Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.
This journal is © the Partner Organisations 2020

Supporting Information

The origin of regioselectivity in Cu-catalyzed hydrocarbonylative coupling of alkynes with alkyl halides

Shengnan Liu, Jianbiao Liu, Qiong Wang, Jin Wang, Fang Huang, Wenjuan Wang, Chuanzhi Sun and Dezhan Chen**

College of Chemistry, Chemical Engineering and Materials Science, Collaborative Innovation Center of Functionalized Probes for Chemical Imaging in Universities of Shandong, Institute of Molecular and Nano Science, Shandong Normal University, Jinan 250014, P. R. China

Table of Contents

I. Free energy profiles for formation of silyl radical…….…….S2

II. Frontier molecular orbitals of catalysis and substrates……..……..…..…..…….S2

III. Free energy profiles for the insertion of acyl bromide…….…….....S3

IV Results of RDG analysis…….…….……..……..……..……..….....S4

V. Free energy profiles for the C-C coupling…….……..……..……..……..…S4

VI. Free energy profiles for the other products……..……..……..……..…….....S5

VII. Results of 1,2- and 1,4-reduction analysis for terminal and internal alkynes..…….……...S9

VIII. Cartesian coordinates of all the structures…….…….……...…….. S12

I. Free energy profiles for formation of silyl radical

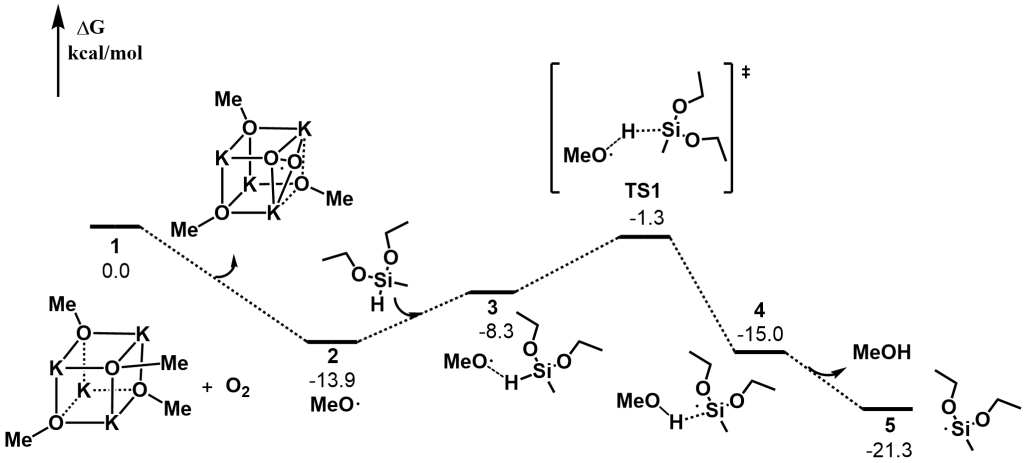

Fig. S1 Free energy profiles for the silyl radical generation.

II. Frontier molecular orbitals of catalysis and substrates

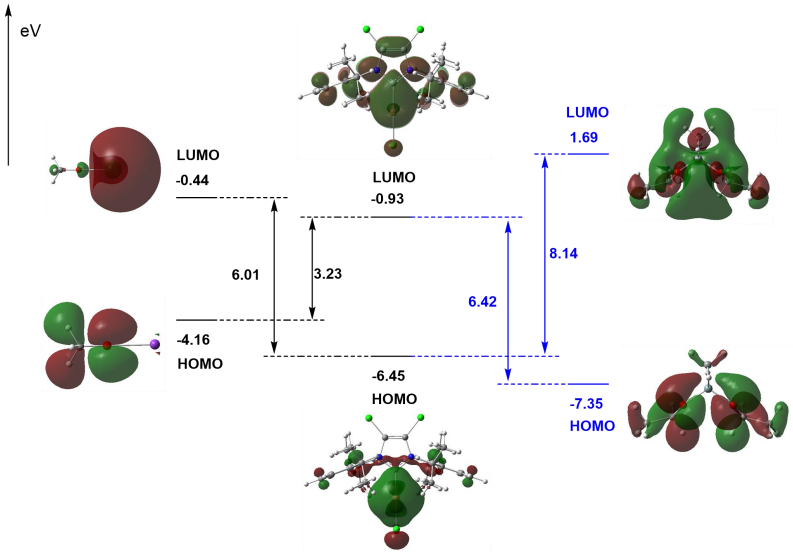

Fig. S2 Frontier molecular orbitals of $(EtO)_2MeSi\text{-}H$, K-OMe and ^{Cl}IPrCuCl.

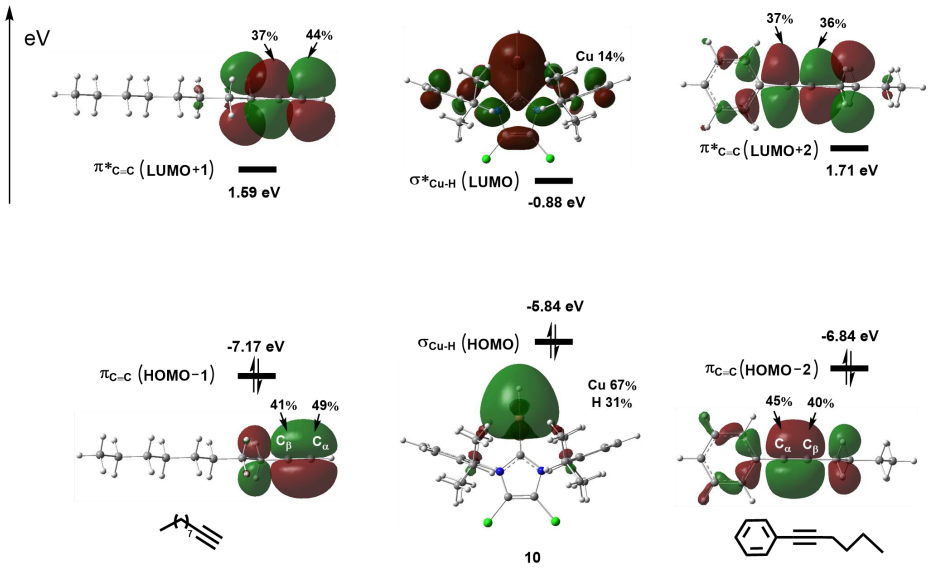

Fig. S3 Frontier molecular orbitals of ^{Cl}IPrCuH (**10**) and two alkyne substrates with spatial plots, atomic contributions/coefficients, and energies given in eV.

III. Free energy profiles for the insertion of acyl bromide

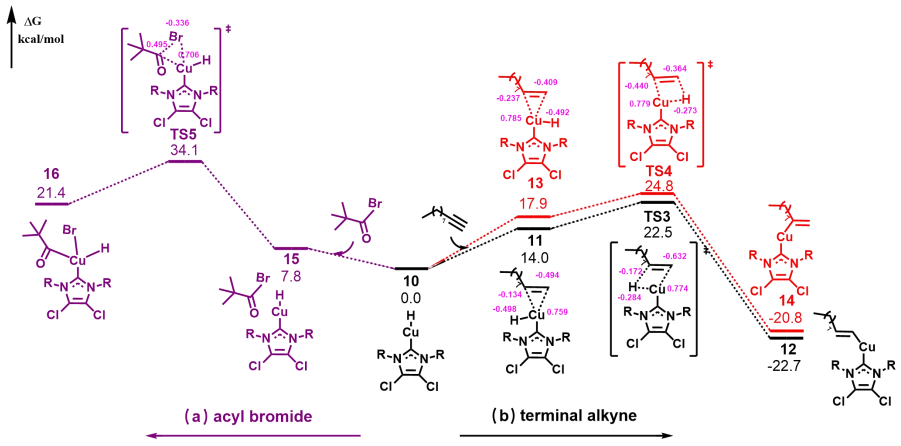

Fig. S4 Free energy profiles for the insertion of terminal alkyne and acyl bromide.

IV. Results of RDG analysis

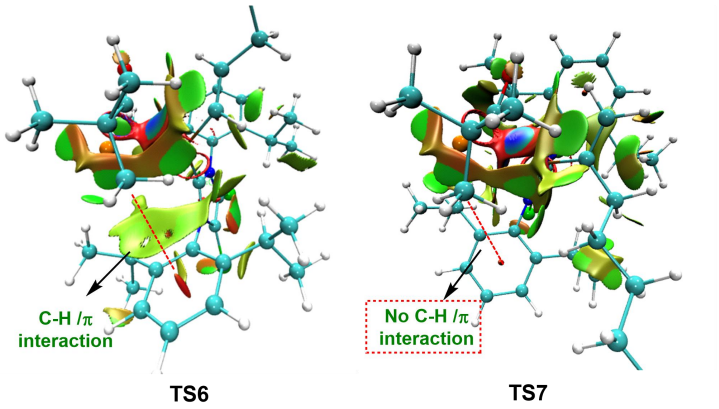

Fig. S5 Color-filled RDG isosurfaces of complexes **TS6** and **TS7** (red, steric effect; green, van der Waals interaction; blue, strong attraction).

V. Free energy profiles for the C-C coupling

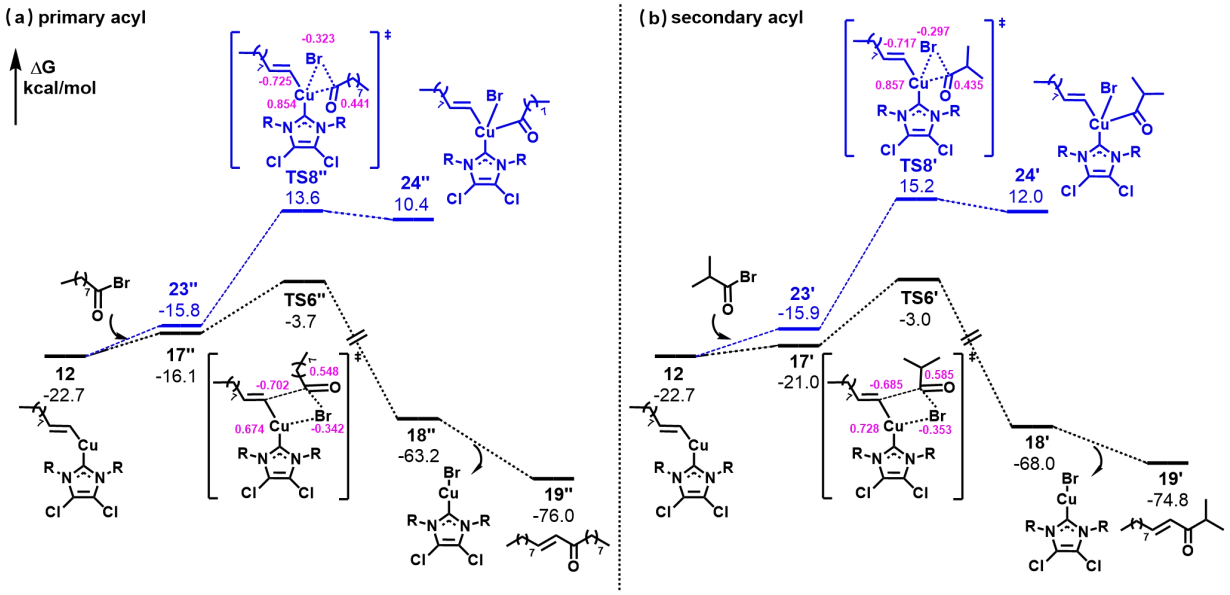

Fig. S6 Free energy profiles for the C-C coupling of acyl bromide with alkenylcopper of (a) primary acyl, (b) secondary acyl. The numbers in purple are selected NBO charges.

VI. Free energy profiles for the other products

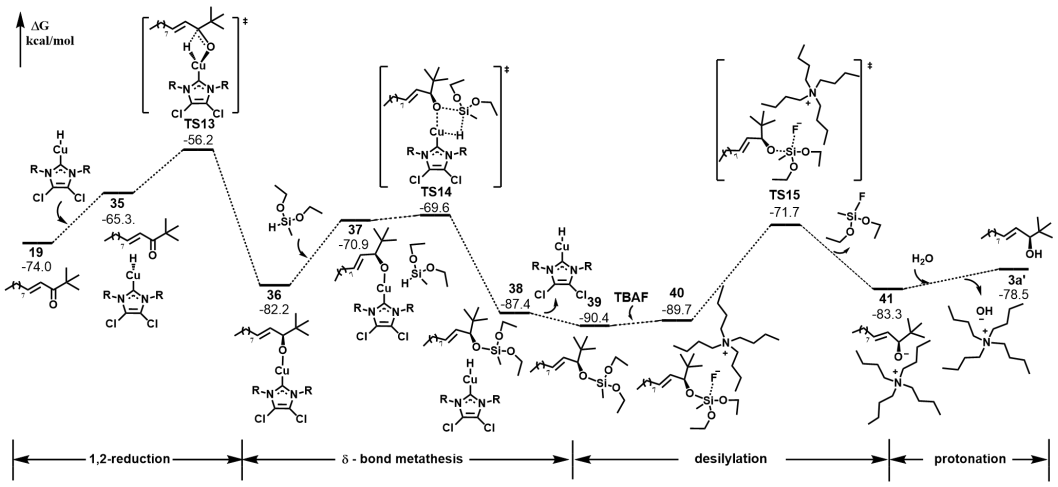

Fig. S7 Free energy profiles for the enantiomer **3a'** of **3a** for terminal alkyne.

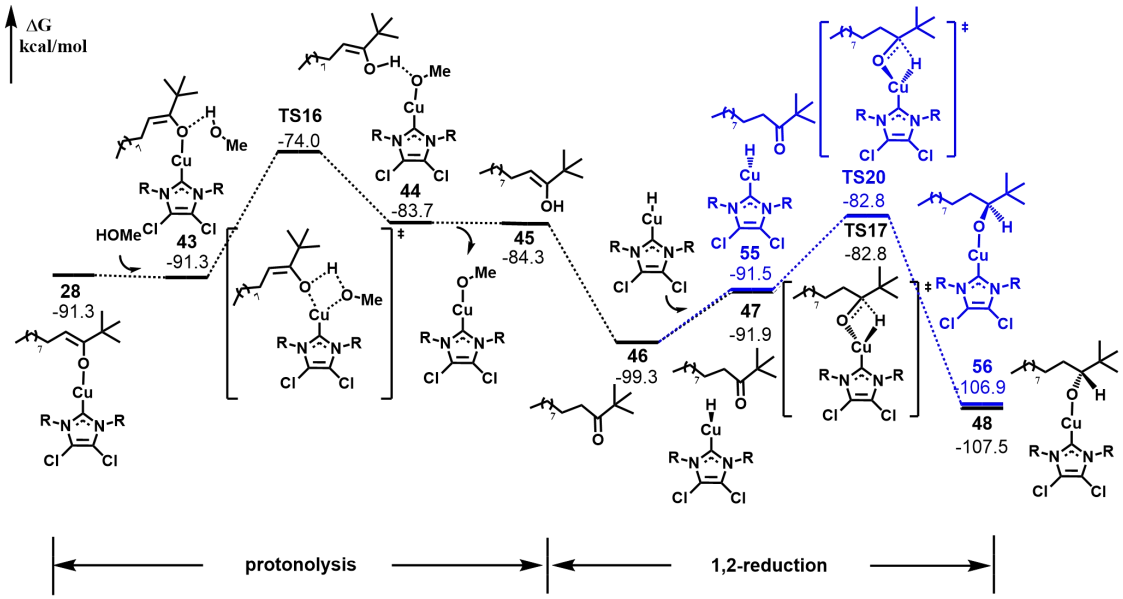

Fig. S8 Free energy profiles for the protonolysis and 1,2-reduction step of by-products for terminal alkyne.

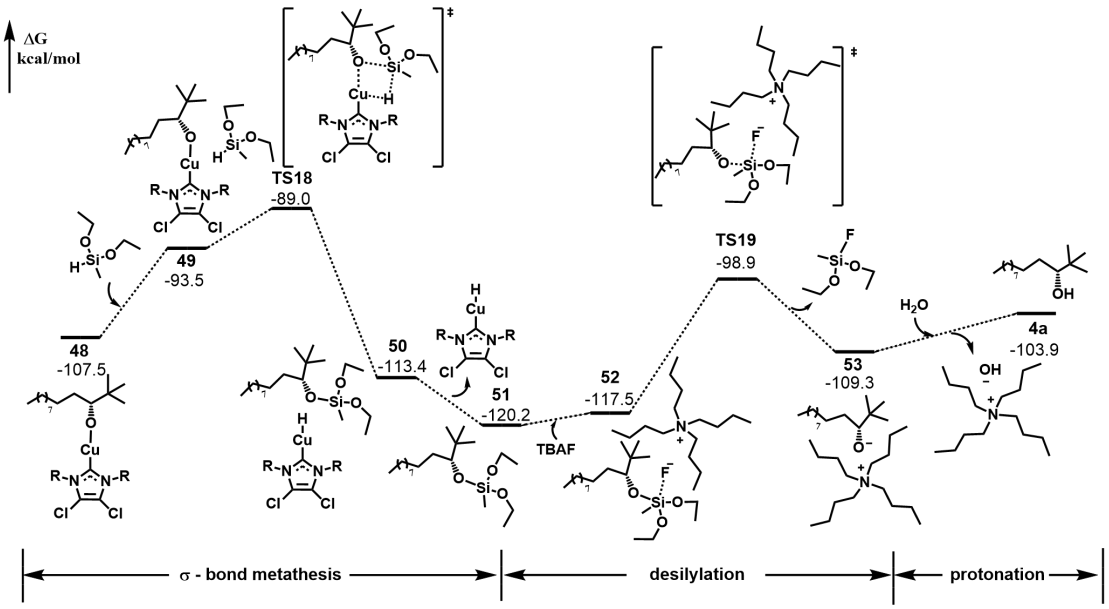

Fig. S9 Free energy profiles for the by-product **4a** generation of terminal alkyne.

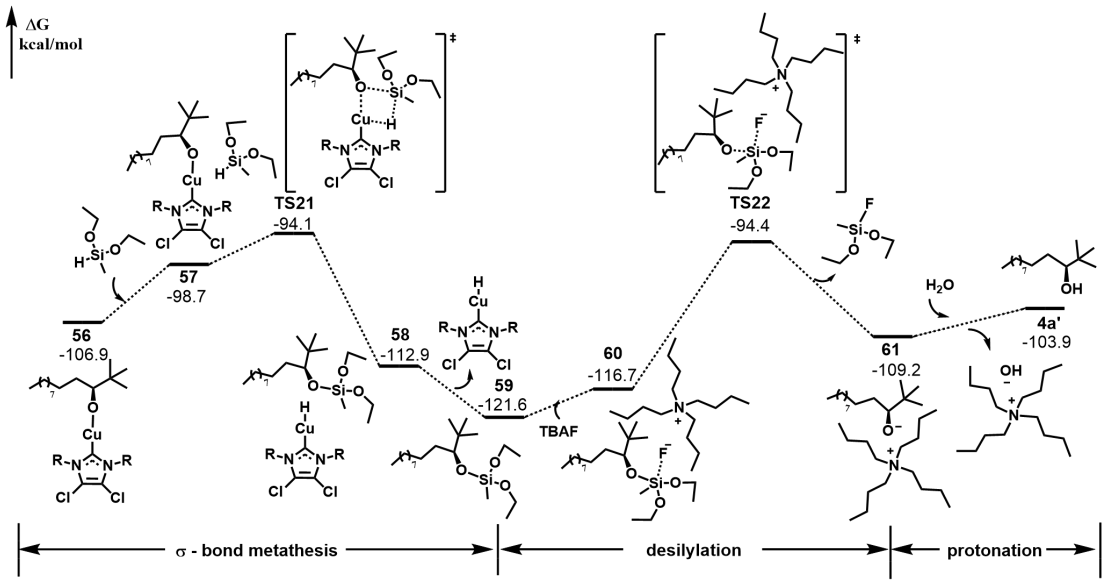

Fig. S10 Free energy profiles for the enantiomer **4a'** generation of **4a** for terminal alkyne.

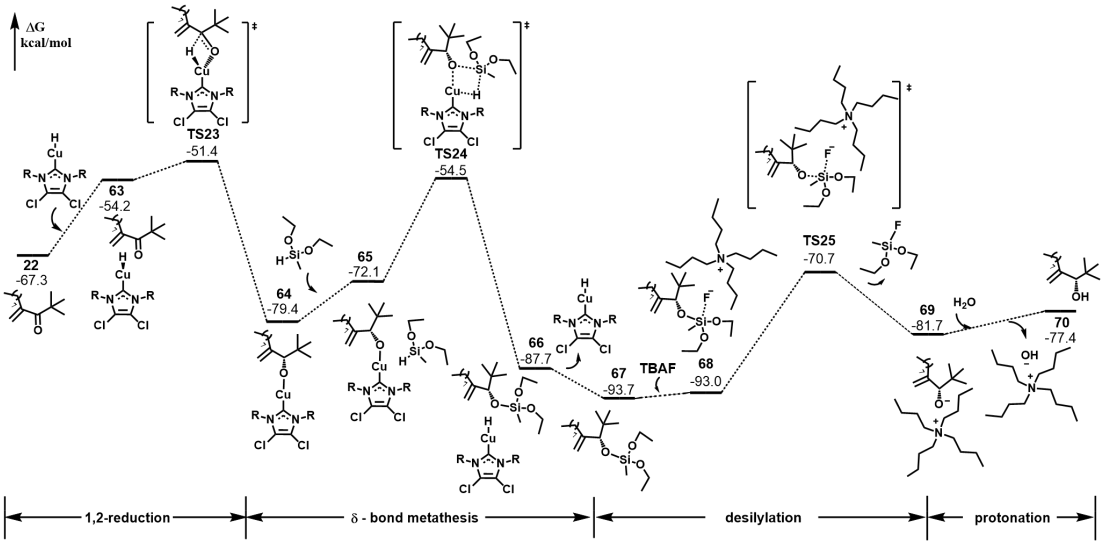

Fig. S11 Free energy profiles for the allylic alcohol **70** produced by enone **22** for terminal alkyne.

