.78974500
C	0.25531400	-1.34465100	2.57616800
O	-0.50559500	-1.22554600	3.52093900
O	0.76367000	-2.47492900	2.10783200
C	0.27439000	-3.70739800	2.69047700
H	0.79948500	-4.49949800	2.15984600
H	0.50220000	-3.74206800	3.75740800
H	-0.80229800	-3.78670700	2.53112600
O	2.64684900	-0.08600800	3.02289700
Si	4.33270200	-0.25854600	2.70057700
C	5.23435500	1.27043000	3.38923400
H	5.23434700	1.99696900	2.56204500
C	4.79984600	-1.83585300	3.63571900
H	5.89414500	-1.91184000	3.55653600
C	4.51071600	-0.30036600	0.80947800
H	4.14524300	0.68215700	0.47789300
C	3.65652500	-1.36376600	0.10071800
H	2.61808600	-1.37506200	0.43876600
H	3.64380100	-1.17914000	-0.97800300
H	4.05816000	-2.36840200	0.25685900
C	5.98169700	-0.40415100	0.36653200
H	6.44371400	-1.33581100	0.71398600
H	6.05117900	-0.39609600	-0.72874100
H	6.58634100	0.42902300	0.73723800
C	4.53211200	1.93086600	4.59010500
H	5.04159300	2.86254100	4.86642800
H	3.48469600	2.17192800	4.38605500
H	4.54712600	1.27983900	5.47018300
C	6.70362700	0.96451500	3.73985800
H	7.25455000	0.51535800	2.90760300
H	7.23182700	1.88311300	4.02463900
H	6.76978000	0.27587500	4.58924900
C	4.44201300	-1.71321100	5.12912900
H	4.72995500	-2.62470600	5.66792900
H	4.94962800	-0.87240400	5.61023900
H	3.36373900	-1.57583500	5.26845900
C	4.19090000	-3.11808900	3.04364600
H	4.56996000	-3.32802800	2.04039900
H	4.43456500	-3.98220900	3.67508700
H	3.10049200	-3.05222500	2.97954800

Rh	1.30367100	0.56554100	-2.62805400
O	3.05371100	1.01815700	-1.61539600
O	1.89546800	-1.40970900	-2.71203100
O	-0.54751200	0.07630100	-3.41049500
O	0.68762000	2.51349800	-2.34860900
Rh	0.32382900	0.06306500	-0.38674800
C	0.19230700	2.80327400	-1.23107800
O	-0.00560400	2.07571300	-0.22025300
C	-1.46740000	-0.20320300	-2.60164000
O	-1.46831300	-0.19393500	-1.33897100
C	3.06499600	0.87057600	-0.36932500
O	2.18842600	0.37770800	0.39694700
O	0.77862800	-1.89875100	-0.78710100
C	1.55271600	-2.14253000	-1.74907000
C	-1.85919700	4.27708600	-0.96461000
C	3.73892300	-3.26579100	-1.16573400
C	-0.30680700	4.24832900	-1.04164400
F	0.19145200	4.76297100	0.11104700
F	0.09733500	5.03124600	-2.07010100
F	-2.35097400	3.33698400	-1.81757400
F	-2.24715800	3.97040000	0.29068000
C	-2.49944100	5.63357700	-1.34010600
F	-3.79822500	5.61623400	-1.01658300
F	-1.89824000	6.62347900	-0.66420500
F	-2.38556400	5.86349100	-2.65184300
C	-2.79869800	-0.69690200	-3.20324800
F	-3.83374900	0.04082400	-2.72554600
F	-2.78428100	-0.59134000	-4.55239200
C	-3.03851500	-2.18301300	-2.82436900
C	-4.07912800	-2.91934900	-3.70017200
F	-3.45790900	-2.25708300	-1.54167500
F	-1.85598900	-2.84851900	-2.93358900
F	-5.20374300	-2.19467000	-3.77869500
F	-4.36481700	-4.10328100	-3.14355100
F	-3.60102100	-3.12661200	-4.93046000
C	2.27920000	-3.49706700	-1.67049800
C	4.27300400	1.45446300	0.38486900
F	1.64165100	-4.33264100	-0.80989400
F	2.33338300	-4.09437900	-2.88216600
F	4.52955800	-3.00600400	-2.22588700
F	3.76164100	-2.17971000	-0.34240600
C	4.34746600	-4.44600700	-0.37352800
F	3.76043000	-4.55178300	0.82717300