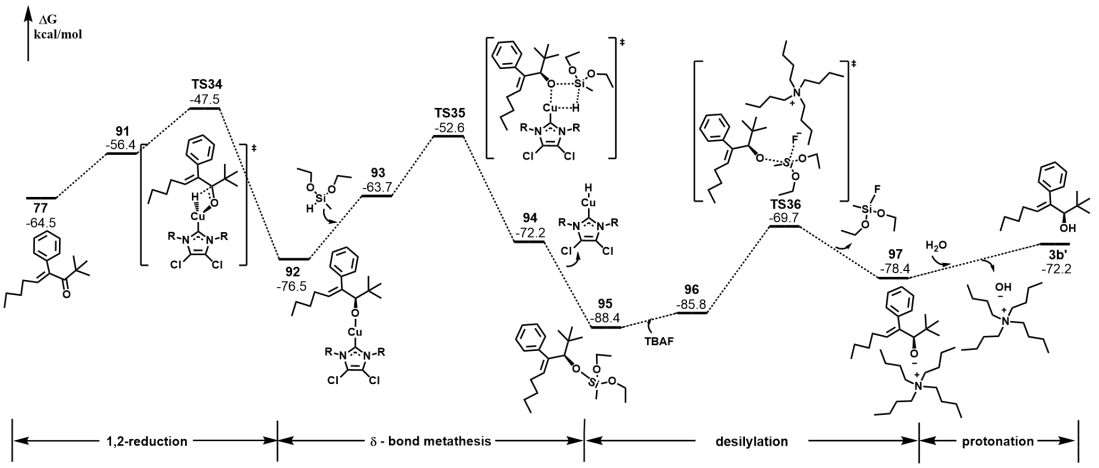

Fig. S12 Free energy profiles for the enantiomer **3b'** generation of **3b** for internal alkyne.

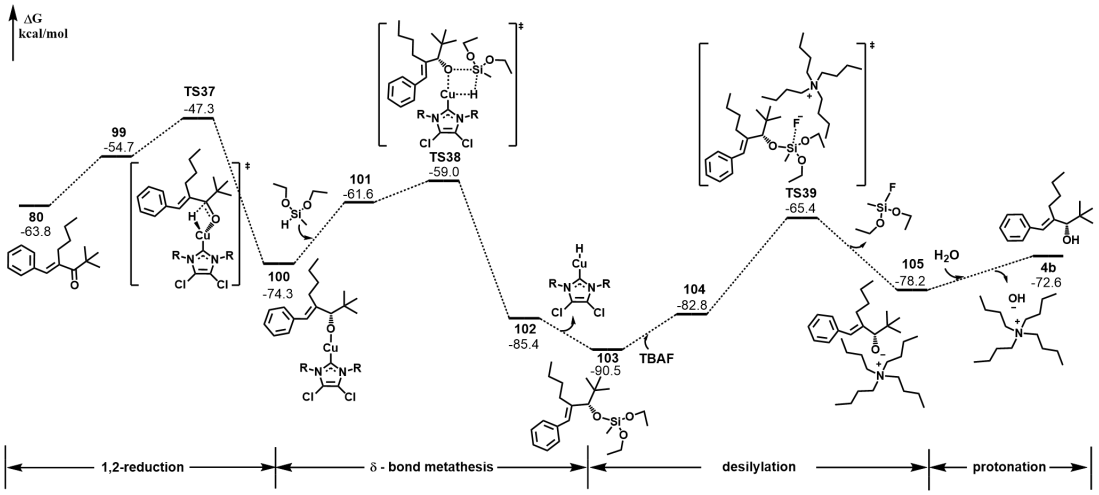

Fig. S13 Free energy profiles for the by-product **4b** generation of internal alkyne.

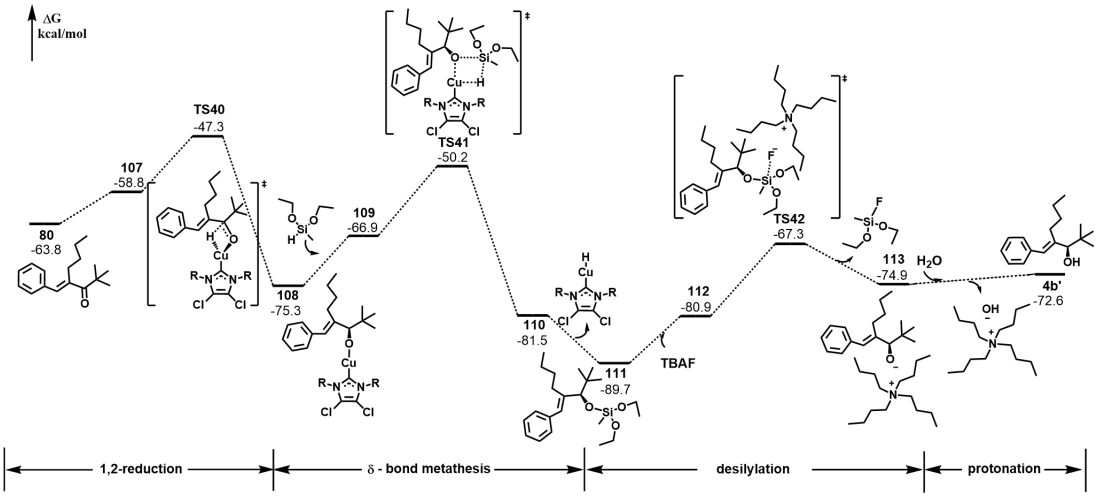

Fig. S14 Free energy profiles for the enantiomer **4b'** generation of **4b** for internal alkyne.

VII. Results of 1,2- and 1,4-reduction analysis for terminal and internal alkynes

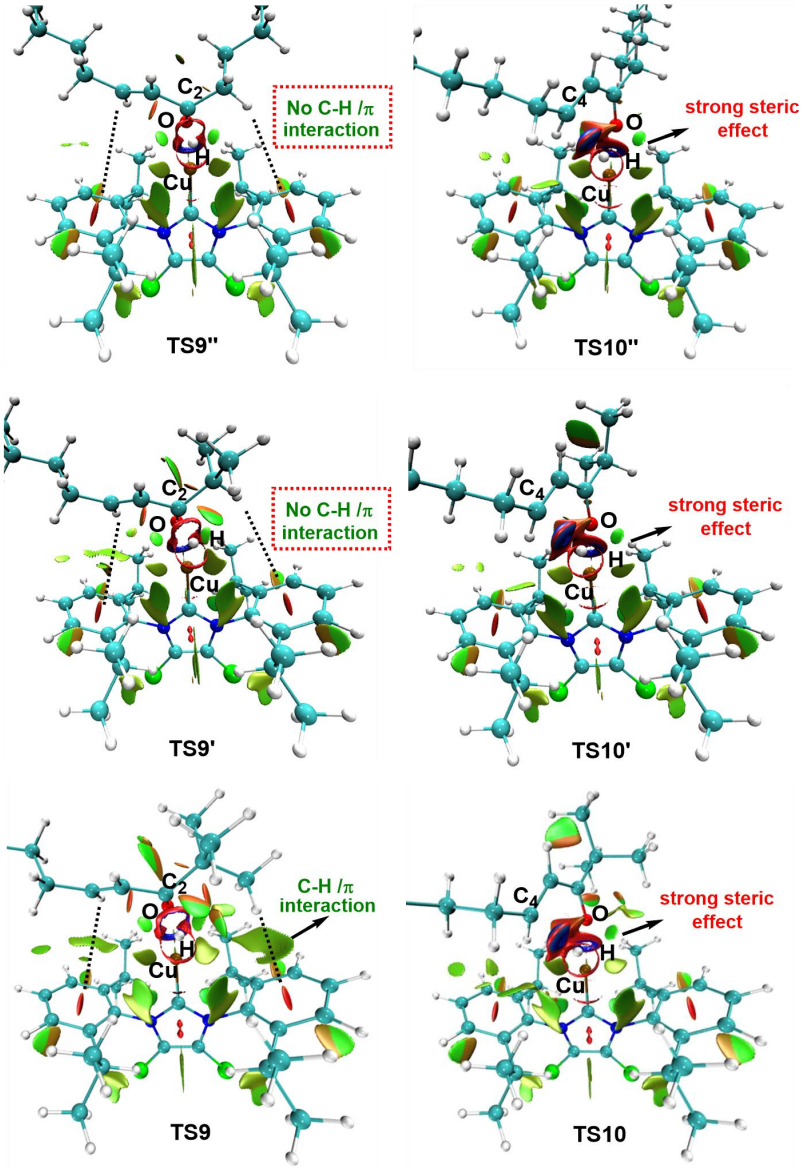

Fig. S15 Color-filled RDG isosurfaces of transition states **TS9"**, **TS9'** and **TS9** in 1,2-reduction and **TS10"**, **TS10'** and **TS10** in 1,4-reduction. (red, steric effect; green, van der Waals interaction; blue, strong attraction).

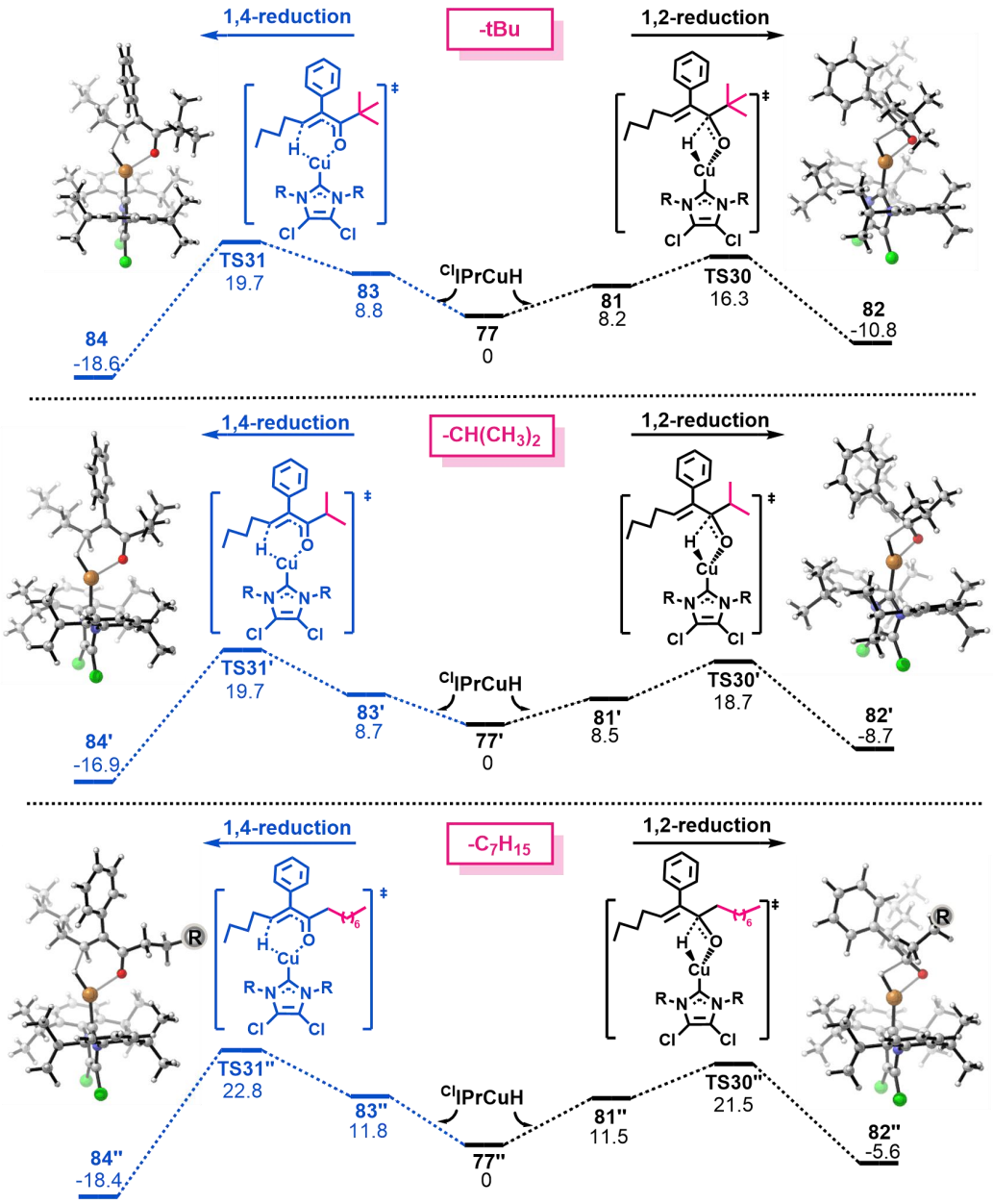

Fig. S16 Free energy profiles for the 1,2-reduction and 1,4-reduction reactions of unsaturated ketones with catalyst ^{Cl}IPrCuH. The red label represents alkyl substituents of three different alkyl halides at the *α*'-site. Optimized 3D geometry on R=C_6H_{13}.

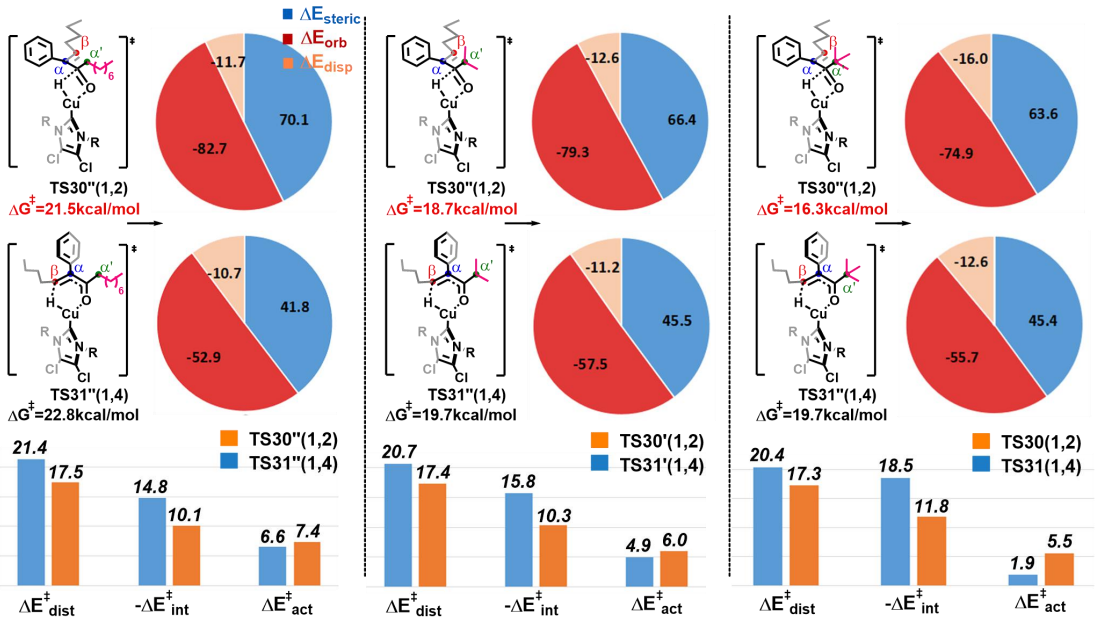

Fig. S17 The comparison of EDA of 1,2- and 1,4-reduction for internal alkynes with primary, secondary and tertiary alkyl halide. The pie chart shows the energy of each component. Histogram shows distortion-interaction analysis. $\Delta\Delta E = \Delta E_{(1,2)} - \Delta E_{(1,4)}$ in parentheses. All energies are in kcal/mol.

VIII. Cartesian coordinates of all the structures

1

O	-1.09711400	-0.91869500	-1.78407900
O	2.21691500	-0.62136100	-0.08957700
O	-0.92415900	-0.75488400	1.94162700
O	-0.14250500	2.27336000	-0.10466800
K	0.91510500	0.73624300	-1.97881000
K	0.19243800	-2.29306500	0.09126200
K	-2.20313900	0.60311200	0.09550300
K	1.13822500	0.92287000	1.76274800
C	-2.00887500	-1.60135800	-2.55443800
H	-1.98259000	-2.71424500	-2.42828100
H	-3.07913600	-1.33446100	-2.35275400
H	-1.89554900	-1.45011600	-3.65561700
C	-0.49505900	3.60037800	-0.18538900
H	-1.59932900	3.78999000	-0.13683400
H	-0.07587500	4.24407200	0.62737100
H	-0.17614500	4.11010100	-1.12872900
C	3.54623700	-0.76217900	-0.41266400
H	3.89580700	-1.82076400	-0.49561200
H	3.83561700	-0.30553000	-1.39627500
H	4.25467900	-0.29626700	0.31668600
C	-1.15962700	-1.16379100	3.23357800
H	-0.50603000	-0.67285100	4.00185400
H	-2.19734100	-0.97164400	3.60138900
H	-1.00519400	-2.25798200	3.41051600

O_2

O	0.00000000	0.00000000	0.60772300
O	0.00000000	0.00000000	-0.60772300

$[KOMe]_3KOO\cdot$

O	1.03821400	-1.52386700	1.17275400
O	0.04609300	-0.30558300	-2.31763800
O	0.90912600	2.07539300	0.33350500
O	-2.22008400	0.11206700	0.53123200
K	-1.01640500	-2.04385000	-0.43559400
K	2.25343800	0.00174400	-0.62759000
K	-0.21140500	0.52623700	2.15678500
K	-1.16762700	1.76772200	-1.20702900
C	1.67883200	-2.69701600	1.50021300
H	2.71624000	-2.78981400	1.08970300
H	1.80203700	-2.86967900	2.59642200
H	1.16286800	-3.62348100	1.13530100
C	-3.58947800	-0.02155300	0.57287600
H	-3.96517800	-1.03787600	0.28644500
H	-4.04431600	0.16200200	1.57593100
H	-4.14420600	0.67052300	-0.10987400
C	1.72130900	3.17153900	0.51720500
H	1.78202500	3.53370300	1.57285100
H	2.79160000	3.00757900	0.22689100
H	1.42037800	4.07645700	-0.06586000
O	0.76571800	-1.43706600	-2.43165600

2

C	0.57509000	0.01289400	-0.00006600
H	1.03417800	1.01277700	-0.00124200
H	0.93822900	-0.56639200	-0.87016000
H	0.93779100	-0.56374400	0.87200500
O	-0.79509200	0.00500000	-0.00002600

$(EtO)_2MeSiH$

Si	-0.00000200	0.89880400	-0.57693200
H	0.00002000	1.62075900	-1.86741300
O	-1.38924600	-0.01467300	-0.62953200
O	1.38906700	-0.01493300	-0.62956100
C	1.96369000	-0.74448700	0.46021200
C	3.39381700	-1.12209500	0.11099300
H	1.37038100	-1.64911000	0.65052700
H	1.94580500	-0.13879500	1.37638900
H	3.84410100	-1.69862500	0.92549100
H	3.41977200	-1.72998600	-0.79825900
H	3.99989300	-0.22647600	-0.05563000
C	-1.96364200	-0.74457100	0.46013000
C	-3.39384800	-1.12205400	0.11109500
H	-1.94556000	-0.13917000	1.37649600
H	-1.37030400	-1.64926200	0.65002900
H	-3.84396900	-1.69882700	0.92551100
H	-3.99994600	-0.22637700	-0.05512800
H	-3.42000100	-1.72966700	-0.79833700
C	0.00012200	2.06154200	0.89549600
H	0.88550500	2.70551900	0.86800500
H	-0.88507500	2.70577200	0.86792300
H	0.00000100	1.53784200	1.85663200

3

C	-0.51288600	0.56654200	2.24103400
H	-0.80805600	-0.38323000	2.69872000

H	0.43936100	0.87784300	2.68323400
H	-1.26578200	1.31456100	2.51279200
Si	-0.35838000	0.42651400	0.38034700
H	0.09519500	1.70386800	-0.22576500
O	2.94318200	2.32261700	-0.22343200
O	0.79792100	-0.67677900	-0.07903500
O	-1.78959100	-0.06557000	-0.31414600
C	-2.99564100	0.70560800	-0.27836800
H	-2.80214000	1.72343300	-0.64602900
H	-3.35543600	0.79149100	0.75624600
C	-4.04620800	0.02839500	-1.14263900
H	-4.25450700	-0.98090000	-0.77494100
H	-4.97868100	0.60160600	-1.12653200
H	-3.70286800	-0.04593400	-2.17874300
C	0.78055000	-2.06102100	0.30193000
H	0.80097000	-2.14474400	1.39671800
H	-0.14741500	-2.52734400	-0.05165800
C	1.98615900	-2.76113800	-0.30123700
H	2.91602200	-2.31093800	0.05938900
H	1.98588200	-3.82012100	-0.02406300
H	1.96693400	-2.69025600	-1.39289300
C	3.44053600	1.26891900	-0.93891800
H	4.33454100	0.81636300	-0.47739300
H	2.65173800	0.48589100	-0.88784500
H	3.61440000	1.49124700	-2.00401300