F	4.18197600	-5.59138600	-1.04629100
F	5.65476700	-4.23136300	-0.19201800
F	5.30759800	1.67930600	-0.45705300
F	4.68478000	0.59829300	1.35572300
C	3.86330600	2.79518000	1.05746400
F	3.09008400	3.49899000	0.18648700
F	3.13016700	2.52489800	2.15862000
C	5.04803900	3.69890100	1.47280700
F	4.59929000	4.69251300	2.24809400
F	5.63591600	4.22426000	0.39333700
F	5.94942400	2.98453100	2.16151900
C	-1.47282200	-2.60127900	1.12138900
H	-1.14155500	-2.51376300	0.09103200
H	-2.47542400	-3.03823900	1.13115400
C	-1.44227500	-1.25390800	1.79719800
C	-0.58967000	-0.27133700	1.47636800
C	-0.27139300	0.77821900	2.45990900
O	0.65800600	0.67396600	3.25525400
O	-1.01751500	1.89332300	2.36908900
C	-0.56331400	3.03443800	3.11771800
H	-1.17489800	3.86926600	2.77805500
H	-0.70182000	2.87729800	4.19045600
H	0.49135800	3.22742300	2.91024300
O	-2.24217800	-1.17534200	2.93327500
Si	-3.87428900	-0.64187900	2.87412300
C	-4.90066900	-2.14038300	3.45150400
H	-4.77720800	-2.91051900	2.67438100
C	-4.04358100	0.70659000	4.21807300
H	-4.95582600	0.42439500	4.76381600
C	-4.20802000	-0.22141900	1.03715700
H	-3.50027300	-0.88846500	0.52943900
C	-3.82998400	1.20154700	0.59239800
H	-2.83987700	1.49505200	0.93986600
H	-3.82990300	1.25641100	-0.50090800
H	-4.54956800	1.93999800	0.95873100
C	-5.60050500	-0.59193600	0.50099600
H	-6.38961300	0.03107100	0.93776800
H	-5.62841300	-0.43784000	-0.58531700
H	-5.85671500	-1.63961300	0.68685100
C	-4.37275900	-2.71113100	4.78022400
H	-4.89502100	-3.64051100	5.04245700
H	-3.30262900	-2.92696000	4.74864700
H	-4.54077800	-2.00604700	5.60258000
C	-6.40332400	-1.83802200	3.59588400

H	-6.85959800	-1.48694800	2.66808800
H	-6.94958900	-2.73598600	3.91305600
H	-6.57889700	-1.07177700	4.36008700
C	-2.87681400	0.63295700	5.22202400
H	-3.03154300	1.34898200	6.03990300
H	-2.77607600	-0.36126100	5.66833700
H	-1.92338200	0.87103200	4.74392100
C	-4.24437000	2.14854000	3.72755100
H	-5.13940900	2.24693000	3.10549600
H	-4.36172500	2.82856900	4.58204100
H	-3.39088400	2.49719700	3.14155000
C	0.71464500	-2.92040800	2.31029900
C	-0.43252200	-3.22868300	4.32800900
C	-0.53035300	-3.61138700	1.85796600
H	-0.10329700	-3.77923200	5.20909000
H	-1.06631800	-2.39029100	4.61495900
H	-0.28557200	-4.43015100	1.17807700
C	-1.06632100	-4.12559100	3.23312800
H	-2.15388200	-4.09053900	3.26887000
H	-0.74585700	-5.15908800	3.38075900
O	1.75970900	-2.50359900	1.67275200
C	2.62542600	-1.80926800	2.63730900
H	3.60573400	-2.28559000	2.60985000
H	2.66938500	-0.76336000	2.33199400
C	1.91257800	-1.98225900	3.97026200
O	2.23150500	-1.64248800	5.07690100
N	0.74109300	-2.69868400	3.61321300

TS17

Rh	1.26256000	0.24293100	-2.64487100
O	3.12748200	0.55363500	-1.83783800
O	1.58990600	-1.78855200	-2.61093900
O	-0.66118700	-0.10056900	-3.28347300
O	0.89450900	2.26472100	-2.48921600
Rh	0.40217700	0.03041400	-0.32436900
C	0.45045600	2.69152300	-1.39464000
O	0.19514600	2.06648200	-0.32964800
C	-1.54042700	-0.31271300	-2.41107700
O	-1.46399000	-0.23246100	-1.15378100
C	3.21611800	0.54482000	-0.58458500
O	2.33491100	0.30845900	0.28579200
O	0.67204300	-1.99577800	-0.53543600
C	1.24595300	-2.41401400	-1.57597200
C	-1.44152900	4.37770400	-1.27857600

C	3.07141300	-4.06283600	-0.89426400
C	0.10052400	4.19034600	-1.32364300
F	0.63539700	4.74007500	-0.20462700
F	0.59219400	4.84527700	-2.40182000
F	-2.01231600	3.43536500	-2.07877400
F	-1.87059000	4.19159700	-0.01317900
C	-1.94131200	5.76279000	-1.75121500
F	-3.23817700	5.89268500	-1.44670500
F	-1.25176300	6.73218200	-1.13273700
F	-1.79405700	5.89240300	-3.07312600
C	-2.89589800	-0.83628000	-2.92968800
F	-3.92414800	-0.14154800	-2.38464500
F	-2.96653400	-0.72132000	-4.27630700
C	-3.06046600	-2.33350700	-2.55082900
C	-4.12418800	-3.10033000	-3.37159800
F	-3.39991700	-2.42537400	-1.24469500
F	-1.86427000	-2.95774600	-2.73023200
F	-5.27182300	-2.40879700	-3.38871300
F	-4.34474400	-4.29216700	-2.80366000
F	-3.70526700	-3.29061800	-4.62567500
C	1.64232200	-3.90177200	-1.53240100
C	4.57951400	0.92885800	0.01912300
F	0.73519500	-4.59736400	-0.79290800
F	1.65851100	-4.42547600	-2.77420100
F	3.93006500	-4.50754100	-1.83257900
F	3.50700800	-2.84657200	-0.46116600
C	3.14897500	-5.02842500	0.31026300
F	2.38755100	-4.59100500	1.32330000
F	2.74489200	-6.25142900	-0.05012100
F	4.41721500	-5.09740500	0.73259000
F	5.52246800	1.02733400	-0.94543400
F	4.97268900	-0.01842200	0.91102400
C	4.46952200	2.28847700	0.76146900
F	3.67614600	3.11481500	0.02691500
F	3.88892700	2.08991900	1.96407300
C	5.82101700	3.00557800	0.99241800
F	5.65157700	4.01116200	1.85797400
F	6.29260900	3.49906400	-0.15677500
F	6.71262800	2.14215600	1.50040500
C	-1.64111300	-2.15184700	1.49756800
H	-1.51957100	-2.19704900	0.41712800
H	-2.59687900	-2.60840500	1.76030900
C	-1.55745000	-0.71258100	1.96344300
C	-0.43617800	-0.00781700	1.65394600