TS1

C	-0.22349900	-0.34938100	2.36276400
H	-0.27227500	-1.43424800	2.50614300
H	0.63476400	0.03425300	2.92289100
H	-1.12987100	0.09069400	2.79022100
Si	-0.04996300	0.08169500	0.54501300
H	0.09350800	1.64738200	0.37771400
O	0.46606200	3.02838100	0.27861600
O	1.34840900	-0.49480200	-0.12260700
O	-1.31570900	-0.49812500	-0.36264700
C	-2.70258700	-0.24821800	-0.09019100
H	-2.89399400	0.83269300	-0.10870300
H	-2.95709400	-0.61467400	0.91302000
C	-3.54754200	-0.95100400	-1.13880700
H	-3.36956800	-2.03033100	-1.11791000
H	-4.61061300	-0.77185100	-0.94917000
H	-3.30705000	-0.58011400	-2.13946200
C	1.72877400	-1.87967600	-0.17812200
H	1.73563600	-2.30276200	0.83522500
H	0.99252200	-2.43793400	-0.76943100
C	3.10741200	-1.98983300	-0.80536600
H	3.84663600	-1.44281800	-0.21266700
H	3.41489000	-3.03911000	-0.85928100
H	3.10348700	-1.57819100	-1.81893900
C	1.18078800	3.16337800	-0.91878000
H	1.50623800	4.21500200	-0.96016600
H	2.08696200	2.54144900	-0.95795800
H	0.57513000	2.97159500	-1.81758000

4

C	0.34703500	0.26641300	2.35845600
H	-0.58781900	0.16660500	2.92155400
H	1.06396800	-0.46818400	2.73519300
H	0.75600200	1.26601900	2.52925200
Si	0.01135600	-0.02270200	0.52546400
H	2.21554000	0.30754800	-0.65922300
O	3.09818800	0.64944100	-0.90249900
O	-0.63514300	-1.54830400	0.40409900
O	-1.12288300	1.03249100	-0.09616700
C	-0.95189200	2.45476200	-0.18695300
H	-0.06983300	2.68456700	-0.79850100
H	-0.78073400	2.87331900	0.81368300
C	-2.19823100	3.06295600	-0.80655300
H	-3.07890200	2.84653800	-0.19453600
H	-2.08952200	4.14942000	-0.88425800
H	-2.36627500	2.65950800	-1.80947200
C	-1.23333500	-2.09323200	-0.78343400
H	-2.02419400	-1.42166200	-1.13710400
H	-0.47625400	-2.16395800	-1.57539400
C	-1.79758500	-3.46691700	-0.46517400
H	-2.56016700	-3.40012800	0.31656000
H	-2.25651100	-3.90178800	-1.35886400
H	-1.00717000	-4.14030700	-0.12040800
C	4.06007600	-0.31145000	-0.48827000
H	5.04714600	0.09361200	-0.72862500
H	4.02747000	-0.50519200	0.59343600
H	3.95055600	-1.27231400	-1.01168600

5

Si	0.00412100	0.85922200	-0.47579000
O	-1.06399300	-0.33007700	0.02735200
O	1.52086100	0.33675200	-0.03931400
C	2.05089400	-0.96350500	-0.30976000
C	3.39322800	-1.10155700	0.38951000
H	2.17154500	-1.09636900	-1.39431100
H	1.35090500	-1.73132700	0.04232000
H	3.82562400	-2.08864300	0.19415200
H	4.09301400	-0.33954400	0.03410500
H	3.27668300	-0.98193600	1.47061100
C	-2.46727000	-0.31587200	-0.22671600
C	-3.08768800	-1.57836900	0.34956900
H	-2.65718600	-0.25992600	-1.30817100
H	-2.92622900	0.57227700	0.23207500
H	-4.16786500	-1.59164300	0.16979600
H	-2.64743700	-2.46643400	-0.11310400
H	-2.91418300	-1.63282600	1.42821400
C	-0.25666900	2.47941500	0.46748900
H	0.49191700	3.21734600	0.16609600
H	-1.24847900	2.89691500	0.27077800
H	-0.15591800	2.29894200	1.54364800

MeOH

O	0.75134800	0.12262100	0.00000000
H	1.13071900	-0.76574100	0.00001000
C	-0.66396500	-0.01902400	0.00000300
H	-1.03518800	-0.54466400	0.89120500
H	-1.08738300	0.98884600	-0.00035300
H	-1.03513900	-0.54526500	-0.89087800

6 ^{Cl}IPrCuCl

C	0.00040500	0.00839600	0.18289000
C	-0.68199000	-0.07011600	-1.97685100
C	0.68010200	-0.06010100	-1.97803200
N	1.08433100	-0.01215800	-0.64721700
N	-1.08453000	-0.02711700	-0.64532200
Cl	1.76104100	-0.09696800	-3.30126900
Cl	-1.76454300	-0.12717000	-3.29806900
C	3.10588200	-1.22757500	0.03633300
C	2.45944700	0.00439300	-0.18911600
C	3.08438100	1.24989200	0.02020900
C	4.40481700	1.23243000	0.48699200
C	5.06853900	0.03250400	0.72818600
C	4.42533400	-1.18185500	0.50328300
H	4.91795200	2.17240100	0.66465800
H	6.09182400	0.04364100	1.09177100
H	4.95418100	-2.11039500	0.69439000
C	-3.08686700	-1.24397300	0.09355800
C	-4.40749200	-1.19745800	0.55755100
C	-5.06861800	0.01563900	0.73041500
C	-4.42259800	1.21395800	0.43781200
C	-3.10290800	1.23049600	-0.03069300
C	-2.45917900	-0.01356200	-0.18575700
H	-4.92268300	-2.12483500	0.78772700
H	-6.09207800	0.02720400	1.09349700
H	-4.94949500	2.15291200	0.57592700
C	2.43152400	-2.57685700	-0.19343600
H	1.43622100	-2.39705200	-0.60991100
C	2.24041900	-3.33780800	1.13328200
H	1.71802800	-4.28365900	0.95503800
H	3.20322000	-3.56971000	1.60075500
H	1.65271800	-2.75138900	1.84646500
C	3.20328100	-3.43180500	-1.21726300
H	2.66738400	-4.36810400	-1.40456300
H	3.31652900	-2.90734100	-2.17091600
H	4.20322900	-3.68968400	-0.85342800
C	2.39046200	2.58522700	-0.23071400
H	1.38513500	2.38409700	-0.61136300
C	2.22965500	3.38744300	1.07541100
H	1.66898000	2.81872900	1.82386900
H	3.20204000	3.64568000	1.50781600
H	1.69133300	4.32109900	0.88127100
C	3.12652600	3.41183000	-1.30335200
H	2.58287600	4.34160600	-1.50075900
H	4.13711400	3.68058000	-0.97876900
H	3.21099200	2.86000900	-2.24457300
C	-2.39588400	-2.59261400	-0.08277700
C	-2.42606900	2.56351300	-0.33590300
C	-3.12793700	-3.47107000	-1.11632500
H	-2.58630300	-4.41149100	-1.26204400
H	-4.14148400	-3.71943500	-0.78475900
H	-3.20438200	-2.96801700	-2.08515000
C	-3.19573900	3.36006600	-1.40725000
H	-3.30950900	2.78186200	-2.32925600

H	-4.19542800	3.64015200	-1.05952100
H	-2.65799300	4.28307400	-1.64772800
C	-2.24628500	-3.32745400	1.26374200
H	-3.22222100	-3.56222000	1.70160300
H	-1.70846800	-4.27064500	1.12100600
H	-1.68987600	-2.72254600	1.98655100
H	-1.38726600	-2.41481800	-0.46635200
Cu	0.00169500	0.06958800	2.07731600
C	-2.23480600	3.39727200	0.94623200
H	-1.71196000	4.33154300	0.71591700
H	-3.19751700	3.65498600	1.40008100
H	-1.64753500	2.85097300	1.69093600
H	-1.43067600	2.35907600	-0.74061100
Cl	0.00355800	0.13082700	4.23024700

7 ^{Cl}IPrCuOMe

C	-0.02713000	0.00277600	0.18277800
C	-0.81470700	-0.01309900	-1.94587600
C	0.54479400	-0.01363000	-2.01417700
N	1.01446900	-0.00383000	-0.70368200
N	-1.15186500	-0.00295300	-0.59484500
Cl	1.56065700	-0.02402900	-3.38947500
Cl	-1.96171500	-0.02271600	-3.21434700
C	3.05697200	-1.23921100	-0.12494500
C	2.40996200	-0.00177400	-0.31566400
C	3.05803900	1.23737400	-0.14055700
C	4.40171600	1.20802600	0.25359800
C	5.06694800	0.00188700	0.45767900
C	4.40070000	-1.20615400	0.26866000
H	4.93191800	2.14316800	0.40412400
H	6.10880400	0.00335500	0.76443300
H	4.93006700	-2.13984000	0.43084000
C	-3.12827600	-1.23730100	0.18211200
C	-4.42769600	-1.20343700	0.70335800
C	-5.07205400	0.00478800	0.95545400
C	-4.42871100	1.21049900	0.68921700
C	-3.12924000	1.23933800	0.16766600
C	-2.50223800	-0.00015900	-0.07093400
H	-4.93980500	-2.13681600	0.91555800
H	-6.07978600	0.00673300	1.36044600
H	-4.94166800	2.14589300	0.89022800
C	2.35708900	-2.58189300	-0.31108200
H	1.34311200	-2.39328200	-0.67503200
C	2.22739500	-3.33129600	1.03000000
H	1.68342800	-4.27107500	0.88729900
H	3.21067800	-3.57325300	1.44742300
H	1.68517100	-2.73113800	1.76775000
C	3.06372200	-3.45270100	-1.36807800
H	2.50959500	-4.38518300	-1.51766400
H	3.12922100	-2.93723300	-2.33115800
H	4.07978800	-3.71766200	-1.05785800
C	2.35942400	2.57830600	-0.34339600
H	1.34567100	2.38609300	-0.70601400
C	2.22933400	3.34363000	0.98858300
H	1.68569300	2.75277500	1.73275800
H	3.21254100	3.58916500	1.40407300
H	1.68668700	4.28234000	0.83435600
C	3.06761800	3.43577400	-1.41016900
H	2.51427700	4.36676600	-1.57152600
H	4.08360400	3.70381200	-1.10233200
H	3.13354600	2.90859800	-2.36686500
C	-2.45458400	-2.58128900	-0.07817800
C	-2.45665000	2.58083100	-0.10797400
C	-3.24342700	-3.42076700	-1.10214500
H	-2.71226500	-4.35505800	-1.31212600
H	-4.23813100	-3.68197900	-0.72609800
H	-3.37126300	-2.88199900	-2.04606200
C	-3.24654800	3.40826400	-1.14086300
H	-3.37474700	2.85873400	-2.07850200
H	-4.24113100	3.67325700	-0.76717300
H	-2.71596200	4.34034900	-1.36183000
C	-2.23842300	-3.36259400	1.23268600
H	-3.19176900	-3.60785100	1.71253300
H	-1.71464500	-4.30281000	1.02992600
H	-1.64105900	-2.78465700	1.94477700
H	-1.46682900	-2.39247200	-0.50794200
Cu	0.08447500	0.01614800	2.05917100
C	-2.24064000	3.37664000	1.19416300
H	-1.71797200	4.31517000	0.98101000
H	-3.19401700	3.62597500	1.67181500
H	-1.64238700	2.80705400	1.91220900
H	-1.46895200	2.38795600	-0.53602800
O	0.11409600	0.03018000	3.87364700

C	1.30562000	0.02597500	4.61363300
H	1.93077400	-0.86810900	4.43521500
H	1.94775500	0.90430200	4.41811900
H	1.08322000	0.03853800	5.69554000

$(EtO)_2MeSiH$

Si	0.00000700	0.90151200	-0.57998300
H	0.00016300	1.63319700	-1.86148800
O	-1.39040900	-0.00659900	-0.61686600
O	1.38990600	-0.00733800	-0.61684600
C	1.95441100	-0.76187300	0.45154800
C	3.39305100	-1.11452200	0.10823000
H	1.37029200	-1.68046700	0.60708300
H	1.92096200	-0.18903500	1.39012200
H	3.84315500	-1.71331700	0.90710800
H	3.43217500	-1.68865500	-0.82179200
H	3.98901100	-0.20699100	-0.02520800
C	-1.95447200	-0.76147600	0.45156900
C	-3.39298600	-1.11474700	0.10838500
H	-1.92118100	-0.18865000	1.39015500
H	-1.36991800	-1.67980900	0.60700000
H	-3.84279200	-1.71369000	0.90732100
H	-3.98932900	-0.20746500	-0.02504700
H	-3.43194600	-1.68892800	-0.82161200
C	0.00034400	2.06266100	0.90029000
H	0.88526800	2.70751600	0.87693900
H	-0.88435500	2.70782800	0.87709300
H	0.00033700	1.53853300	1.86166700

8

C	-1.02127800	0.11243500	0.00038100
C	-3.25009300	0.22449700	0.40673900
C	-2.76482200	1.49645200	0.43454500
N	-1.39753700	1.41300000	0.18648600
N	-2.17127700	-0.61281700	0.13967100
Cl	-3.59692500	2.96459000	0.70611900
Cl	-4.85026800	-0.32883600	0.64227300
C	-0.26225600	3.14819400	-1.13058400
C	-0.49319900	2.54447300	0.12200700
C	0.10890700	2.99503400	1.31439100
C	0.98425300	4.08392400	1.21698300
C	1.24225100	4.69546900	-0.00687600
C	0.62395500	4.23226800	-1.16535000
H	1.46921200	4.45707000	2.11345900
H	1.92431700	5.53913900	-0.05739300
H	0.82974000	4.72098900	-2.11244100
C	-2.51125400	-2.59814200	-1.26514200
C	-2.55924600	-3.99405700	-1.36725600
C	-2.35841600	-4.80547900	-0.25363000
C	-2.10942200	-4.23645000	0.99232600
C	-2.04935700	-2.84662700	1.15652700
C	-2.24576200	-2.05403000	0.00783700
H	-2.75616500	-4.45052400	-2.33228200
H	-2.39874100	-5.88584400	-0.35691300
H	-1.95778700	-4.88021500	1.85306000
C	-0.92997500	2.67931500	-2.41967600
H	-1.58881800	1.84001900	-2.18031100
C	0.10715400	2.16609000	-3.43714400
H	-0.39731700	1.79313100	-4.33487600
H	0.79190600	2.96284200	-3.74552200
H	0.70570900	1.35241500	-3.01592800
C	-1.80898800	3.78693000	-3.03384200
H	-2.32542500	3.40842300	-3.92216300
H	-2.56432900	4.13730000	-2.32369900
H	-1.20961900	4.65042500	-3.34107700
C	-0.15640300	2.36290600	2.67742700
H	-0.84783300	1.52645200	2.54078400
C	1.13236800	1.78825500	3.29628500
H	1.60129700	1.05613600	2.63279800
H	1.86391100	2.57726000	3.50117900
H	0.90397000	1.29343800	4.24636500
C	-0.82986400	3.36416500	3.63762400
H	-1.06288500	2.87490300	4.58916700
H	-0.17176200	4.21287800	3.85228800
H	-1.76115100	3.75793900	3.21946700
C	-2.74405800	-1.74269500	-2.50698200
C	-1.78518200	-2.26115800	2.54033100
C	-4.14947600	-1.97353200	-3.09680300
H	-4.31356200	-1.30688400	-3.94984300
H	-4.27137500	-3.00245700	-3.45098300
H	-4.93066600	-1.77722400	-2.35608900
C	-2.91295100	-2.62537400	3.52644000
H	-3.88798900	-2.29135600	3.15848300
H	-2.96730900	-3.70673400	3.69031100

H	-2.73317000	-2.15044200	4.49656100
C	-1.65177100	-1.98157200	-3.56736200
H	-0.65616300	-1.77558300	-3.16214300
H	-1.66232800	-3.01582200	-3.92680000
H	-1.81246800	-1.32609600	-4.42985300
H	-2.68485200	-0.69006600	-2.21642400
Cu	0.69854800	-0.55424000	-0.39496400
C	-0.40977600	-2.69428100	3.08379600
H	-0.22717900	-2.22961000	4.05855400
H	-0.35605600	-3.77990500	3.21720700
H	0.39734400	-2.39652300	2.40745600
H	-1.76968900	-1.17086200	2.45526000
O	2.37584600	-1.26316600	-0.88913300
C	2.71124300	-1.42653000	-2.26308900
H	1.86655200	-1.87191400	-2.80283200
H	2.96594700	-0.46669900	-2.72937200
H	3.57104000	-2.09868600	-2.34759400
Si	3.72035700	-0.82881700	0.45889100
H	2.45635900	-0.88774700	1.29901600
O	4.46455100	-2.27861200	-0.04212400
O	4.01843400	0.55226900	-0.50077800
C	5.08165000	1.47555600	-0.32643800
C	4.98789800	2.55113400	-1.40191100
H	6.05540200	0.96800000	-0.39793300
H	5.03951600	1.94405800	0.66675600
H	5.80296300	3.27595400	-1.29607400
H	5.05034600	2.10552500	-2.40000700
H	4.03620400	3.08730000	-1.32579000
C	5.75526200	-2.72719700	0.33860100
C	6.05666400	-4.04022200	-0.37390000
H	5.81605300	-2.87664200	1.42587700
H	6.52229900	-1.98256800	0.07783700
H	7.04740800	-4.41386200	-0.09237400
H	5.31370400	-4.80021400	-0.11042300
H	6.03499200	-3.90609200	-1.46039300
C	4.81205600	-0.40812600	2.00979100
H	4.43000500	0.50695600	2.48239800
H	4.70154300	-1.20983400	2.75293300
H	5.88664400	-0.26452100	1.84404200

TS2

C	-1.01693000	0.08376700	-0.00276400
C	-3.28829300	0.00935400	0.07510000
C	-2.92638800	1.31832400	0.00294300
N	-1.53470100	1.35140400	-0.04296800
N	-2.11179700	-0.73697200	0.06815900
Cl	-3.91592200	2.71360700	-0.03505500
Cl	-4.85354700	-0.67562500	0.16548100
C	-0.37896300	3.05896800	-1.37785000
C	-0.73278500	2.55526300	-0.10981200
C	-0.34348400	3.17400500	1.09565500
C	0.44006200	4.33093000	0.99923800
C	0.81372300	4.84757100	-0.23850600
C	0.40590500	4.21833500	-1.41173600
H	0.76117000	4.83211200	1.90703500
H	1.42256800	5.74555600	-0.28927900
H	0.70202400	4.63288600	-2.37021300
C	-2.10300100	-2.90517900	-1.08598100
C	-2.02647000	-4.30133000	-1.00466100
C	-1.90503500	-4.94600300	0.22339200
C	-1.86192900	-4.20505400	1.40124500
C	-1.93424100	-2.80626800	1.38242200
C	-2.04617400	-2.18233700	0.12315900
H	-2.06365800	-4.88998200	-1.91605600
H	-1.84733600	-6.02986000	0.26284100
H	-1.77291200	-4.71966800	2.35285300
C	-0.81665500	2.40497500	-2.68444400
H	-1.39679500	1.51011400	-2.44204500
C	0.39381100	1.94655400	-3.52016400
H	0.05351300	1.42405400	-4.42067500
H	1.00550900	2.79658500	-3.84070300
H	1.03385900	1.26738200	-2.94949900
C	-1.73323900	3.33784400	-3.50077700
H	-2.07885000	2.82907200	-4.40686100
H	-2.61220300	3.63975800	-2.92297100
H	-1.20538800	4.24620000	-3.81009900
C	-0.74079500	2.64690800	2.47128000
H	-1.33723400	1.74074100	2.33314600
C	0.49483900	2.25509700	3.30511700
H	1.10135000	1.50664500	2.78642000
H	1.12941800	3.12373600	3.51064800
H	0.18161500	1.83669000	4.26772600
C	-1.61954500	3.66203300	3.22956000