C	-0.07933000	1.20329300	2.41820500
O	0.96717400	1.31877800	3.04577700
O	-0.98014000	2.20027000	2.33297900
C	-0.59375700	3.45515800	2.91971200
H	-1.41710700	4.13971700	2.72071800
H	-0.44206200	3.35140400	3.99681900
H	0.32346100	3.82455200	2.45570300
O	-2.44862500	-0.30422500	2.88803400
Si	-4.12621800	0.04140000	2.71523400
C	-5.06964000	-1.52492500	3.24529100
H	-4.96515900	-2.23001800	2.40608100
C	-4.43561800	1.43866400	3.96855400
H	-5.42635600	1.22302500	4.39319100
C	-4.37944300	0.38622800	0.86552500
H	-3.89831100	-0.48099200	0.39010400
C	-3.65533400	1.63958300	0.34550500
H	-2.61623400	1.68641600	0.67033200
H	-3.66363500	1.64578500	-0.74821500
H	-4.15350700	2.55221700	0.68223800
C	-5.85051000	0.38288100	0.41679300
H	-6.43499700	1.16125400	0.92160600
H	-5.91579300	0.57736600	-0.66096700
H	-6.33912900	-0.57774200	0.60291700
C	-4.46334000	-2.18351000	4.49606900
H	-4.95126200	-3.14362300	4.70794600
H	-3.39272500	-2.36798600	4.38805300
H	-4.60075500	-1.55074500	5.38032400
C	-6.57229600	-1.27548300	3.47466300
H	-7.06625300	-0.80653300	2.61970200
H	-7.09284600	-2.21990800	3.67805500
H	-6.73283900	-0.62703100	4.34342300
C	-3.41351200	1.38740000	5.12060300
H	-3.65212400	2.14629900	5.87664600
H	-3.39822100	0.41506100	5.62284400
H	-2.40212100	1.58458300	4.75279100
C	-4.49072300	2.85273800	3.36896600
H	-5.28208700	2.95225800	2.61961300
H	-4.68626100	3.59342200	4.15544200
H	-3.54375800	3.11975700	2.89217800
C	0.64932900	-1.92324900	2.52439100
C	-0.41262500	-2.30429600	4.59354500
C	-0.47883200	-2.90210400	2.18495500
H	-0.05004800	-2.66933400	5.55484000
H	-1.19944700	-1.56627600	4.75702900

H	-0.09115800	-3.69428600	1.54433800
C	-0.82069300	-3.42845100	3.61430900
H	-1.87401300	-3.69539600	3.70070900
H	-0.22013400	-4.31684600	3.82650000
O	1.83520700	-1.81228100	1.96451600
C	2.73388400	-1.19034900	2.93106000
H	3.65167800	-1.77861900	2.96494300
H	2.92122000	-0.16594300	2.61425000
C	1.95954300	-1.23206400	4.24118700
O	2.32964700	-0.97261200	5.36283800
N	0.70090800	-1.69022900	3.85997600

23

Rh	1.99815100	-0.12507800	-2.21251500
O	0.51102900	-1.40967900	-2.80523400
O	0.72058400	1.42910200	-2.54903600
O	3.38249900	1.21133800	-1.49600500
O	3.24810100	-1.68637400	-1.72679400
Rh	1.11017600	-0.27665700	0.03442300
C	3.16203200	-2.15706600	-0.56436200
O	2.33281100	-1.87642600	0.34561600
C	3.29851300	1.52141900	-0.27778700
O	2.58276600	1.00612000	0.62053600
C	-0.33561000	-1.75010900	-1.93873300
O	-0.36483700	-1.48098100	-0.70533400
O	-0.06467800	1.33851100	-0.41598900
C	-0.02812400	1.77784900	-1.59513100
C	5.20085300	-2.44839800	0.89042500
C	-2.36165100	2.11768000	-2.49865600
C	4.25508600	-3.14786300	-0.12623900
F	3.69655400	-4.22599800	0.47315300
F	4.97704900	-3.56408200	-1.19056200
F	5.41514500	-1.17256500	0.46760000
F	4.59161100	-2.40509900	2.09498600
C	6.57853600	-3.12979500	1.06761200
F	7.20177600	-2.59984500	2.12551900
F	6.41339500	-4.44382100	1.27218200
F	7.33411900	-2.94498700	-0.01898200
C	4.09004300	2.77444000	0.13448700
F	4.14241600	2.87578100	1.48441300
F	5.34962000	2.72876000	-0.35167000
C	3.37631400	4.03302700	-0.44091500
C	3.70139900	5.35270100	0.29863800
F	2.02967600	3.83781500	-0.36800200