H	-1.93843500	3.24155000	4.18914900
H	-1.07175000	4.58724400	3.43765400
H	-2.51518400	3.92307800	2.65759600
C	-2.24643100	-2.23768600	-2.45027100
C	-1.90385000	-2.03313400	2.69741400
C	-3.56077700	-2.64772500	-3.14420900
H	-3.66665500	-2.11502200	-4.09510700
H	-3.58042200	-3.72111900	-3.36041800
H	-4.43071600	-2.41321500	-2.52350800
C	-3.13513800	-2.36026900	3.56585100
H	-4.06791100	-2.14962100	3.03364600
H	-3.14664400	-3.41524000	3.85980800
H	-3.12203700	-1.75954400	4.48143500
C	-1.03221700	-2.53264300	-3.35168100
H	-0.09967900	-2.21718100	-2.87478800
H	-0.95066000	-3.60141800	-3.57599200
H	-1.12915200	-1.99895000	-4.30311700
H	-2.28251100	-1.15492800	-2.30101900
Cu	0.81729400	-0.39890500	0.08063400
C	-0.59602100	-2.28397100	3.47226900
H	-0.57876000	-1.68102700	4.38641400
H	-0.49771200	-3.33460900	3.76532600
H	0.27651100	-2.01550900	2.86910900
H	-1.94100800	-0.96486700	2.46707800
O	2.49803100	-1.03790400	-0.96211300
C	2.89656800	-1.14366200	-2.32757100
H	1.99422600	-1.16194400	-2.94672000
H	3.51105000	-0.28567700	-2.62597400
H	3.47071300	-2.05938200	-2.49249600
Si	3.61291300	-0.78541400	0.40420600
H	2.10382400	-0.61560300	1.13421900
O	4.73263800	-1.83013700	-0.37989700
O	4.03421600	0.82117600	0.07173400
C	5.22228200	1.43764800	0.55016100
C	5.24930700	2.89445100	0.10731400
H	6.10835000	0.91592300	0.15732200
H	5.27485100	1.38262700	1.64750600
H	6.15818500	3.38986300	0.46595200
H	5.22516500	2.96574200	-0.98484200
H	4.38189500	3.43204100	0.50361900
C	5.93995700	-2.36426500	0.12776300
C	6.64666600	-3.14709700	-0.97355800
H	5.74547400	-3.02996400	0.98184600
H	6.60758800	-1.56879000	0.49408500
H	7.58329800	-3.57801900	-0.60273400
H	6.01092600	-3.96256600	-1.33399400
H	6.87834000	-2.49591600	-1.82265300
C	4.14029800	-1.14519600	2.22311500
H	3.67837200	-0.40138200	2.88188900
H	3.74848900	-2.12591400	2.52411500
H	5.22006300	-1.15167600	2.41059800

9

C	1.92051600	0.00523800	-0.39583100
C	2.20956600	-0.60232300	1.77278400
C	2.12373400	0.75616400	1.73735200
N	1.94669300	1.11314900	0.40382100
N	2.08361100	-1.04756500	0.46031500
Cl	2.20816600	1.87952300	3.02410600
Cl	2.42963700	-1.63826500	3.11566600
C	0.54447200	3.04637400	-0.17705300
C	1.82767500	2.47142800	-0.08719500
C	3.00309200	3.15471900	-0.45911300
C	2.85849400	4.45756600	-0.95188600
C	1.60360100	5.05048300	-1.06301700
C	0.46256500	4.35203800	-0.67808800
H	3.74074700	5.01246200	-1.25529900
H	1.51486800	6.06137000	-1.45014500
H	-0.50975000	4.82555600	-0.76946700
C	0.92546900	-3.16337200	-0.00725400
C	1.00147600	-4.49730300	-0.42754200
C	2.21954500	-5.07618600	-0.77360800
C	3.39411400	-4.33157500	-0.70355200
C	3.38022200	-2.99344500	-0.29067700
C	2.13040700	-2.43487300	0.04454900
H	0.09292500	-5.08833100	-0.48576800
H	2.25387300	-6.11218300	-1.09786400
H	4.33788700	-4.79442400	-0.97464700
C	-0.73015500	2.31291100	0.22860300
H	-0.45044600	1.34236400	0.64845500
C	-1.62753400	2.03650500	-0.99441200
H	-2.52238100	1.48731000	-0.68466700
H	-1.95138500	2.97033300	-1.46695000

H	-1.09821400	1.44451400	-1.74821000
C	-1.50574500	3.07358500	1.32195300
H	-2.39623400	2.50587200	1.60952500
H	-0.88956000	3.22964500	2.21299600
H	-1.83940000	4.05509900	0.96848700
C	4.39387500	2.53683000	-0.35592200
H	4.29613000	1.54107900	0.08580000
C	5.02748100	2.35502500	-1.74925400
H	4.39418500	1.73703300	-2.39377800
H	5.17748700	3.31881500	-2.24742400
H	6.00471200	1.86853600	-1.66054000
C	5.31290000	3.35669100	0.57066700
H	6.28190100	2.85773500	0.67653100
H	5.49855900	4.35849700	0.16927800
H	4.87669000	3.46887200	1.56809800
C	-0.42765800	-2.56223800	0.35948500
C	4.68723600	-2.20956200	-0.22519200
C	-1.08741800	-3.32223600	1.52663300
H	-2.02806000	-2.83713400	1.80713800
H	-1.31794300	-4.35726300	1.25312000
H	-0.43847200	-3.34321500	2.40770300
C	5.68237000	-2.85073100	0.76181600
H	5.24973800	-2.93968300	1.76312000
H	5.98271000	-3.85166900	0.43484700
H	6.58796300	-2.23943200	0.83469200
C	-1.36116800	-2.50296000	-0.86578200
H	-0.90222700	-1.93565900	-1.68221600
H	-1.58812500	-3.50734900	-1.23980000
H	-2.30842600	-2.02057700	-0.60384800
H	-0.26686700	-1.53322300	0.69330400
Cu	1.69951800	-0.05861600	-2.32297200
C	5.31431200	-2.05060200	-1.62413900
H	6.22448100	-1.44441100	-1.56416500
H	5.58682800	-3.02113400	-2.05230500
H	4.62055100	-1.56018200	-2.31444600
H	4.46709300	-1.20400100	0.14455500
O	-4.95986100	1.48898700	0.86164100
C	-5.45760800	2.68822000	0.27112300
H	-5.10697800	3.53284500	0.87059700
H	-5.07989900	2.80972900	-0.75117500
H	-6.55189800	2.69815100	0.24879300
Si	-5.54302600	-0.03918000	0.60303000
H	1.52352000	-0.11128700	-3.83584000
O	-7.18410000	0.14895200	0.42018800
O	-4.89423400	-0.76281100	-0.74347700
C	-5.06361000	-0.28077800	-2.08482000
C	-4.90003100	-1.43241300	-3.06329600
H	-4.31352000	0.49563600	-2.28232900
H	-6.05494100	0.17729500	-2.19999300
H	-5.00811000	-1.07313700	-4.09193900
H	-3.91093400	-1.88860000	-2.96050000
H	-5.65604100	-2.20352500	-2.88502000
C	-8.08776100	-0.92265400	0.12329800
C	-9.50571600	-0.37817100	0.06900300
H	-8.01091000	-1.70073000	0.89509700
H	-7.81844600	-1.38297100	-0.83646800
H	-10.21277300	-1.18255300	-0.15813100
H	-9.78472100	0.06707100	1.02881100
H	-9.59493400	0.38933500	-0.70598100
C	-5.05171400	-1.09263700	2.05534100
H	-5.39025800	-2.12570300	1.93084500
H	-3.96322000	-1.10841100	2.16814500
H	-5.48267700	-0.69977600	2.98099300

10 ^{Cl}IPrCuH

C	0.00002200	-0.00005800	-0.43084300
C	-0.68095600	-0.00449000	1.73547700
C	0.68074600	0.00476400	1.73555700
N	1.08284700	0.00670200	0.40319400
N	-1.08290100	-0.00666400	0.40306900
Cl	1.76289800	0.01348700	3.05972600
Cl	-1.76326500	-0.01296900	3.05952000
C	3.08751200	1.24541000	-0.29296300
C	2.45830000	0.00770400	-0.05269500
C	3.10383300	-1.23063500	-0.24205000
C	4.42443300	-1.20052900	-0.70726800
C	5.07071400	0.00588400	-0.96393200
C	4.40887700	1.21311800	-0.75628700
H	4.95180000	-2.13500200	-0.87167800
H	6.09482300	0.00515600	-1.32550500
H	4.92422200	2.14705600	-0.95796800
C	-3.10379900	1.23059700	-0.24258000
C	-4.42433600	1.20044200	-0.70797200

C	-5.07059000	-0.00600000	-0.96457100
C	-4.40879100	-1.21321200	-0.75668000
C	-3.08748900	-1.24545400	-0.29317000
C	-2.45829900	-0.00772200	-0.05298400
H	-4.95167600	2.13489700	-0.87257200
H	-6.09464900	-0.00531100	-1.32628300
H	-4.92411700	-2.14717100	-0.95830900
C	2.39493300	2.58800500	-0.08016500
H	1.39532800	2.39906900	0.32113900
C	2.21494500	3.34129700	-1.41271200
H	1.67887500	4.28165000	-1.24604800
H	3.18139100	3.58309600	-1.86768700
H	1.64387200	2.74417600	-2.13079400
C	3.14284500	3.45488200	0.95154200
H	2.59770500	4.38882700	1.12366200
H	3.24321800	2.93733600	1.91055000
H	4.14737300	3.71678000	0.60336200
C	2.42493500	-2.57159000	0.02091900
H	1.43663200	-2.37812700	0.44774000
C	2.21119600	-3.35215800	-1.29090300
H	1.61597000	-2.77279600	-2.00386900
H	3.16659800	-3.59513600	-1.76802500
H	1.68711400	-4.29288400	-1.09126600
C	3.20446900	-3.41473300	1.04844100
H	2.66301600	-4.34250500	1.26072800
H	4.19656600	-3.68901100	0.67521000
H	3.33648300	-2.87424600	1.99074500
C	-2.42492400	2.57157900	0.02031600
C	-2.39494800	-2.58802700	-0.08010100
C	-3.20460300	3.41486500	1.04761000
H	-2.66316400	4.34265200	1.25986700
H	-4.19663400	3.68912000	0.67418600
H	-3.33678200	2.87450000	1.98996000
C	-3.14305100	-3.45479900	0.95155600
H	-3.24361300	-2.93715100	1.91048900
H	-4.14751000	-3.71674600	0.60321300
H	-2.59793600	-4.38872000	1.12388000
C	-2.21097800	3.35197600	-1.29157400
H	-3.16630700	3.59490900	-1.76886600
H	-1.68691200	4.29272000	-1.09197800
H	-1.61565600	2.77251600	-2.00437900
H	-1.43668900	2.37815700	0.44731300
Cu	0.00013800	-0.00020700	-2.37195200
C	-2.21471000	-3.34145700	-1.41253600
H	-1.67868100	-4.28179700	-1.24567500
H	-3.18107300	-3.58329000	-1.86766900
H	-1.64349500	-2.74441300	-2.13057000
H	-1.39542100	-2.39904500	0.32137500
H	0.00022600	-0.00030700	-3.89526900

11

C	-8.69109400	-0.00141700	0.65036000
C	-7.39177700	-0.00116400	-0.16532400
H	-8.70369700	-0.87965400	1.31163900
H	-8.70382700	0.87658100	1.31195500
C	-6.12572100	-0.00131500	0.70112300
H	-7.37832800	-0.87928400	-0.82658200
H	-7.37841300	0.87727800	-0.82615700
H	-6.13714600	0.87703600	1.36192100
H	-6.13691100	-0.88015300	1.36127600
C	-4.83042400	-0.00082000	-0.11983200
C	-3.56968400	-0.00112600	0.76589200
H	-4.80738000	0.87899100	-0.77546800
H	-4.80721800	-0.87999800	-0.77631200
H	-3.57416900	0.87246300	1.42931400
H	-3.57371800	-0.87560500	1.42813100
C	-9.95741000	-0.00135500	-0.21526800
C	-11.25798300	-0.00151400	0.59842600
H	-9.94516400	-0.87935800	-0.87719200
H	-9.94523800	0.87682200	-0.87696300
C	-12.51717500	-0.00149200	-0.27456000
H	-11.27031100	-0.87907800	1.25927000
H	-11.27040800	0.87590900	1.25945500
H	-13.42760900	-0.00160300	0.33408600
H	-12.54957000	0.88255100	-0.92193000
H	-12.54947500	-0.88540700	-0.92211000
C	1.50967500	0.00012500	0.03077900
C	3.63703000	0.68035900	-0.40789900
C	3.63781900	-0.67788800	-0.40751300
N	2.33017700	-1.08335800	-0.13978100
N	2.32890300	1.08445300	-0.14042000
Cl	4.94580500	-1.75235100	-0.66771500
Cl	4.94388100	1.75616600	-0.66824700

C	1.42328800	-3.12102800	-1.17972300
C	1.90306600	-2.46297500	-0.02720300
C	2.00547500	-3.09920000	1.22774600
C	1.59652100	-4.43686900	1.30545500
C	1.11567000	-5.11102800	0.18707200
C	1.03275300	-4.45897500	-1.04026000
H	1.66022600	-4.95700700	2.25611900
H	0.80676400	-6.14899300	0.27089600
H	0.66121100	-4.99838200	-1.90556600
C	1.41786000	3.12056000	-1.18000000
C	1.02625700	4.45818500	-1.04055100
C	1.11039900	5.11089700	0.18636800
C	1.59347900	4.43771500	1.30436000
C	2.00375400	3.10044400	1.22660800
C	1.90028200	2.46360800	-0.02792100
H	0.65282000	4.99683100	-1.90550200
H	0.80059300	6.14859600	0.27015900
H	1.65786100	4.95826600	2.25475500
C	1.34876900	-2.45406100	-2.55094900
H	1.49760900	-1.37879600	-2.41513000
C	-0.02686400	-2.64211800	-3.21789700
H	-0.07787400	-2.05284000	-4.13965600
H	-0.20627100	-3.68730200	-3.48999000
H	-0.83825900	-2.32184800	-2.55878400
C	2.47027400	-2.96848300	-3.47742300
H	2.42684700	-2.45825500	-4.44568600
H	3.46087300	-2.79805200	-3.04672400
H	2.36349700	-4.04353300	-3.65927800
C	2.55527300	-2.41184800	2.47483300
H	2.77154600	-1.36939700	2.22542700
C	1.52586100	-2.39613300	3.62095300
H	0.61038500	-1.88287000	3.31459800
H	1.26811600	-3.41033700	3.94466100
H	1.94013800	-1.86778400	4.48654800
C	3.87750300	-3.06261000	2.93067000
H	4.28437200	-2.52462700	3.79347400
H	3.72482500	-4.10513300	3.23009500
H	4.62851300	-3.04765900	2.13529500
C	1.34181100	2.45255600	-2.55063500
C	2.55543900	2.41400300	2.47335900
C	2.46505800	2.96290000	-3.47727500
H	2.42028700	2.45210000	-4.44517500
H	2.36135700	4.03812900	-3.65987200
H	3.45512100	2.79000200	-3.04636400
C	3.87565000	3.06829100	2.92994500
H	4.62674700	3.05638400	2.13459500
H	3.71988400	4.11003800	3.23046000
H	4.28408300	2.53065700	3.79222300
C	-0.03288900	2.64382800	-3.21858600
H	-0.20878000	3.68899400	-3.49302100
H	-0.08525600	2.05286100	-4.13918400
H	-0.84575700	2.32752900	-2.55936800
H	1.48737200	1.37699700	-2.41351400
Cu	-0.39554300	-0.00082900	0.58031100
H	-0.52261100	-0.00303600	2.14103000
C	1.52568100	2.39461600	3.61914400
H	1.94141600	1.86754200	4.48482700
H	1.26435900	3.40791300	3.94282600
H	0.61202700	1.87829800	3.31241100
H	2.77483600	1.37232400	2.22343900
C	-2.31298100	-0.00020300	-0.01808700
C	-1.59280800	0.00118900	-1.04278300
H	-1.37477900	0.00247900	-2.09201700

TS3

C	8.72767300	0.00001600	0.46506500
C	7.43270100	0.00003100	-0.35765800
H	8.73619300	0.87810100	1.12674300
H	8.73609000	-0.87798600	1.12685300
C	6.16354000	0.00016400	0.50400900
H	7.42243300	0.87826500	-1.01886100
H	7.42233400	-0.87830500	-1.01872400
H	6.17455300	-0.87812200	1.16517600
H	6.17466100	0.87852700	1.16507200
C	4.86702300	0.00018500	-0.31600000
C	3.61120000	0.00021400	0.57020800
H	4.84559900	-0.87867500	-0.97338300
H	4.84562800	0.87903100	-0.97340300
H	3.62117100	-0.87459700	1.23391700
H	3.62109100	0.87514700	1.23375600
C	10.00035900	-0.00011800	-0.39105000
C	11.29425300	0.00009400	0.43334000
H	9.99335500	0.87783800	-1.05308900

H	9.99341100	-0.87835400	-1.05272000
C	12.56100700	-0.00005800	-0.42859800
H	11.30099400	0.87771200	1.09423900
H	11.30104300	-0.87724500	1.09460900
H	13.46606900	0.00028900	0.18804900
H	12.59915700	-0.88427000	-1.07540600
H	12.59892200	0.88368900	-1.07605600
C	-1.55814700	0.00000300	0.00561700
C	-3.72707700	-0.67931400	0.11869100
C	-3.72710800	0.67921900	0.11873900
N	-2.39481900	1.08531700	0.05018800
N	-2.39477000	-1.08535300	0.05010000
Cl	-5.05269600	1.76059800	0.18157100
Cl	-5.05262300	-1.76075000	0.18146800
C	-1.81430100	3.09689900	-1.23364400
C	-1.94289800	2.45917600	0.01742100
C	-1.65101000	3.10425400	1.23703700
C	-1.20485400	4.43033300	1.17191000
C	-1.05797100	5.08315600	-0.04905900
C	-1.36147600	4.42241100	-1.23628900
H	-0.97128200	4.95803500	2.09141900
H	-0.70938800	6.11157300	-0.07499700
H	-1.24835000	4.94322400	-2.18198600
C	-1.81398000	-3.09695100	-1.23359200
C	-1.36120900	-4.42248100	-1.23613200
C	-1.05795200	-5.08322000	-0.04883700
C	-1.20500900	-4.43036200	1.17209100
C	-1.65113200	-3.10426700	1.23711500
C	-1.94281500	-2.45920700	0.01743900
H	-1.24794400	-4.94331600	-2.18180000
H	-0.70941300	-6.11165400	-0.07469300
H	-0.97159500	-4.95804700	2.09165100
C	-2.15568000	2.41672700	-2.55643700
H	-2.47588500	1.39320600	-2.34285200
C	-0.92520500	2.32207800	-3.47898600
H	-1.18853700	1.79723100	-4.40370400
H	-0.55431300	3.31511100	-3.75496900
H	-0.11331500	1.77397100	-2.99241000
C	-3.32679200	3.12748900	-3.26377600
H	-3.59588300	2.59121300	-4.17995700
H	-4.21266000	3.17338400	-2.62295800
H	-3.06087900	4.15232500	-3.54419000
C	-1.82324700	2.43405100	2.59700400
H	-2.10002600	1.38910700	2.43123200
C	-0.51202300	2.42966000	3.40611000
H	0.28826300	1.92819700	2.85413800
H	-0.18114600	3.44600500	3.64518000
H	-0.65903600	1.89870600	4.35274100
C	-2.96328400	3.09450500	3.39891500
H	-3.10743000	2.57343700	4.35138400
H	-2.73478500	4.14219300	3.62240500
H	-3.90890000	3.06706200	2.84907200
C	-2.15509000	-2.41679300	-2.55646100
C	-1.82347900	-2.43401700	2.59704500
C	-3.32642400	-3.12724400	-3.26374800
H	-3.59541200	-2.59090800	-4.17992500
H	-3.06078700	-4.15215500	-3.54415300
H	-4.21227700	-3.17290300	-2.62289200
C	-2.96334800	-3.09463200	3.39905800
H	-3.90892700	-3.06768600	2.84912800
H	-2.73450300	-4.14217000	3.62289500
H	-3.10775300	-2.57332100	4.35135300
C	-0.92456800	-2.32264000	-3.47899500
H	-0.55395800	-3.31581500	-3.75484300
H	-1.18772600	-1.79784500	-4.40379100
H	-0.11252300	-1.77470800	-2.99247800
H	-2.47494700	-1.39314600	-2.34297100
Cu	0.34407900	0.00006600	-0.06190700
H	1.31232700	0.00019600	1.18329200
C	-0.51220800	-2.42932700	3.40608300
H	-0.65930600	-1.89849100	4.35276800
H	-0.18104800	-3.44560600	3.64503500
H	0.28791900	-1.92761800	2.85410300
H	-2.10047600	-1.38913800	2.43122300
C	2.34150300	0.00008200	-0.21937600
C	1.82389100	-0.00005200	-1.39869600
H	2.22928300	-0.00015900	-2.40198500

12

C	9.06605300	-0.00148500	0.47300200
C	7.58077300	0.01813700	0.08877200
H	9.27973500	0.84778800	1.13822300
H	9.27698300	-0.90676500	1.06064900

C	6.63277900	-0.03465100	1.29421500
H	7.36973200	0.92375800	-0.49823100
H	7.36740600	-0.83066100	-0.57696400
H	6.84452000	-0.94048900	1.88095800
H	6.84696700	0.81397300	1.96011400
C	5.14818600	-0.01495700	0.90660600
C	4.20934800	-0.07260100	2.11538300
H	4.93632600	-0.86115100	0.23890700
H	4.93787500	0.89120600	0.32237300
H	4.44297100	-0.97339300	2.70656100
H	4.44301300	0.76709200	2.79046900
C	10.01392500	0.05009200	-0.73248500
C	11.49903800	0.03121900	-0.34716200
H	9.80419900	0.95525100	-1.32084000
H	9.80223700	-0.79936700	-1.39816300
C	12.43960000	0.08501000	-1.55606300
H	11.70981800	0.87955900	0.31876500
H	11.70868300	-0.87386600	0.23944100
H	13.49052700	0.07180700	-1.24740800
H	12.27740900	-0.77038400	-2.22246700
H	12.27629600	0.99600200	-2.14356700
C	-1.67792100	0.00376100	-0.05684400
C	-3.80559800	-0.69309300	-0.44293300
C	-3.81768000	0.66836600	-0.43255800
N	-2.50944700	1.08043300	-0.19557600
N	-2.49022700	-1.08533900	-0.21160600
Cl	-5.13252200	1.74007100	-0.65449700
Cl	-5.10139000	-1.78405700	-0.68198500
C	-1.67527600	3.12431200	-1.27371800
C	-2.07431400	2.45885900	-0.09733200
C	-2.06403700	3.07118300	1.17179900
C	-1.61627100	4.39671000	1.24002900
C	-1.20693400	5.07895700	0.09737500
C	-1.23956900	4.44913400	-1.14419900
H	-1.58641400	4.89950600	2.20170700
H	-0.86233400	6.10611400	0.17453800
H	-0.91807600	4.99212900	-2.02762600
C	-1.60023100	-3.09802200	-1.30584200
C	-1.14874100	-4.41875100	-1.18835400
C	-1.13143200	-5.06803300	0.04311200
C	-1.57017500	-4.40909900	1.18837500
C	-2.03466000	-3.08894700	1.13206400
C	-2.03228400	-2.45742300	-0.12754500
H	-0.80327500	-4.94303700	-2.07378800
H	-0.77484400	-6.09176000	0.11067600
H	-1.55029600	-4.92592300	2.14263100
C	-1.69090700	2.46403700	-2.64884800
H	-2.09938600	1.45529300	-2.54010000
C	-0.26386400	2.31910100	-3.21355800
H	-0.28893700	1.79918500	-4.17707500
H	0.20171800	3.29741900	-3.37276900
H	0.37492100	1.74871900	-2.53153700
C	-2.60424900	3.22100300	-3.63304800
H	-2.64964700	2.68970400	-4.58986900
H	-3.62339000	3.30933300	-3.24402600
H	-2.23041000	4.23074100	-3.83255700
C	-2.50624700	2.35677900	2.44532700
H	-2.85657000	1.35680300	2.17403800
C	-1.32675700	2.17588700	3.42138400
H	-0.50930500	1.61944800	2.95175200
H	-0.93130800	3.14198500	3.75255100
H	-1.65203500	1.62571700	4.31073200
C	-3.68475900	3.08257100	3.12405100
H	-4.02489700	2.51416400	3.99601300
H	-3.39709100	4.08016700	3.47161800
H	-4.53106700	3.19496300	2.43913300
C	-1.60155600	-2.41885700	-2.67161700
C	-2.50176000	-2.39732800	2.40895700
C	-2.52855100	-3.14833400	-3.66442000
H	-2.56363100	-2.60721600	-4.61582600
H	-2.17276800	-4.16313700	-3.87266100
H	-3.54936800	-3.22253900	-3.27677400
C	-3.66442800	-3.15757600	3.07655100
H	-4.50474300	-3.28611800	2.38715000
H	-3.35349200	-4.15041600	3.41825700
H	-4.02220300	-2.60375100	3.95081700
C	-0.17278800	-2.29142100	-3.23563900
H	0.27623200	-3.27458000	-3.41326400
H	-0.18977000	-1.75523100	-4.19054900
H	0.47664100	-1.74374400	-2.54517000
H	-1.99044000	-1.40381000	-2.54943000
Cu	0.22487700	0.01190000	0.28852100

H	2.11407900	-0.11437700	2.73326100
C	-1.33158300	-2.19422900	3.39189400
H	-1.67552400	-1.66083000	4.28476700
H	-0.91229900	-3.15303200	3.71527200
H	-0.52654100	-1.61177500	2.93223800
H	-2.87663700	-1.40413400	2.14487200
C	2.71894500	-0.05934900	1.82182100
C	2.10170500	0.00903500	0.62230100
H	2.79450400	0.06069300	-0.22958200

13

C	7.84111500	-0.19504900	0.13046400
C	6.70618200	0.12950100	-0.84932300
H	7.63087300	0.28151200	1.09875200
H	7.85703200	-1.27758500	0.32206000
C	5.32484500	-0.32448500	-0.35953000
H	6.68640300	1.21284500	-1.03482300
H	6.91829300	-0.34112400	-1.81980400
H	5.33910700	-1.41023700	-0.18775000
H	5.11583700	0.13645300	0.61640000
C	4.19409000	0.02145600	-1.33581900
C	2.81152200	-0.44691900	-0.83915900
H	4.39303500	-0.43496900	-2.31359500
H	4.16532800	1.10634500	-1.49906700
H	2.82650400	-1.53548200	-0.69540000
H	2.60444100	-0.01609800	0.14612000
C	9.22276900	0.25166300	-0.36397100
C	10.35830300	-0.06087800	0.61901800
H	9.20514900	1.33287200	-0.56345700
H	9.43662400	-0.23073700	-1.32864600
C	11.73449000	0.38629600	0.11511300
H	10.14585300	0.42357600	1.58193700
H	10.37533200	-1.14082700	0.82006500
H	12.52241900	0.15143200	0.83854500
H	11.99050400	-0.10947900	-0.82841500
H	11.75825100	1.46753800	-0.06376800
C	1.71663500	-0.12119200	-1.78537200
C	1.28633900	0.15641900	-2.93280100
C	-1.40802100	0.01037400	-0.17459400
C	-2.90008800	0.64216100	1.42713500
C	-2.91376900	-0.71399000	1.37440200
N	-1.98693900	-1.09273700	0.40250500
N	-1.98280400	1.07686500	0.47156000
Cl	-3.88196500	-1.80891000	2.26703800
Cl	-3.78207800	1.68215300	2.46295500
C	-0.73484600	-3.15388000	0.89315700
C	-1.66439500	-2.46856800	0.07954700
C	-2.31676800	-3.08199300	-1.01141800
C	-1.97629900	-4.41002400	-1.30068500
C	-1.04204200	-5.10077500	-0.53496500
C	-0.43617800	-4.47946700	0.55308100
H	-2.45855800	-4.91183100	-2.13323200
H	-0.79446700	-6.12979200	-0.77916000
H	0.27604400	-5.03453700	1.15537300
C	-0.60200300	3.08543600	0.80143200
C	-0.37320800	4.43828600	0.52000700
C	-1.20967000	5.14806400	-0.33669800
C	-2.29980000	4.51749500	-0.92852600
C	-2.58135900	3.16674700	-0.68553100
C	-1.70985600	2.47026500	0.18002500
H	0.46777700	4.94367400	0.98356400
H	-1.01384100	6.19700900	-0.53975500
H	-2.94842900	5.08305100	-1.58998200
C	-0.08697500	-2.54304400	2.13484700
H	-0.37128200	-1.48809900	2.18871500
C	1.45083600	-2.60021200	2.08207300
H	1.87358500	-2.09982800	2.95973600
H	1.81523800	-3.63273900	2.08546700
H	1.84012800	-2.10797900	1.18941700
C	-0.59305100	-3.23180600	3.42029000
H	-0.16056100	-2.74692800	4.30198000
H	-1.68136700	-3.18607000	3.50573900
H	-0.29732000	-4.28627800	3.44095600
C	-3.40491900	-2.39352900	-1.83155000
H	-3.40430000	-1.33020800	-1.57880700
C	-3.15587200	-2.49799200	-3.34753100
H	-2.17968400	-2.08671700	-3.61709900
H	-3.20559300	-3.53418300	-3.69836000
H	-3.92173800	-1.93202600	-3.88808000
C	-4.79439400	-2.95931600	-1.46824300
H	-5.57513900	-2.43099600	-2.02586500
H	-4.86401400	-4.02346800	-1.71946600
H	-5.00724300	-2.85262200	-0.40042800

C	0.30797700	2.35712000	1.78629100
C	-3.81115000	2.53651200	-1.33609600
C	-0.00185100	2.78246700	3.23683400
H	0.62985800	2.22810100	3.93928400
H	0.19268900	3.85096300	3.38017600
H	-1.04749800	2.59483400	3.49766200
C	-5.11281900	3.15454600	-0.78388100
H	-5.17927200	3.06142300	0.30324700
H	-5.18057300	4.21852500	-1.03531100
H	-5.98208500	2.65326000	-1.22281800
C	1.79993400	2.56478300	1.46852000
H	2.11166400	3.60138000	1.63382600
H	2.41217600	1.93377600	2.12147800
H	2.02556200	2.30694000	0.42992000
H	0.10785700	1.28541100	1.70459200
Cu	-0.32273600	0.13901700	-1.82324100
H	-1.35296100	0.47724400	-2.94968300
C	-3.77261500	2.65286500	-2.87212700
H	-4.64763900	2.15460700	-3.30375200
H	-3.79554800	3.69867400	-3.19710600
H	-2.87421000	2.17794300	-3.27427500
H	-3.81846600	1.46980500	-1.09394000
H	1.35597600	0.36008600	-3.98398700

TS4

C	8.43488500	-0.02328800	0.26203500
C	7.20442000	-0.02299000	-0.65417000
H	8.38855200	0.84817400	0.93097300
H	8.40097200	-0.90783300	0.91432000
C	5.87281200	-0.03882200	0.10772400
H	7.23788500	0.86168400	-1.30610100
H	7.24947100	-0.89443800	-1.32298000
H	5.83804100	-0.92534400	0.75755100
H	5.83018300	0.83111000	0.77917400
C	4.64194200	-0.03232400	-0.80700000
C	3.31226000	-0.04461000	-0.03204900
H	4.67399700	-0.90321200	-1.47552000
H	4.66891800	0.85444200	-1.45456900
H	3.27728100	-0.92569400	0.62419100
H	3.28073700	0.81226700	0.65546100
C	9.76727100	-0.00642700	-0.49783000
C	10.99716500	-0.00443600	0.41910700
H	9.80189500	0.87750500	-1.15104000
H	9.81567400	-0.87847300	-1.16596600
C	12.32391400	0.01279900	-0.34716200
H	10.94870700	0.86708900	1.08633800
H	10.96270200	-0.88776900	1.07150300
H	13.18100200	0.01441800	0.33461600
H	12.41715000	-0.86517000	-0.99688400
H	12.40236300	0.90266700	-0.98249700
C	2.07836800	-0.02788100	-0.87635500
C	1.77634700	-0.01522500	-2.12900400
C	-1.53466900	0.00238500	-0.11840700
C	-3.40821800	0.69482000	0.97424700
C	-3.42057900	-0.66331300	0.96959600
N	-2.27033900	-1.07798200	0.29862300
N	-2.25098100	1.09299900	0.30535200
Cl	-4.57668700	-1.73606400	1.63501000
Cl	-4.54383100	1.78378500	1.64850300
C	-1.12770100	-3.11472500	1.05855000
C	-1.89406200	-2.45696800	0.07412400
C	-2.31832000	-3.09036800	-1.11271200
C	-1.93083000	-4.42296700	-1.30334700
C	-1.16302400	-5.09418200	-0.35566200
C	-0.76996300	-4.44635600	0.81226900
H	-2.23928100	-4.94195000	-2.20548500
H	-0.87448000	-6.12749800	-0.52544400
H	-0.17802800	-4.98258000	1.54753500
C	-1.06045900	3.10453900	1.05987300
C	-0.68988400	4.43377200	0.81952200
C	-1.09491900	5.09757800	-0.33525100
C	-1.88639100	4.44467200	-1.27628300
C	-2.28823200	3.11567000	-1.09070100
C	-1.85426700	2.46674900	0.08416400
H	-0.07809200	4.95533300	1.54905700
H	-0.79621500	6.12874800	-0.50044500
H	-2.20185600	4.97531400	-2.16919700
C	-0.69649900	-2.44908000	2.36216100
H	-1.06170700	-1.41822200	2.35777300
C	0.83781800	-2.38532800	2.48540600
H	1.12017600	-1.86412300	3.40646100
H	1.27995200	-3.38688800	2.52104100
H	1.27502600	-1.84792100	1.63940800

C	-1.32060500	-3.15347700	3.58344200
H	-1.04656800	-2.62678000	4.50367500
H	-2.41243100	-3.17774800	3.51684300
H	-0.96570100	-4.18569400	3.67278000
C	-3.19152900	-2.40392500	-2.15923800
H	-3.31508200	-1.35738100	-1.86742200
C	-2.53418300	-2.40865800	-3.55238700
H	-1.55438000	-1.92340200	-3.52545600
H	-2.40447900	-3.42640600	-3.93548800
H	-3.16488300	-1.86570200	-4.26451200
C	-4.59564200	-3.04030200	-2.21112400
H	-5.22623500	-2.50635800	-2.92998500
H	-4.54423200	-4.08823200	-2.52587800
H	-5.08850000	-3.00648100	-1.23481000
C	-0.61351200	2.42042600	2.34835200
C	-3.18252300	2.44782400	-2.13140700
C	-1.22955000	3.10291900	3.58610900
H	-0.94283500	2.56513000	4.49603200
H	-0.88016500	4.13612900	3.68589200
H	-2.32215700	3.12141100	3.53101200
C	-4.57495200	3.10978000	-2.17328100
H	-5.06169100	3.08418400	-1.19369700
H	-4.50686000	4.15678600	-2.48789800
H	-5.21998600	2.58792200	-2.88817600
C	0.92212400	2.36213300	2.45624900
H	1.36043700	3.36452300	2.50970500
H	1.21507000	1.82259000	3.36331600
H	1.35384700	1.84478800	1.59497900
H	-0.97270700	1.38766700	2.33038800
Cu	0.08332300	-0.00637100	-1.12455500
H	0.12453800	0.00500900	-2.69610600
C	-2.53399000	2.44293300	-3.52885600
H	-3.18019200	1.91526600	-4.23859700
H	-2.38567200	3.45910300	-3.90941500
H	-1.56411000	1.93763700	-3.50950300
H	-3.32334600	1.40315700	-1.84046800
H	2.16006300	-0.01047500	-3.13616500
14			
C	-8.25412700	0.24909500	0.07255500
C	-7.07479000	1.15214100	-0.31097800
H	-8.22603600	-0.66473200	-0.53847800
H	-8.13403300	-0.08001900	1.11491100
C	-5.70379100	0.48500000	-0.13906600
H	-7.19157300	1.47743000	-1.35483200
H	-7.10865500	2.06807200	0.29658100
H	-5.59298800	0.15292300	0.90369500
H	-5.66535500	-0.42726000	-0.75234100
C	-4.52621100	1.39709800	-0.50771300
C	-3.15777900	0.72535400	-0.31195900
H	-4.57642600	2.31130900	0.09997000
H	-4.63426000	1.72142400	-1.55196400
H	-3.09402300	0.36709900	0.72754800
H	-3.13068600	-0.19623100	-0.91466300
C	-9.62208400	0.92412600	-0.08914600
C	-10.80273800	0.02582400	0.30117700
H	-9.74557000	1.25057200	-1.13194900
H	-9.64860700	1.83978200	0.51931400
C	-12.16365500	0.71149200	0.14130200
H	-10.77911300	-0.88774300	-0.30877500
H	-10.67826700	-0.30183700	1.34247300
H	-12.98489100	0.04543500	0.42664800
H	-12.23008400	1.60899100	0.76722500
H	-12.33148400	1.02088300	-0.89687600
C	-1.89438500	1.53173700	-0.61658300
C	-1.99550600	2.79729600	-1.07619900
C	1.55055800	-0.09537400	-0.01042500
C	3.18679100	-1.63159500	0.34228500
C	3.77046000	-0.40177000	0.36325900
N	2.75752700	0.52785800	0.14611500
N	1.82877000	-1.42845200	0.11329300
Cl	5.41296600	0.01299300	0.60134200
Cl	3.90120000	-3.17227700	0.54791500
C	2.80235200	2.70192200	1.28831400
C	2.93960100	1.96406600	0.09549200
C	3.23802300	2.56077800	-1.14558300
C	3.38272900	3.95367100	-1.16891700
C	3.24182300	4.71227300	-0.00978000
C	2.95732800	4.09140000	1.20358300
H	3.60560800	4.44964100	-2.10834800
H	3.35585600	5.79154600	-0.05198100
H	2.85097000	4.69387600	2.10029200
C	0.17015400	-2.88238100	1.19523300

C	-0.80055800	-3.88444100	1.06978500
C	-1.09167800	-4.45586800	-0.16615500
C	-0.41386700	-4.03774200	-1.30830300
C	0.56727000	-3.04034500	-1.24429100
C	0.83321900	-2.47662300	0.01960100
H	-1.33677400	-4.21962100	1.95216400
H	-1.84928200	-5.23068300	-0.23926600
H	-0.65024400	-4.49043000	-2.26611000
C	2.48868100	2.05732500	2.63497500
H	2.46325600	0.97254000	2.49829600
C	1.09876200	2.48416200	3.14612000
H	0.87210000	1.98161300	4.09256100
H	1.05368700	3.56446200	3.32076800
H	0.31754900	2.22521500	2.42436100
C	3.58274300	2.35753000	3.67804000
H	3.36664900	1.82843500	4.61210300
H	4.56844900	2.03817300	3.32563300
H	3.63750300	3.42655300	3.90853800
C	3.39047600	1.76209100	-2.43638800
H	3.32210200	0.69831800	-2.19171500
C	2.24642000	2.07606900	-3.42048900
H	1.27146100	1.86177800	-2.97151300
H	2.25744500	3.12969100	-3.71941600
H	2.34800800	1.46905400	-4.32646800
C	4.76692400	1.98909100	-3.09066800
H	4.87014100	1.35366700	-3.97645100
H	4.89482200	3.02784400	-3.41241800
H	5.58142200	1.74705300	-2.40096200
C	0.45700700	-2.27550300	2.56524600
C	1.28314200	-2.60119400	-2.51785500
C	0.93364600	-3.34037100	3.57178500
H	1.18729900	-2.86823200	4.52667600
H	0.15652500	-4.08653100	3.76750100
H	1.82089400	-3.86607400	3.20571000
C	2.00703600	-3.77824400	-3.19995200
H	2.71720000	-4.25793200	-2.51926400
H	1.30033300	-4.54117600	-3.54275500
H	2.56047900	-3.42259900	-4.07528900
C	-0.76751800	-1.50890800	3.10281000
H	-1.62128200	-2.17754000	3.25633800
H	-0.52977600	-1.04337800	4.06526100
H	-1.07528600	-0.72065800	2.40830600
H	1.26757600	-1.54954200	2.45611900
Cu	-0.17534000	0.72116200	-0.32332900
H	-1.11423100	3.39704000	-1.30212900
C	0.31032000	-1.90604400	-3.49101400
H	0.84885200	-1.55495200	-4.37775200
H	-0.47602100	-2.59100600	-3.82607800
H	-0.17142300	-1.04362100	-3.01922300
H	2.04632300	-1.86660000	-2.24634300
H	-2.94683400	3.30741500	-1.25291200

15

C	1.28111300	-0.00667300	-0.17601000
C	2.81574500	-0.66813500	1.36229600
C	2.80914400	0.69319000	1.35168500
N	1.86337200	1.08389900	0.40858900
N	1.87459300	-1.08231100	0.42477000
Cl	3.75208800	1.78400400	2.27184300
Cl	3.76622200	-1.73636700	2.30093600
C	0.55501100	3.12277400	0.82573400
C	1.54357100	2.45700300	0.07313600
C	2.23829300	3.06819700	-0.99019100
C	1.89651700	4.38964100	-1.30426400
C	0.91554900	5.07028900	-0.58827400
C	0.25662400	4.44304400	0.46552000
H	2.40673700	4.89084000	-2.12082700
H	0.66610900	6.09436500	-0.85028000
H	-0.50265600	4.98589900	1.01959600
C	0.57483100	-3.12338700	0.85658400
C	0.29281200	-4.45238100	0.51588800
C	0.97390300	-5.09318000	-0.51542800
C	1.96055900	-4.41724400	-1.22810900
C	2.28649600	-3.08754500	-0.93274000
C	1.57022600	-2.46323800	0.10836300
H	-0.47071800	-4.99150700	1.06777200
H	0.73726400	-6.12397700	-0.76248300
H	2.48780300	-4.92872400	-2.02727300
C	-0.17841200	2.47925400	1.99892700
H	0.18624700	1.45424700	2.11158000
C	-1.69569800	2.39789800	1.74544800
H	-2.19109900	1.89485500	2.58259400
H	-2.13806200	3.39534400	1.64982400