F	3.71783500	4.17027900	-1.73776500
F	3.09927000	5.37739300	1.49343000
F	3.26614100	6.38754400	-0.42632400
F	5.02505700	5.46499200	0.47018000
C	-1.09524900	2.82844800	-1.95513300
C	-1.53825000	-2.57692100	-2.43519500
F	-1.43287000	3.55579500	-0.86839700
F	-0.61953100	3.65944100	-2.91261700
F	-2.02404300	1.45958400	-3.63417300
F	-2.76978800	1.20882600	-1.57967200
C	-3.55348700	3.04892400	-2.82561700
F	-4.02791400	3.61084600	-1.70910900
F	-3.17368800	4.01157900	-3.67436700
F	-4.52573800	2.32918900	-3.40042300
F	-1.36897400	-2.92177900	-3.73061800
F	-2.65020900	-1.80120700	-2.33619200
C	-1.74359500	-3.86868000	-1.60651800
F	-0.53154900	-4.46206300	-1.45317800
F	-2.23172200	-3.55337700	-0.38645500
C	-2.70902800	-4.89843800	-2.24311600
F	-2.98903100	-5.85137400	-1.34734100
F	-2.15396400	-5.46368000	-3.31856300
F	-3.85046100	-4.29280700	-2.60260900
O	0.61276100	-0.58060300	2.19052800
C	-0.70396500	-0.60110800	2.82051400
C	1.61939800	-0.15820700	3.13268600
N	-0.40287500	-0.39799100	4.24042900
C	-1.66370200	0.38108400	2.21870000
C	-1.40275300	-1.99555300	2.74212900
C	0.93737200	-0.26381000	4.47969300
H	1.93901400	0.86206100	2.92108300
H	2.46823100	-0.84226900	3.07713200
C	-1.24481300	-1.28104500	5.05491900
C	-2.82975700	-0.24373700	1.89113900
C	-1.41744100	1.82195900	2.12284100
C	-2.82867900	-1.70788800	2.24138300
C	-1.32565000	-2.54543400	4.18119500
H	-0.86560800	-2.62256200	2.02905400
O	1.48885300	-0.25818700	5.56951200
H	-0.76905600	-1.43006400	6.02488300
H	-2.22610600	-0.82174300	5.20606100
O	-0.13610500	2.12161200	2.45756900
O	-2.22890800	2.67489700	1.80728300
H	-3.57588900	-1.89091000	3.02318500

H	-3.10959900	-2.31943300	1.38331200
H	-0.40736800	-3.12602200	4.31434900
H	-2.17600000	-3.18399400	4.43176000
C	0.24706600	3.49775700	2.31043100
H	-0.00862500	3.85986800	1.31424000
H	1.32567600	3.52168300	2.46002000
H	-0.25110200	4.11848700	3.06068800
O	-3.88197400	0.33755900	1.34184000
Si	-5.56556500	0.03844600	1.57364200
C	-5.90137700	0.10349100	3.44725600
H	-5.82630000	-0.93549400	3.80141400
C	-5.97864300	-1.68338900	0.88980500
C	-6.36078400	1.47400700	0.63980800
H	-7.42051000	1.47572500	0.93241200
C	-5.74131600	2.81595000	1.07443400
H	-4.66231700	2.83137600	0.89925400
H	-6.19340100	3.64578400	0.51642200
H	-5.90261000	3.00990000	2.13993600
C	-6.29356700	1.29661700	-0.88646000
H	-6.91404600	0.46143500	-1.22403700
H	-6.65009300	2.19996100	-1.39626000
H	-5.27275300	1.11059800	-1.22699700
C	-4.87725900	0.94134500	4.23393400
H	-5.13164900	0.94998600	5.30154200
H	-3.85998400	0.55142100	4.14277600
H	-4.85604000	1.98137100	3.89339000
C	-7.33236700	0.59374000	3.74167300
H	-7.54946500	0.52500600	4.81492900
H	-7.45831200	1.64232800	3.45071800
H	-8.09457300	0.01071900	3.21461100
C	-7.50021600	-1.91835500	0.84152900
H	-7.99449700	-1.21185000	0.16519100
H	-7.72300400	-2.92843700	0.47510800
H	-7.96773500	-1.81901800	1.82681900
H	-5.56403500	-2.38124800	1.63111900
C	-5.32650800	-2.00753200	-0.46586800
H	-5.80018600	-1.45232800	-1.28030900
H	-4.26249100	-1.76593400	-0.48537000
H	-5.42800800	-3.07473000	-0.69724200