H	-1.92380500	1.83896100	0.83389900
C	0.11991600	3.21908600	3.31875300
H	-0.37037700	2.70950200	4.15487800
H	1.19386900	3.25598000	3.52470500
H	-0.25352900	4.24822800	3.29158500
C	3.32664700	2.36112300	-1.79253100
H	3.45682500	1.35514300	-1.38371900
C	2.92114800	2.20033700	-3.27058900
H	1.98139600	1.64663600	-3.36348600
H	2.79056100	3.17246300	-3.75755900
H	3.69671800	1.65388400	-3.81777400
C	4.68167000	3.08421800	-1.66167000
H	5.45874700	2.52800800	-2.19641600
H	4.64149200	4.09198300	-2.08816600
H	4.98640300	3.17419600	-0.61439800
C	-0.18284200	-2.46402800	2.00519500
C	3.38003400	-2.38477100	-1.73177600
C	0.09765600	-3.17774700	3.34314700
H	-0.41074000	-2.65715500	4.16150700
H	-0.26698300	-4.21029500	3.32810600
H	1.16823600	-3.20210600	3.56792700
C	4.73861600	-3.09577800	-1.57388800
H	5.03204700	-3.16650900	-0.52191300
H	4.71071300	-4.11051900	-1.98445800
H	5.51766700	-2.54241900	-2.10872100
C	-1.69621200	-2.39742100	1.72411800
H	-2.12991900	-3.39916900	1.63407600
H	-2.20811600	-1.88647900	2.54653300
H	-1.91099000	-1.85165000	0.80087200
H	0.17237700	-1.43458700	2.10557200
Cu	-0.00634700	-0.03412500	-1.63085600
C	2.99138700	-2.24951300	-3.21702400
H	2.87580300	-3.23020300	-3.69050200
H	2.04786900	-1.70608500	-3.33032900
H	3.76897000	-1.70451400	-3.76278300
H	3.49824100	-1.37192200	-1.33636500
H	-0.95401900	-0.07311800	-2.82426000
C	-7.05639600	0.65923800	-1.59794400
C	-6.76329500	-0.17393300	-0.33137700
H	-7.10940300	1.72804900	-1.36949000
H	-6.29631300	0.50443000	-2.36603500
H	-8.02467600	0.34924100	-2.00222900
C	-6.66197300	-1.67297600	-0.68691000
C	-7.86649100	0.05133900	0.72180100
H	-6.44686400	-2.27940000	0.19817100
H	-7.62157400	-1.99993800	-1.09865200
H	-5.88598800	-1.85733300	-1.43231500
H	-8.82607800	-0.27346300	0.30967800
H	-7.67043300	-0.52154200	1.63192000
H	-7.94731800	1.10719100	0.99308600
C	-5.44306500	0.29121000	0.28958300
O	-5.25879500	0.74125500	1.37286000
Br	-3.82124400	0.09492800	-0.93162900

TS5

C	0.06505100	-0.44194100	-0.09670500
C	-0.42756100	-2.61605200	0.36223300
C	0.91272400	-2.46626800	0.51014000
N	1.20807400	-1.13592900	0.22096700
N	-0.94307500	-1.36701900	0.00943300
Cl	2.06662600	-3.63315500	0.99459900
Cl	-1.36469300	-4.03869900	0.52876600
C	2.99554000	0.09477400	1.38364600
C	2.55275600	-0.58711700	0.22775700
C	3.37960700	-0.79971200	-0.89781300
C	4.68349400	-0.28970100	-0.83926000
C	5.14588000	0.39014000	0.28239400
C	4.30970000	0.57779300	1.37937900
H	5.34613200	-0.43345500	-1.68659200
H	6.16206700	0.77321200	0.30392100
H	4.68487100	1.10573600	2.24923900
C	-3.14446900	-0.99626400	1.03922600
C	-4.51536500	-0.75496200	0.87372300
C	-5.08223700	-0.64328400	-0.39199600
C	-4.29043900	-0.78867200	-1.52820800
C	-2.91463400	-1.03441100	-1.43089300
C	-2.36217800	-1.10627400	-0.13250900
H	-5.14623100	-0.65661200	1.75158400
H	-6.14701100	-0.45495900	-0.49436700
H	-4.75097500	-0.72403000	-2.50797000
C	2.12843600	0.27598900	2.62807700
H	1.08228000	0.15871200	2.33256300
C	2.26399100	1.67804700	3.24916900

H	1.52365900	1.79892700	4.04632200
H	3.25112200	1.83135400	3.69788800
H	2.09467600	2.46175900	2.50718900
C	2.44762300	-0.80629800	3.68164700
H	1.80255800	-0.68289100	4.55824900
H	2.29933900	-1.81661500	3.29056300
H	3.48821700	-0.72675500	4.01551800
C	2.94696000	-1.57130300	-2.14400700
H	1.88330300	-1.81019900	-2.05019600
C	3.11332800	-0.73540900	-3.42822500
H	2.54247600	0.19371200	-3.36526800
H	4.16486400	-0.49483400	-3.61788200
H	2.74642200	-1.30530900	-4.28908000
C	3.72336400	-2.89902400	-2.27675000
H	3.35618300	-3.46283400	-3.14093500
H	4.79179700	-2.71323100	-2.43158300
H	3.61731800	-3.52826000	-1.38984700
C	-2.59022500	-1.16078100	2.45576100
C	-2.09414500	-1.29852800	-2.69180800
C	-3.29009200	-2.31889000	3.19791200
H	-2.81149100	-2.48182700	4.16917100
H	-4.34510100	-2.09227600	3.38395300
H	-3.24034700	-3.25279500	2.63277700
C	-2.23342900	-2.77584500	-3.11981600
H	-1.92657600	-3.46178700	-2.32533700
H	-3.27167800	-3.00967500	-3.38093600
H	-1.61122700	-2.97416000	-3.99903300
C	-2.69715600	0.13537000	3.28241500
H	-3.73815000	0.46287600	3.37604200
H	-2.31199800	-0.03724500	4.29308100
H	-2.12058300	0.94773000	2.83631000
H	-1.52807600	-1.41127600	2.38767800
Cu	0.26405600	1.28490800	-1.04744400
C	-2.46039800	-0.37108600	-3.86302700
H	-3.46966600	-0.56244600	-4.24264700
H	-2.39502300	0.68302200	-3.58004200
H	-1.76486400	-0.53741300	-4.69153200
H	-1.04328400	-1.11048200	-2.45941800
H	0.57490700	1.04204700	-2.58612100
C	-1.82330200	4.90578300	0.38522500
C	-1.93526500	3.42163900	-0.04023700
H	-1.77911300	5.00400200	1.47313900
H	-0.94175300	5.37871500	-0.05027600
H	-2.71551000	5.42812100	0.02499200
C	-2.01992800	3.30153900	-1.56511600
C	-3.17982700	2.78469100	0.61251100
H	-2.08104100	2.25721600	-1.88461100
H	-2.93210300	3.80592000	-1.89948400
H	-1.16839400	3.76870800	-2.06072100
H	-4.06707800	3.30067700	0.23350800
H	-3.26945000	1.72641000	0.36210500
H	-3.15795900	2.88898300	1.69919500
C	-0.70637500	2.71042600	0.59038000
O	-0.51218600	2.45145400	1.72549800
Br	1.24474000	3.51158600	-0.53144600

16

C	0.16510500	-0.41387500	-0.06438300
C	-0.07711600	-2.66126700	-0.12700400
C	1.22559600	-2.40010100	0.15072600
N	1.37042300	-1.01290800	0.18379900
N	-0.72958500	-1.42963800	-0.23255900
Cl	2.49922400	-3.50371900	0.42908700
Cl	-0.84505400	-4.16891000	-0.36168300
C	3.01062100	0.12471300	1.62985400
C	2.64278800	-0.32927500	0.34339600
C	3.47804700	-0.19168400	-0.78762300
C	4.71531900	0.43617700	-0.59556100
C	5.10484200	0.89814400	0.65717300
C	4.26169800	0.74240500	1.75357800
H	5.38288200	0.56058400	-1.44207500
H	6.07058800	1.37937300	0.78121600
H	4.58179900	1.10329000	2.72453300
C	-2.97920200	-1.48744000	0.74938700
C	-4.35774100	-1.30428600	0.58123500
C	-4.89703100	-0.96019800	-0.65613600
C	-4.06874700	-0.81233000	-1.76495400
C	-2.68061700	-0.97629100	-1.66140600
C	-2.16319300	-1.28128500	-0.38609100
H	-5.01878200	-1.44549000	1.43046600
H	-5.96947700	-0.82401500	-0.75948800
H	-4.50530900	-0.57395400	-2.72952700
C	2.13768300	-0.07528000	2.86770000

H	1.10374900	-0.20531100	2.53686500
C	2.15007400	1.14035200	3.81112400
H	1.41231500	0.99112200	4.60568600
H	3.12376500	1.27354100	4.29406500
H	1.89037800	2.05940900	3.28219600
C	2.55880700	-1.34569200	3.63750800
H	1.90960400	-1.49096500	4.50750300
H	2.50009400	-2.24357800	3.01680800
H	3.58972900	-1.25591700	3.99783000
C	3.12088600	-0.70327700	-2.18224100
H	2.09770000	-1.08959700	-2.15795400
C	3.15560100	0.42411400	-3.23354000
H	2.50125000	1.25272100	-2.95021500
H	4.16894400	0.81750300	-3.36561100
H	2.82305000	0.03767500	-4.20286400
C	4.05008300	-1.85821000	-2.61120700
H	3.74321800	-2.24288900	-3.58956600
H	5.08694100	-1.51647400	-2.69861200
H	4.02841100	-2.68602900	-1.89788600
C	-2.44656800	-1.95490100	2.10566500
C	-1.81432600	-0.89057600	-2.91596700
C	-3.07797600	-3.30484200	2.50736100
H	-2.61080000	-3.67596500	3.42538800
H	-4.15052200	-3.20035400	2.70150100
H	-2.94788100	-4.06051900	1.72846000
C	-2.07495600	-2.10481100	-3.83221200
H	-1.89371500	-3.04876700	-3.30913700
H	-3.10925300	-2.11375500	-4.19272900
H	-1.41552400	-2.06670100	-4.70562900
C	-2.65378200	-0.91729800	3.22461000
H	-3.71476000	-0.68357400	3.36351600
H	-2.27643500	-1.31775300	4.17159400
H	-2.12227400	0.01273900	3.01535500
H	-1.36836800	-2.11418700	2.01995700
Cu	0.01358600	1.47218000	-0.41056800
C	-2.01495300	0.42836600	-3.68453800
H	-3.03735800	0.52630900	-4.06415700
H	-1.80254000	1.29614500	-3.05402400
H	-1.33933500	0.46333400	-4.54533800
H	-0.76427900	-0.92720800	-2.61415200
H	0.74567200	0.91362600	-1.61715800
C	-2.05526700	4.43735400	1.29139400
C	-2.38016800	2.95775100	0.97998900
H	-1.66220200	4.54094800	2.30696000
H	-1.32015900	4.83693200	0.58970100
H	-2.97235500	5.03280000	1.21356800
C	-2.94394200	2.81785300	-0.43903900
C	-3.41088200	2.44192500	2.00349700
H	-3.15433100	1.77217500	-0.68449600
H	-3.88663900	3.37123900	-0.51792700
H	-2.25549500	3.22124400	-1.18551800
H	-4.30625400	3.07235900	1.96555700
H	-3.71560200	1.41547600	1.78299700
H	-3.00616200	2.47543800	3.01812700
C	-1.03786800	2.15675800	1.17683700
O	-0.57523700	2.04443600	2.29172400
Br	0.60885700	3.61836800	-1.16007000

17

C	-7.92401100	-3.44017000	-0.68036200
C	-6.61065900	-2.86443400	-0.13530100
H	-8.06414400	-3.10433700	-1.71799900
H	-7.84808200	-4.53618700	-0.72478200
C	-5.37862300	-3.25142500	-0.96354000
H	-6.68690100	-1.76825600	-0.08981500
H	-6.47024300	-3.20081500	0.90204400
H	-5.30204500	-4.34751200	-1.00842000
H	-5.51917500	-2.91540500	-2.00109300
C	-4.06544700	-2.67585300	-0.41846000
C	-2.82855600	-3.06334700	-1.25140900
H	-3.92258500	-3.01540800	0.61752500
H	-4.13467300	-1.58009000	-0.37194800
H	-2.79326000	-4.16323600	-1.31478800
H	-2.94724000	-2.69528700	-2.27988800
C	-9.15583000	-3.05226400	0.14732400
C	-10.46932200	-3.62783000	-0.39745400
H	-9.23287800	-1.95612100	0.19239200
H	-9.01694500	-3.38849000	1.18505200
C	-11.69406700	-3.23482700	0.43514500
H	-10.60847500	-3.29199300	-1.43426400
H	-10.39281200	-4.72294100	-0.44133600
H	-12.61405200	-3.66191400	0.02207800
H	-11.59903900	-3.58630500	1.46912900

H	-11.81795400	-2.14608000	0.46749700
C	2.65484100	-0.38231100	0.12953400
C	4.22413300	0.44493300	1.54884900
C	4.83957900	0.19630700	0.36010900
N	3.86751300	-0.30957100	-0.49826800
N	2.88818400	0.08704800	1.39246300
Cl	6.47543300	0.43116300	-0.08159300
Cl	4.88232900	1.07153000	2.99804500
C	3.93191300	0.23151300	-2.89364800
C	4.10012200	-0.71985500	-1.86781700
C	4.48406100	-2.05334100	-2.11451700
C	4.69237800	-2.42425500	-3.44888800
C	4.52743200	-1.50952800	-4.48549100
C	4.15171500	-0.19776500	-4.20865900
H	4.98565100	-3.44408300	-3.67776900
H	4.69276900	-1.82005200	-5.51305900
H	4.02488400	0.50521600	-5.02595700
C	1.15624100	1.40811800	2.52640000
C	0.15785700	1.47736700	3.50612700
C	-0.10945100	0.39468600	4.33986400
C	0.62066400	-0.78425500	4.21375000
C	1.62957200	-0.91278200	3.25061800
C	1.86896000	0.19737500	2.41627300
H	-0.41932000	2.39026200	3.61365700
H	-0.88923700	0.47057100	5.09210500
H	0.40368900	-1.61965100	4.87226500
C	3.51646500	1.67552700	-2.63008100
H	3.44854600	1.82145000	-1.54852600
C	2.12129900	1.96798300	-3.21642800
H	1.81838500	2.99383600	-2.98118200
H	2.11702300	1.85841800	-4.30618300
H	1.36975200	1.28663000	-2.80492000
C	4.56398400	2.67480700	-3.15835500
H	4.27152600	3.69794000	-2.90006100
H	5.55098000	2.48315800	-2.72609100
H	4.65750400	2.62252000	-4.24820600
C	4.66974000	-3.08564600	-1.00691300
H	4.47411100	-2.59856700	-0.04748600
C	3.65848800	-4.24068900	-1.14423400
H	2.62960000	-3.86754900	-1.14212400
H	3.81386600	-4.79861800	-2.07377400
H	3.77055200	-4.94268800	-0.31099700
C	6.11645900	-3.61598000	-0.96319900
H	6.23809900	-4.31035400	-0.12522500
H	6.37362200	-4.15508400	-1.88106700
H	6.83699700	-2.80187000	-0.83797500
C	1.41844100	2.61179300	1.62670500
C	2.40900300	-2.21948400	3.14164400
C	1.78227500	3.86625800	2.44441100
H	2.02685100	4.69460000	1.77128200
H	0.94974500	4.19030000	3.07746000
H	2.64719500	3.68472900	3.08999100
C	3.16364300	-2.53849900	4.44709600
H	3.83941500	-1.72421900	4.72624400
H	2.47257000	-2.70324200	5.28039900
H	3.75952000	-3.44912400	4.32515200
C	0.22104000	2.88307300	0.69503600
H	-0.67977500	3.13953800	1.26148900
H	0.44426500	3.72168100	0.02706600
H	-0.00682700	2.00712200	0.07930500
H	2.27794500	2.38283700	0.99034500
Cu	0.98380400	-1.03735900	-0.58877300
H	-1.32419500	-2.89945700	0.33786100
C	1.49168900	-3.38761800	2.73016900
H	2.07852100	-4.30448800	2.60950900
H	0.72505100	-3.57919200	3.48848400
H	0.98547000	-3.17817500	1.78245200
H	3.15941800	-2.10609700	2.35401600
C	-1.52984900	-2.54231500	-0.67745200
C	-0.65783800	-1.70807000	-1.28460900
H	-0.97936300	-1.42242800	-2.29970400
C	-4.68621700	1.90658300	-1.52878800
C	-5.13210600	2.76447800	-0.32504600
H	-4.32008200	2.52497400	-2.35051600
H	-3.90025300	1.19970400	-1.24636200
H	-5.54809300	1.33417300	-1.88462900
C	-5.65448700	1.86075100	0.81020000
C	-6.22419300	3.76825200	-0.75352100
H	-5.96368000	2.44994300	1.67751500
H	-6.52088900	1.29986400	0.44820500
H	-4.89162200	1.14784800	1.13330000
H	-7.09312900	3.20507000	-1.10689600

H	-6.54277000	4.39461800	0.08523100
H	-5.88121800	4.41657500	-1.56212700
C	-3.92722200	3.52790800	0.22923000
O	-3.44815700	3.47325000	1.31211300
Br	-3.05640400	4.80685700	-1.11203600

TS6

C	9.08695500	0.59035700	-0.91458600
C	7.82782100	0.13980000	-0.16273100
H	9.01821100	0.26543900	-1.96286000
H	9.12078100	1.68909800	-0.93983900
C	6.52419200	0.66875900	-0.77449100
H	7.79574700	-0.95894600	-0.13648900
H	7.89495800	0.46569900	0.88520100
H	6.55200500	1.76785200	-0.79434200
H	6.46094500	0.34842500	-1.82460400
C	5.26534600	0.20831600	-0.02851800
C	3.95760300	0.73754400	-0.64709600
H	5.32484000	0.53252100	1.02014000
H	5.23495200	-0.88951800	-0.00602900
H	4.02183500	1.83666700	-0.69262400
H	3.87285200	0.39054800	-1.68596200
C	10.39006900	0.05815600	-0.30517900
C	11.64914800	0.50468100	-1.05943400
H	10.35608100	-1.04064800	-0.27796600
H	10.46156900	0.38452500	0.74248700
C	12.94565300	-0.03368900	-0.44558400
H	11.57716100	0.17928000	-2.10639000
H	11.68467800	1.60247500	-1.08509000
H	13.82452900	0.29970200	-1.00759300
H	13.06436100	0.30615500	0.58984300
H	12.95323500	-1.12982200	-0.43530800
C	-1.89661400	0.39556300	-0.17654800
C	-3.47771200	1.98048900	-0.59805900
C	-3.87789400	0.83684000	-1.21189700
N	-2.91141900	-0.12995000	-0.93782100
N	-2.26565800	1.70115700	0.02814600
Cl	-5.25867100	0.58408800	-2.19293800
Cl	-4.25802900	3.50422300	-0.56250400
C	-3.72421500	-2.45124000	-0.73576100
C	-2.96389200	-1.49052100	-1.43881800
C	-2.28751000	-1.78667400	-2.64291200
C	-2.36591300	-3.10145000	-3.11961100
C	-3.09230500	-4.07391000	-2.43878700
C	-3.76524400	-3.74813800	-1.26522600
H	-1.85858000	-3.36347500	-4.04238000
H	-3.14154000	-5.08645000	-2.82887700
H	-4.34070000	-4.51204500	-0.75256100
C	-1.61143800	2.83298300	2.11908900
C	-0.83219000	3.81209100	2.74904900
C	0.04218300	4.61767800	2.02505100
C	0.14922400	4.46857900	0.64562400
C	-0.60559400	3.50977700	-0.04185400
C	-1.46772000	2.69402200	0.72218300
H	-0.91648400	3.94877800	3.82195800
H	0.63630500	5.36913400	2.53706700
H	0.82587000	5.11016500	0.08973700
C	-4.53176400	-2.13915200	0.52373800
H	-4.25526200	-1.13803600	0.86917200
C	-4.23428600	-3.12026800	1.67363300
H	-4.77902800	-2.81032300	2.57185100
H	-4.56059000	-4.13695400	1.43045100
H	-3.16969000	-3.14529300	1.91431500
C	-6.04644500	-2.13763400	0.22327400
H	-6.60754100	-1.86786900	1.12434400
H	-6.30932600	-1.42976800	-0.56584400
H	-6.37990000	-3.13240100	-0.09220300
C	-1.53758700	-0.73739700	-3.46059200
H	-1.40535600	0.15159900	-2.83848900
C	-0.13223700	-1.20704500	-3.87885300
H	0.45289100	-1.53398100	-3.01548100
H	-0.17496000	-2.03436200	-4.59481100
H	0.40530900	-0.38486900	-4.36242300
C	-2.35661500	-0.32444600	-4.70214600
H	-1.82944100	0.45623800	-5.26099500
H	-2.50366800	-1.17752000	-5.37354000
H	-3.34315200	0.06015400	-4.42849800
C	-2.60316200	2.01501300	2.94233800
C	-0.48384500	3.41615500	-1.56137300
C	-3.85498000	2.85374100	3.27806100
H	-4.57971600	2.24689600	3.83140800
H	-3.59081700	3.71426500	3.90274400
H	-4.34572900	3.23272100	2.37730600

C	-0.99372700	4.70320700	-2.24209600
H	-2.02793700	4.92615600	-1.96536700
H	-0.37767000	5.56584900	-1.96641700
H	-0.94780600	4.59638800	-3.33114800
C	-1.97828000	1.44935100	4.23045600
H	-1.70258700	2.24353600	4.93228600
H	-2.70235700	0.80376100	4.73852200
H	-1.08984500	0.85189900	4.01352000
H	-2.92455000	1.16174500	2.33803300
Cu	-0.14958900	-0.43206700	0.35914000
H	2.74071200	0.62185000	1.18139900
C	0.95796000	3.10353400	-2.00451300
H	0.99419100	2.97686700	-3.09218300
H	1.64051700	3.92061200	-1.74623500
H	1.32591800	2.18852400	-1.53370400
H	-1.11256000	2.59071300	-1.90735800
C	2.71905900	0.33730600	0.12421500
C	1.65372500	-0.32468300	-0.35826900
H	1.73551100	-0.61470200	-1.41562600
C	0.50100400	-3.67073300	0.09058200
C	1.51981000	-3.36867100	1.19029700
H	-0.51791800	-3.68889100	0.48072600
H	0.55625800	-2.93024200	-0.71037700
H	0.72468200	-4.65508100	-0.33278600
C	2.95553500	-3.38639500	0.61965700
C	1.40407600	-4.40790200	2.33361800
H	3.69468400	-3.21111900	1.40538600
H	3.14311000	-4.37013500	0.17860500
H	3.07797800	-2.62168900	-0.14841700
H	1.61522300	-5.39951900	1.92133700
H	2.12620500	-4.20411400	3.12913000
H	0.40016500	-4.41372400	2.76230300
C	1.34567500	-1.99164500	1.86428100
O	2.08152300	-1.39072600	2.56337700
Br	-0.83295600	-1.78179500	2.56909700

18

C	3.39380200	-4.89881100	-0.68434900
C	4.48425200	-3.83246500	-0.84938900
H	2.93452500	-4.79544000	0.30930200
H	2.58946800	-4.70934500	-1.40933300
C	3.97219500	-2.39991400	-0.65219700
H	5.29533900	-4.02943900	-0.13348000
H	4.93273500	-3.92410600	-1.84887600
H	3.16027900	-2.19927600	-1.36448300
H	3.52744700	-2.30806000	0.34879900
C	5.06359300	-1.33595600	-0.82237300
C	4.54301100	0.09824400	-0.58960800
H	5.48900700	-1.40662400	-1.83260500
H	5.88884200	-1.53662500	-0.12606400
H	3.70414700	0.27939400	-1.27817200
H	4.14156800	0.18905600	0.42717200
C	3.90630700	-6.33401000	-0.85841700
C	2.81721700	-7.40059000	-0.68615800
H	4.71321200	-6.52195300	-0.13523100
H	4.36134600	-6.43964600	-1.85377700
C	3.33817700	-8.83150700	-0.85607500
H	2.36094800	-7.29313900	0.30768100
H	2.01262200	-7.21563700	-1.41101100
H	2.53749500	-9.56790400	-0.72923700
H	3.77115700	-8.97898800	-1.85223600
H	4.11877400	-9.05847200	-0.12064200
C	-2.29386500	0.25722700	0.13672700
C	-3.62344800	-0.36123600	1.86467900
C	-4.22703500	0.68718200	1.23875100
N	-3.40041700	1.05562900	0.18168000
N	-2.43946900	-0.61344000	1.17820800
Cl	-5.70473900	1.46226300	1.60882400
Cl	-4.14258000	-1.25076400	3.22860700
C	-4.38030100	1.85722700	-1.92338300
C	-3.66039800	2.13906300	-0.74523300
C	-3.17791900	3.42454300	-0.42719000
C	-3.43217400	4.44870600	-1.34801700
C	-4.13442400	4.20200900	-2.52469000
C	-4.60230300	2.92132600	-2.80662500
H	-3.07292800	5.45177400	-1.14057600
H	-4.31800100	5.01150900	-3.22501700
H	-5.14737700	2.74301100	-3.72815300
C	-1.64067300	-2.92199900	0.92277300
C	-0.70296200	-3.90440800	1.26467900
C	0.33405300	-3.63299800	2.15338100
C	0.45729500	-2.36792500	2.72218500
C	-0.45130400	-1.34596600	2.42007600

C	-1.48696300	-1.65235100	1.51463000
H	-0.78698500	-4.89447100	0.82803400
H	1.04794000	-4.41160300	2.40571000
H	1.27055400	-2.16909500	3.41322800
C	-4.90545700	0.46689600	-2.26826900
H	-4.66319100	-0.20766800	-1.44195800
C	-4.21729300	-0.09271300	-3.52894400
H	-4.57471400	-1.10690900	-3.73611200
H	-4.43286900	0.52437300	-4.40752800
H	-3.13060100	-0.13173700	-3.40406200
C	-6.43882700	0.46159200	-2.42386500
H	-6.79413400	-0.55721500	-2.61030700
H	-6.93318200	0.83470100	-1.52169000
H	-6.75973500	1.08368300	-3.26589500
C	-2.40381300	3.73264700	0.85059200
H	-2.32596900	2.81258400	1.43679000
C	-0.96660700	4.19369500	0.53850100
H	-0.42683100	3.44220700	-0.04619000
H	-0.96141600	5.12989600	-0.02968700
H	-0.41463200	4.36475600	1.46877900
C	-3.14241400	4.76638500	1.72341400
H	-2.59800500	4.92595900	2.66001700
H	-3.22298400	5.73406700	1.21735100
H	-4.15406200	4.42982700	1.97021000
C	-2.76413400	-3.25688100	-0.05363200
C	-0.28891900	0.02619200	3.06605200
C	-3.67316700	-4.37500000	0.49360200
H	-4.50009700	-4.56035000	-0.19972200
H	-3.12341700	-5.31432700	0.61414100
H	-4.09705900	-4.10550400	1.46579800
C	-0.40186300	-0.05494900	4.60117800
H	-1.35098700	-0.50471700	4.90840300
H	0.40869400	-0.65244700	5.03144400
H	-0.34276600	0.94779700	5.03702300
C	-2.20877100	-3.62436100	-1.44378100
H	-1.59196600	-4.52814500	-1.40160200
H	-3.03203700	-3.81449400	-2.14046900
H	-1.59413800	-2.81642000	-1.85264600
H	-3.38638200	-2.36639700	-0.18079600
Cu	-0.86538000	0.34378900	-1.11341700
H	6.05665400	1.15694900	-1.81205500
C	1.03350900	0.69389000	2.64086900
H	1.10350000	1.69964200	3.06861700
H	1.89959400	0.12185800	2.99034000
H	1.10302000	0.77901100	1.55205000
H	-1.10103800	0.66938200	2.71529700
C	5.59454600	1.13636400	-0.82436700
C	6.02556800	2.03551600	0.07528000
H	5.59497200	2.05281700	1.07273300
C	6.25532000	4.87543900	1.23802100
C	7.49258900	4.04207700	0.82879000
H	5.84483200	5.41996600	0.38117100
H	5.45754200	4.25729700	1.66006200
H	6.54240800	5.61054600	1.99782500
C	8.03820400	3.27755600	2.05789300
C	8.58193500	4.97618800	0.28034600
H	8.91174700	2.67285400	1.79211100
H	8.34596300	3.99266000	2.82855200
H	7.28980800	2.61471600	2.50188400
H	8.87567900	5.69825300	1.04927800
H	9.46975600	4.41467200	-0.02327900
H	8.22597800	5.52839900	-0.59374700
C	7.08350300	3.02648500	-0.25968300
O	7.61606600	3.03843100	-1.36634300
Br	0.83316600	0.45228400	-2.61359700

19

C	-4.72545300	-0.21715400	0.42323600
C	-3.36992400	-0.05079900	-0.27477500
H	-4.92036000	-1.28687700	0.58575300
H	-4.67648600	0.23735800	1.42311200
C	-2.20013500	-0.65873600	0.50867600
H	-3.41652800	-0.51063300	-1.27212800
H	-3.17702000	1.01837900	-0.44214900
H	-2.14997400	-0.19526300	1.50403600
H	-2.39165100	-1.72754300	0.67950900
C	-0.84792200	-0.49474700	-0.19525000
C	0.32429100	-1.09359700	0.60978600
H	-0.65153800	0.57024500	-0.37460700
H	-0.88860300	-0.97139700	-1.18384800
H	0.39043700	-0.60802700	1.59069200
H	0.10981700	-2.15693500	0.79345900
C	-5.89500600	0.39802600	-0.35469100

C	-7.25162900	0.22954500	0.34052700
H	-5.94336500	-0.05387800	-1.35587600
H	-5.70166500	1.46853900	-0.51486000
C	-8.41338200	0.85096100	-0.44069000
H	-7.44656900	-0.84013300	0.49743500
H	-7.20245300	0.67871700	1.34190000
H	-9.36654200	0.71248300	0.08023000
H	-8.26453900	1.92775400	-0.58146100
H	-8.50870600	0.39894500	-1.43467100
H	1.70276700	-1.47927200	-1.08104800
C	1.63171400	-0.98679500	-0.11088400
C	2.71551700	-0.32630800	0.32561300
H	2.68974300	0.18368400	1.28453700
C	4.73618000	1.99897600	0.29410200
C	5.15922000	0.52440100	0.09596600
H	4.42946300	2.45316700	-0.65391000
H	3.90974000	2.10412700	1.00289600
H	5.58271800	2.57421000	0.68409000
C	5.57404100	-0.08805700	1.45434200
C	6.34226100	0.45611400	-0.88133500
H	5.86813000	-1.13682800	1.34198800
H	6.43189600	0.46045200	1.85781300
H	4.77172400	-0.03876700	2.19604300
H	7.18908600	1.02409500	-0.48263800
H	6.66432700	-0.57645400	-1.04148900
H	6.07524800	0.87377600	-1.85579000
C	3.96799900	-0.27160900	-0.47698400
O	4.05053400	-0.84065700	-1.56185500
20			
C	6.55860200	-2.34308900	-1.45373900
C	5.31279100	-1.53020900	-1.07916600
H	6.25087400	-3.34834500	-1.77628600
H	7.04246000	-1.88094800	-2.32632300
C	4.29485500	-1.41159300	-2.22115400
H	4.82608200	-1.98976000	-0.20684600
H	5.61972200	-0.52363500	-0.75994100
H	4.78436800	-0.95824000	-3.09538900
H	3.98753000	-2.41961700	-2.53630900
C	3.04674400	-0.59691000	-1.85928000
C	2.03109600	-0.48966700	-3.01166000
H	3.34658200	0.41532700	-1.55234500
H	2.55460900	-1.04627000	-0.98568200
H	2.53400700	-0.02945100	-3.88059400
H	1.76443700	-1.51332700	-3.31767000
C	7.58171800	-2.46874600	-0.31767500
C	8.82729900	-3.27785800	-0.70101300
H	7.10156800	-2.93546400	0.55473700
H	7.88963700	-1.46445000	0.00777000
C	9.84536100	-3.40126700	0.43746000
H	8.51987600	-4.28093700	-1.02732100
H	9.30714600	-2.81013600	-1.57166300
H	10.72113600	-3.98316900	0.13112400
H	10.19814600	-2.41537600	0.76188700
H	9.40519700	-3.89728300	1.31034900
C	0.76501700	0.27570900	-2.65327400
C	0.49920100	1.39942700	-3.35298900
C	-1.65246400	-1.02779600	0.05755200
C	-2.50286200	-2.02958800	1.91138400
C	-3.54795100	-1.50082200	1.21764000
N	-3.01283000	-0.89199500	0.08613700
N	-1.35012100	-1.73416800	1.18899100
Cl	-5.21774900	-1.52905000	1.58752400
Cl	-2.51115800	-2.89662000	3.38606100
C	-4.24320100	-0.94227300	-2.03985900
C	-3.78331500	-0.20504500	-0.93039800
C	-4.03774900	1.17088900	-0.76440000
C	-4.76854500	1.81353200	-1.77172900
C	-5.22888800	1.11536600	-2.88504900
C	-4.97031100	-0.24676300	-3.01419000
H	-4.97681100	2.87517800	-1.68302500
H	-5.79295100	1.63455300	-3.65442700
H	-5.33689400	-0.78020000	-3.88564800
C	0.47269100	-3.37827100	1.13224300
C	1.77350800	-3.73239100	1.51181700
C	2.55241000	-2.88346200	2.29420000
C	2.04462200	-1.65728800	2.71576300
C	0.75032700	-1.24994900	2.36800800
C	-0.00997800	-2.12894900	1.57116100
H	2.18079600	-4.68598900	1.19051900
H	3.55804800	-3.17962900	2.57823400
H	2.66238400	-1.00406700	3.32392700
C	-3.98127000	-2.43487200	-2.21568100

H	-3.42607200	-2.79117300	-1.34336100
C	-3.10390700	-2.70815800	-3.45317000
H	-2.88958900	-3.77913500	-3.53553000
H	-3.60504100	-2.39568300	-4.37550800
H	-2.15197500	-2.17180100	-3.38812300
C	-5.29598200	-3.23675000	-2.27638700
H	-5.08079000	-4.30840900	-2.34268600
H	-5.90794600	-3.06654300	-1.38518600
H	-5.89364200	-2.96359700	-3.15244600
C	-3.54074000	1.96867100	0.43695400
H	-3.06068900	1.27552700	1.13357500
C	-2.47680500	2.99932800	0.01309800
H	-1.63595000	2.51493100	-0.49278100
H	-2.89560200	3.74512200	-0.67068500
H	-2.08710100	3.53106900	0.88713300
C	-4.70015800	2.64334100	1.19516900
H	-4.31769100	3.16059500	2.08124000
H	-5.20989700	3.38632700	0.57310100
H	-5.44382200	1.91006700	1.52249100
C	-0.34945800	-4.33350600	0.27250200
C	0.23253300	0.10578100	2.83791800
C	-0.56116900	-5.68973300	0.97310800
H	-1.20239600	-6.33317500	0.36161000
H	0.38730500	-6.21554500	1.12536600
H	-1.03769600	-5.56412100	1.95023300
C	0.25263400	0.22620100	4.37396400
H	-0.32296800	-0.57666300	4.84503700
H	1.27329800	0.18552600	4.76828200
H	-0.18235000	1.18302900	4.68079100
C	0.28694700	-4.51945100	-1.11893100
H	1.27653800	-4.98330900	-1.04657100
H	-0.34146000	-5.16742600	-1.73914500
H	0.40029000	-3.55942900	-1.63224600
H	-1.33793100	-3.89206200	0.11737300
Cu	-0.42898400	-0.36194200	-1.28670600
H	-0.37947700	2.01651600	-3.16821000
C	1.02009900	1.25409800	2.17714200
H	0.60796200	2.22387600	2.47445600
H	2.07474200	1.23290600	2.47257900
H	0.97321000	1.18354000	1.08570900
H	-0.80926300	0.20488900	2.52015000
H	1.15404300	1.75818100	-4.15800400
C	3.28546900	4.12579100	0.11166000
C	2.52932800	5.20176600	-0.69465300
H	3.28484100	4.34786400	1.18037400
H	2.85006500	3.13392100	-0.04088200
H	4.32282100	4.09911700	-0.23530300
C	2.56247900	4.86086200	-2.19853900
C	3.14683600	6.59567800	-0.44480700
H	2.02629700	5.60940400	-2.78760200
H	3.60338700	4.83881900	-2.53372500
H	2.11479700	3.88251100	-2.39409000
H	4.18635900	6.58046700	-0.78551300
H	2.61682400	7.37334700	-1.00303700
H	3.13406100	6.85654200	0.61539500
C	1.05755100	5.23341800	-0.27790100
O	0.09022200	5.09833900	-0.94675500
Br	0.75952000	5.59119000	1.72542200

TS7

C	7.17334200	0.26086600	1.45689700
C	5.93598400	-0.35776700	0.79391500
H	6.93776500	1.28531100	1.77964700
H	7.41091000	-0.29822800	2.37342100
C	4.70364200	-0.39554100	1.70691100
H	5.69432500	0.20529800	-0.11912600
H	6.17413000	-1.37979300	0.46555800
H	4.94756200	-0.95701600	2.62019900
H	4.46477700	0.62564400	2.03578300
C	3.46933900	-1.02480100	1.04611000
C	2.23679200	-1.05176200	1.96624200
H	3.71737900	-2.04878600	0.73756500
H	3.22872100	-0.47631000	0.12456900
H	2.54506200	-1.48324800	2.93405500
H	1.95196700	-0.01164200	2.17905300
C	8.40867300	0.28861800	0.54800300
C	9.64604800	0.90815000	1.20997700
H	8.17233700	0.84634700	-0.36983100
H	8.64580400	-0.73598900	0.22674500
C	10.87539600	0.92884000	0.29565100
H	9.41039200	1.93265900	1.52939300
H	9.88187700	0.35144200	2.12735400
H	11.74099100	1.37456400	0.79713400

H	11.15554500	-0.08483200	-0.01359700
H	10.68244000	1.50930000	-0.61401500
C	1.02105100	-1.81151100	1.44849400
C	0.53773400	-2.80330000	2.21491800
C	-1.32512800	0.57874400	0.05536800
C	-2.38114200	2.58175700	-0.21193700
C	-3.13621600	1.83689200	0.63463400
N	-2.48209600	0.61804000	0.79480300
N	-1.27996500	1.80305600	-0.57020100
Cl	-4.61068300	2.26234300	1.39504100
Cl	-2.65795500	4.19044000	-0.73272300
C	-2.59837400	-0.32009500	3.06488800
C	-2.94779000	-0.41879900	1.70020300
C	-3.78397200	-1.44037400	1.19913000
C	-4.24878200	-2.39381700	2.11451100
C	-3.90837100	-2.33114300	3.46247900
C	-3.09424100	-1.30431400	3.92927700
H	-4.89299700	-3.19378800	1.76621500
H	-4.28358300	-3.08225200	4.15164600
H	-2.84136700	-1.26056100	4.98386200
C	0.86009700	2.99265400	-0.77448200
C	1.85663900	3.53932400	-1.59338800
C	1.79394700	3.42765100	-2.97797900
C	0.72665900	2.76406800	-3.57468200
C	-0.30170400	2.19401100	-2.81218100
C	-0.20522900	2.31262900	-1.40651100
H	2.68817600	4.06729400	-1.13819700
H	2.57532700	3.86276500	-3.59433500
H	0.68611700	2.69140500	-4.65586500
C	-1.74129800	0.80605900	3.64016700
H	-1.37086500	1.41502300	2.81043400
C	-0.51062300	0.26521600	4.39282800
H	0.13795000	1.09515500	4.69355700
H	-0.80330400	-0.26776800	5.30395200
H	0.06378200	-0.42228900	3.76865900
C	-2.56975900	1.72472300	4.56216700
H	-1.94828800	2.54807600	4.93031800
H	-3.43164500	2.15324700	4.04427600
H	-2.94058400	1.17235900	5.43233800
C	-4.23591000	-1.51404200	-0.25786500
H	-3.55355300	-0.90361700	-0.85581200
C	-4.17683300	-2.94363600	-0.82681800
H	-3.19303400	-3.39453200	-0.68143200
H	-4.92912800	-3.59410000	-0.36772400
H	-4.38311300	-2.91829900	-1.90166200
C	-5.66015400	-0.94151100	-0.42197600
H	-5.96103600	-0.97512400	-1.47465300
H	-6.38277800	-1.53133300	0.15313300
H	-5.72958100	0.09488400	-0.08208300
C	0.95354500	3.19481600	0.73648400
C	-1.47192200	1.52276100	-3.53097200
C	0.62405300	4.65040100	1.12917000
H	0.67462100	4.76729000	2.21696600
H	1.34425800	5.34518800	0.68346500
H	-0.37485400	4.94784500	0.80106500
C	-2.49909700	2.56035700	-4.03392600
H	-2.92238200	3.15600600	-3.22345200
H	-2.03243200	3.24858700	-4.74756700
H	-3.32232200	2.05208800	-4.54748600
C	2.33684200	2.80284800	1.28678600
H	3.11687400	3.49442300	0.95186800
H	2.32524700	2.82972400	2.38129800
H	2.62024400	1.79640900	0.97175300
H	0.21890800	2.54273900	1.21707100
Cu	-0.09761100	-1.06998400	0.00880600
H	-0.32060700	-3.40623600	1.92751900
C	-1.01440000	0.65367400	-4.71870300
H	-1.86025500	0.06677100	-5.09085600
H	-0.65483500	1.26590000	-5.55248200
H	-0.22227800	-0.04074500	-4.43235700
H	-1.97273900	0.86327500	-2.81610000
H	0.98984800	-3.06307300	3.17901600
C	2.28011600	-2.73868400	-2.08675600
C	1.39755000	-3.86970300	-1.55671300
H	1.82052000	-2.23752400	-2.94003900
H	2.47482600	-1.99731900	-1.31101400
H	3.23744100	-3.16021800	-2.40910600
C	2.13178600	-4.67246500	-0.45985500
C	0.99878800	-4.82497700	-2.71030200
H	1.52411800	-5.51341000	-0.11572600
H	3.06291000	-5.06622000	-0.87881100
H	2.36264600	-4.04171500	0.39925700

H	1.91212100	-5.24480200	-3.14349200
H	0.37892500	-5.64840900	-2.34506500
H	0.45453600	-4.29383200	-3.49403800
C	0.06469900	-3.39931200	-0.93397300
O	-0.71697300	-4.03176100	-0.30557200
Br	-0.91333500	-1.93315400	-2.36176600

21

C	-3.70897000	4.79038000	0.51919500
C	-3.93326200	3.66685800	-0.50117400
H	-4.63671100	4.95995000	1.08516900
H	-2.95900500	4.46473700	1.25436100
C	-4.38408600	2.34662300	0.13621700
H	-4.68340400	3.98981900	-1.23765100
H	-3.00365200	3.49622100	-1.06094900
H	-3.63053800	2.02256400	0.86774900
H	-5.31147000	2.51203000	0.70368600
C	-4.60647700	1.22311700	-0.88592900
C	-5.03752500	-0.08778600	-0.22308700
H	-3.67920100	1.06333100	-1.45071300
H	-5.36560000	1.53833700	-1.61454000
H	-4.27700000	-0.39959400	0.50445900
H	-5.94860200	0.08706300	0.36865900
C	-3.25330100	6.11097800	-0.11392700
C	-3.02142700	7.23391900	0.90533900
H	-4.00219600	6.43962400	-0.84921600
H	-2.32656000	5.94014300	-0.68005700
C	-2.56428800	8.54823400	0.26407300
H	-3.94719500	7.40535300	1.47186300
H	-2.27272600	6.90540100	1.63922400
H	-2.40552600	9.32854900	1.01609400
H	-1.62287800	8.41500200	-0.28145000
H	-3.30851500	8.92044300	-0.44967800
C	-5.28525400	-1.26547800	-1.14987700
C	-5.11220500	-1.23806300	-2.47660800
C	2.11012200	-0.40801900	0.19185400
C	3.77655400	-1.76011700	0.92008900
C	2.70693300	-1.94854100	1.74245300
N	1.69327900	-1.11317000	1.28361200
N	3.39566500	-0.81270100	-0.02540500
Cl	2.54915900	-2.98292500	3.09392800
Cl	5.31887200	-2.49577900	0.96353800
C	-0.64555100	-1.85554800	1.38232500
C	0.36913100	-1.00413600	1.86357400
C	0.15546600	-0.04566000	2.87469900
C	-1.13767800	0.04632500	3.40376000
C	-2.16440900	-0.77368200	2.94222300
C	-1.92254400	-1.71253800	1.94183700
H	-1.34296500	0.77305800	4.18360900
H	-3.16076700	-0.68066200	3.36484400
H	-2.73827400	-2.32993700	1.57884000
C	4.19977900	-0.97798800	-2.34088600
C	5.00842600	-0.46357400	-3.36215500
C	5.81214100	0.65372700	-3.15195500
C	5.82695900	1.28280400	-1.90991600
C	5.04053600	0.81387100	-0.85017300
C	4.23400900	-0.31497700	-1.09756300
H	5.00566200	-0.94426700	-4.33536400
H	6.42955300	1.03586400	-3.95958100
H	6.45697700	2.15366900	-1.75922500
C	-0.41010500	-2.90318000	0.29899200
H	0.64630500	-2.87594900	0.01646400
C	-1.23148100	-2.59635500	-0.96865600
H	-1.01512000	-3.33888400	-1.74464400
H	-2.30573500	-2.62616800	-0.76247700
H	-0.98814700	-1.60654500	-1.36766600
C	-0.70733900	-4.32434500	0.81757200
H	-0.46865800	-5.06345300	0.04547700
H	-0.11489100	-4.55820400	1.70760600
H	-1.76510600	-4.44142400	1.07417700
C	1.25269900	0.87729800	3.39577200
H	2.18120500	0.63930400	2.86922200
C	0.92905500	2.35460800	3.09813000
H	0.77943500	2.51939300	2.02653900
H	0.02059800	2.67653600	3.61808300
H	1.75078200	2.99675000	3.43249000
C	1.51266800	0.65721000	4.89890800
H	2.33990300	1.29121600	5.23488300
H	0.63353800	0.91257000	5.49978300
H	1.77401100	-0.38416500	5.11047800
C	3.33061400	-2.20252000	-2.61049700
C	5.08119700	1.53163200	0.49561600
C	4.18452800	-3.43290600	-2.97499800

H	3.54233500	-4.30926700	-3.11144300
H	4.73517800	-3.27594300	-3.90845200
H	4.91119700	-3.66224900	-2.18957400
C	6.49708700	1.51206200	1.10442500
H	6.87054500	0.48928800	1.21343600
H	7.20859900	2.06639300	0.48343100
H	6.48719500	1.97912400	2.09477900
C	2.27773600	-1.91591000	-3.69931100
H	2.74852700	-1.69208400	-4.66242200
H	1.63219200	-2.78952100	-3.83835000
H	1.64620100	-1.06444600	-3.42717600
H	2.78607900	-2.44660300	-1.69409600
Cu	1.11050100	0.85786500	-0.81319300
H	-5.25531500	-2.11486800	-3.09776100
C	4.54699600	2.97278400	0.37896400
H	4.54559900	3.45517800	1.36213800
H	5.17056800	3.57684300	-0.28857800
H	3.52431800	2.98721100	-0.01067100
H	4.42376500	0.99962100	1.18916000
H	-4.78230800	-0.33806200	-2.98532400
C	-8.09463400	-2.10528600	-0.26227200
C	-7.02825300	-3.18546100	-0.56067100
H	-7.99879100	-1.71782200	0.75766000
H	-8.02115900	-1.26580800	-0.95963600
H	-9.09422000	-2.54115400	-0.36197700
C	-7.24049300	-3.72397900	-1.99506600
C	-7.15804300	-4.34358100	0.44242300
H	-6.46020500	-4.43891500	-2.27663900
H	-8.20288200	-4.24466500	-2.04045200
H	-7.26355200	-2.92179200	-2.73562200
H	-8.15560500	-4.78785900	0.36564600
H	-6.41745000	-5.12375700	0.24656100
H	-7.01311100	-3.99837900	1.46985500
C	-5.63197700	-2.54443500	-0.41594800
O	-4.80425900	-3.01199900	0.35719500
Br	-0.08270900	2.36710400	-2.01659900

22

C	4.04912900	-0.47745100	-0.13323700
C	2.87617800	0.48425300	0.09355000
H	3.94851100	-1.33824800	0.54318700
H	3.99195100	-0.88468400	-1.15285400
C	1.50295300	-0.16077300	-0.13075200
H	2.92710800	0.88351500	1.11652200
H	2.98224200	1.34979900	-0.57568100
H	1.45047700	-0.55328300	-1.15608600
H	1.39631700	-1.02971300	0.53387100
C	0.33489500	0.80586900	0.10322900
C	-1.02864800	0.15259700	-0.15109800
H	0.45051200	1.67999100	-0.55049200
H	0.37834300	1.18148700	1.13384300
H	-1.04023200	-0.25066100	-1.17342500
H	-1.12452600	-0.72275300	0.50318000
C	5.42254400	0.17225200	0.07490700
C	6.59717400	-0.78861200	-0.14722900
H	5.47979300	0.58348900	1.09307300
H	5.52442300	1.03074700	-0.60444500
C	7.96449800	-0.12919200	0.05738900
H	6.49745300	-1.64443400	0.53423400
H	6.53850900	-1.20176400	-1.16345700
H	8.78147900	-0.83892700	-0.10946400
H	8.10600500	0.70973800	-0.63365600
H	8.06654500	0.26235700	1.07606600
C	-2.23575300	1.05922800	0.01476500
C	-2.15707800	2.32587600	0.44634900
H	-3.04762300	2.94089600	0.51866900
H	-1.21912200	2.78122500	0.74337300
O	-4.35713700	1.33465500	-0.98544000
C	-4.16706900	-0.79651800	0.11127500
C	-5.69643300	-0.80692300	-0.06892200
C	-3.56586900	-1.92526800	-0.76305500
C	-3.83542600	-1.03128100	1.60137100
H	-6.17117700	-0.01616000	0.51921800
H	-5.97477900	-0.65571100	-1.11422200
H	-6.09841300	-1.76982300	0.26236300
H	-2.49028400	-2.04570500	-0.62418200
H	-4.04149200	-2.87512800	-0.49665000
H	-3.75640500	-1.74236200	-1.82560900
H	-4.24692100	-1.99443200	1.92099600
H	-2.76109000	-1.04958300	1.79929100
H	-4.28007200	-0.25295900	2.23010200
C	-3.62950000	0.58025100	-0.35258300

23

C	-8.16854100	2.31753500	1.52431500	C	1.74478800	1.92599500	-2.70919500
C	-6.80567200	2.09780000	0.85499800	C	1.09588500	3.01331300	-3.30791300
H	-8.30430700	1.57322700	2.32220800	C	1.20933900	4.29823600	-2.78356400
H	-8.17387400	3.29824500	2.02159000	C	1.98223600	4.52602800	-1.64789700
C	-5.62321300	2.18091600	1.82893400	C	2.65398700	3.47785900	-1.00634200
H	-6.79895600	1.11583200	0.36005000	C	2.50863500	2.18760300	-1.55429300
H	-6.67010600	2.84035800	0.05551300	H	0.49251300	2.84969700	-4.19540400
H	-5.62754100	3.16462600	2.32063600	H	0.69557100	5.12603000	-3.26369000
H	-5.76243400	1.44154100	2.63092800	H	2.06564500	5.53301000	-1.25098600
C	-4.25974700	1.95386900	1.16390500	C	2.50594400	-3.21707500	-0.34561000
C	-3.07525500	2.03522500	2.14654800	H	2.71397500	-2.35183800	-0.98126300
H	-4.11700900	2.69514800	0.36439400	C	1.00186600	-3.52427000	-0.47779000
H	-4.24671300	0.97078000	0.67367900	H	0.75029400	-3.74177400	-1.52104500
H	-3.11654800	3.01485400	2.65008900	H	0.71825500	-4.39645000	0.12102900
H	-3.19848200	1.27547100	2.93075300	H	0.39002100	-2.67814600	-0.15242100
C	-9.35243600	2.23812200	0.55220200	C	3.35949600	-4.38738100	-0.87303900
C	-10.71463000	2.45464900	1.22381600	H	3.11643000	-4.58756300	-1.92183100
H	-9.34753900	1.25841700	0.05261800	H	4.42878600	-4.16432900	-0.80715300
H	-9.21944100	2.98441800	-0.24438800	H	3.17183700	-5.30637400	-0.30776300
C	-11.89151600	2.37685900	0.24574600	C	4.29224900	0.08914800	3.19368500
H	-10.84836200	1.70753800	2.01816100	H	4.37716400	0.70743100	2.29575200
H	-10.71913400	3.43279700	1.72408400	C	3.33845400	0.82077000	4.15824000
H	-12.84791900	2.53610300	0.75503600	H	2.34577100	0.94239000	3.71347200
H	-11.80277100	3.13541400	-0.54062000	H	3.22357700	0.27260700	5.09946300
H	-11.93484700	1.39741700	-0.24477200	H	3.73119000	1.81506300	4.39641800
C	2.59789600	0.33654500	0.10246600	C	5.70574600	-0.03500900	3.79548500
C	4.45335500	0.62707300	-1.17654300	H	6.10593400	0.95832700	4.02433200
C	4.69447700	-0.41911500	-0.33968100	H	5.69709900	-0.61160900	4.72652700
N	3.55047800	-0.58664000	0.43566000	H	6.39359700	-0.52724200	3.10093300
N	3.16753900	1.07897800	-0.89483400	C	1.60221400	0.53269800	-3.31364700
Cl	6.09753100	-1.38758600	-0.19584500	C	3.49515400	3.76540400	0.23341200
Cl	5.47045700	1.31816300	-2.36602000	C	2.13958300	0.48597700	-4.75767300
C	2.87794400	-2.85752000	1.08952000	H	2.08597200	-0.53650800	-5.14602300
C	3.38250700	-1.59532300	1.46180400	H	1.55309200	1.12538400	-5.42586100
C	3.73458500	-1.27150100	2.78763000	H	3.18238700	0.81457200	-4.80622500
C	3.55146300	-2.26251400	3.76029200	C	4.62579500	4.76819100	-0.06984500
C	3.04872900	-3.51698200	3.42552600	H	5.26610300	4.41448100	-0.88383100
C	2.71833700	-3.80902200	2.10494900	H	4.22834300	5.74781900	-0.35534900
H	3.80668700	-2.04747800	4.79326100	H	5.25087100	4.91018700	0.81799600
H	2.91545500	-4.27030900	4.19651400	C	0.14520000	0.03551000	-3.24605200
H	2.32845900	-4.79121900	1.85651200	H	-0.52316000	0.67998500	-3.82706700

H	0.07254900	-0.97746500	-3.65583700
H	-0.22048000	0.01046200	-2.21518100
H	2.20695000	-0.16051800	-2.72226500
Cu	0.85308000	0.58572700	0.89656700
H	-1.49836600	2.62365900	0.73535400
C	2.62007900	4.25108600	1.40536500
H	3.23778200	4.41634900	2.29461500
H	2.12009800	5.19549700	1.16516000
H	1.85068600	3.51368600	1.65513500
H	3.96832400	2.83193200	0.55057200
C	-1.72842000	1.85577400	1.48222000
C	-0.84567400	0.85964400	1.71425900
H	-1.19722600	0.14990500	2.48108800
C	-5.74621500	-2.64500300	-1.80297400
C	-4.90432900	-3.77200700	-1.16628100
H	-5.56369400	-1.68369000	-1.31867200
H	-5.53411400	-2.54274800	-2.87160800
H	-6.80553100	-2.89404400	-1.68890900
C	-5.20540000	-5.11761800	-1.85624500
C	-5.19643700	-3.87163400	0.34649600
H	-4.60832400	-5.92641400	-1.42698700
H	-6.26310800	-5.36030200	-1.72067400
H	-4.99699700	-5.07073400	-2.92828600
H	-6.25292600	-4.12226400	0.48186400
H	-4.59756600	-4.65678900	0.81785500
H	-4.99757400	-2.92787000	0.85784200
C	-3.41709400	-3.47734600	-1.38101400
O	-2.61496500	-4.12902700	-1.96508200
Br	-2.77445900	-1.73605900	-0.53909900

TS8

C	-9.11483700	0.16765500	-0.78639700
C	-7.75239600	-0.47622000	-0.49783400
H	-9.16285800	1.14866600	-0.29213100
H	-9.20062200	0.36734500	-1.86434600
C	-6.56231000	0.37404100	-0.96076800
H	-7.66341300	-0.66749200	0.58114300
H	-7.70580800	-1.46089800	-0.98492600
H	-6.64521000	0.55410600	-2.04254900
H	-6.61718400	1.36353200	-0.48424900
C	-5.19750900	-0.25692200	-0.65595000
C	-4.00726300	0.59502800	-1.13514500
H	-5.14279400	-1.25017700	-1.12436900
H	-5.10345700	-0.42427500	0.42578600
H	-4.12845500	0.77397900	-2.21637300
H	-4.04472400	1.57974300	-0.65025700
C	-10.30727900	-0.68479500	-0.33451800
C	-11.66841800	-0.03463500	-0.61474900
H	-10.21986100	-0.89039500	0.74216200
H	-10.26466100	-1.66355600	-0.83397500
C	-12.85443800	-0.89408800	-0.16489200
H	-11.71223700	0.94151600	-0.11260100
H	-11.75457000	0.17356500	-1.69010600
H	-13.80993100	-0.40371300	-0.37945600
H	-12.85613600	-1.86413600	-0.67550500
H	-12.81528900	-1.08943600	0.91305300
C	1.65342800	0.29925900	-0.27343800
C	3.25535500	0.77180100	-1.82612600
C	2.97499000	1.92599500	-1.17278500
N	1.97981100	1.63743800	-0.24204600
N	2.46819100	-0.22790300	-1.25127100
Cl	3.72420500	3.45208400	-1.36387500
Cl	4.30696200	0.54309800	-3.15761800
C	1.69087200	2.66258800	1.97534500
C	1.34915800	2.63649200	0.60339200
C	0.45000200	3.56076200	0.02329600
C	-0.17973600	4.46566400	0.88925800
C	0.09123300	4.47514000	2.25277100
C	1.03104100	3.59541800	2.78375900
H	-0.88847900	5.17927100	0.48158600
H	-0.41461600	5.18407300	2.90182700
H	1.25882100	3.63890700	3.84256800
C	3.83534100	-2.27525000	-1.16804500
C	3.98383800	-3.62830800	-1.50462400
C	3.00453000	-4.30899800	-2.21808100
C	1.85594700	-3.64201900	-2.63520800
C	1.64930800	-2.28817300	-2.34163200
C	2.64160400	-1.63337600	-1.57651100
H	4.88356100	-4.15357900	-1.20041500
H	3.14066900	-5.35849500	-2.46217000
H	1.11235100	-4.18108000	-3.21002300
C	2.80355100	1.79353100	2.56244700
H	2.85010000	0.86666300	1.98347500

C	2.57042100	1.39986400	4.03049200
H	3.33488200	0.68020500	4.34090500
H	2.65148200	2.26067300	4.70264400
H	1.58924400	0.93937200	4.16878400
C	4.16740500	2.50476200	2.41934600
H	4.96853400	1.87097400	2.81488400
H	4.40382800	2.73929900	1.37813200
H	4.17198000	3.44480700	2.98221600
C	0.18270400	3.68989300	-1.47924500
H	0.77378500	2.93491200	-2.00549200
C	-1.29098700	3.45453500	-1.86008900
H	-1.61142900	2.44316400	-1.60919800
H	-1.95258200	4.16422800	-1.35126700
H	-1.41779800	3.60183000	-2.93842800
C	0.62462600	5.07907500	-1.99243900
H	0.54511300	5.11448800	-3.08404900
H	-0.01990500	5.86753600	-1.58956400
H	1.65501300	5.31424300	-1.71795200
C	4.98128000	-1.58894300	-0.41792800
C	0.43488900	-1.55612400	-2.91220300
C	6.30782600	-1.68657600	-1.20220800
H	7.07836100	-1.09037100	-0.70255600
H	6.66810700	-2.71968000	-1.24440100
H	6.20686200	-1.32299700	-2.22678800
C	0.80253000	-0.85846200	-4.24028400
H	1.62657300	-0.15049700	-4.12086100
H	1.10153800	-1.59541200	-4.99424600
H	-0.06142300	-0.30845400	-4.62809400
C	5.18273300	-2.15965000	0.99854800
H	5.42072700	-3.22814700	0.96964500
H	6.01533600	-1.64683500	1.49147200
H	4.29417500	-2.02897500	1.61741200
H	4.74250100	-0.52838300	-0.30416700
Cu	-0.03808900	-0.38509700	0.58473900
H	-2.52463500	-1.01232200	-1.36250800
C	-0.78495900	-2.46780800	-3.12463200
H	-1.64658900	-1.85880300	-3.41225000
H	-0.62234800	-3.19423000	-3.92815400
H	-1.04668500	-3.01558700	-2.21453900
H	0.13270000	-0.78317700	-2.19978300
C	-2.66004300	-0.04528600	-0.86991300
C	-1.68324800	0.45722100	-0.09479100
H	-1.91125200	1.42946900	0.36393900
C	0.19515500	-3.94956400	3.46209400
C	1.12526400	-3.10478900	2.55696300
H	-0.38211300	-3.31214200	4.13460000
H	-0.49496900	-4.55318100	2.86655100
H	0.81636000	-4.62233400	4.06217200
C	1.86991700	-4.03427200	1.57199700
C	2.10298900	-2.28994700	3.40826600
H	2.48912300	-3.47066800	0.87360800
H	2.51916400	-4.70319900	2.14485400
H	1.16667900	-4.64138700	0.99689600
H	2.82789100	-2.96724200	3.86987300
H	2.64777800	-1.56137900	2.80423600
H	1.58173500	-1.74695500	4.19739100
C	0.21546900	-2.22738900	1.69107100
O	-0.56997500	-2.57333400	0.85407100
Br	-0.76155200	-0.51543200	3.07779600

24

C	-8.80980100	0.11015500	-0.82812900
C	-7.44431200	-0.43296300	-0.38781600
H	-8.91719800	1.14791700	-0.48094000
H	-8.84553100	0.15282000	-1.92636000
C	-6.25799600	0.38816200	-0.90953800
H	-7.40497800	-0.46982700	0.71017500
H	-7.34141300	-1.47297100	-0.72962600
H	-6.30112600	0.42966200	-2.00763300
H	-6.35410400	1.42696200	-0.56229800
C	-4.89486600	-0.16789900	-0.47840000
C	-3.70228300	0.64334400	-1.01822400
H	-4.80421200	-1.20915300	-0.81901600
H	-4.83878800	-0.19979900	0.61800400
H	-3.78935000	0.69945900	-2.11512500
H	-3.75900400	1.67355300	-0.64500800
C	-9.99392400	-0.71981600	-0.31631300
C	-11.36022200	-0.18232600	-0.76089400
H	-9.96149600	-0.76087400	0.78203300
H	-9.88489900	-1.75833800	-0.66116100
C	-12.53604500	-1.02125900	-0.24963900
H	-11.47164400	0.85394700	-0.41325200
H	-11.39148700	-0.13886300	-1.85828300

H	-13.49584400	-0.61257000	-0.58313000	H	-1.70720700	2.53263100	-1.62953400
H	-12.47099500	-2.05456500	-0.60987300	H	-1.98695900	4.26465500	-1.37507300
H	-12.55128500	-1.05481000	0.84594800	H	-1.54086400	3.66863400	-2.97764600
C	1.54044300	0.28543900	-0.29723000	C	0.58964100	5.08392900	-2.16342000
C	3.02611300	0.65187500	-1.97897900	H	0.47773500	5.08720800	-3.25265500
C	2.81407200	1.84013600	-1.36307800	H	-0.02070300	5.90241100	-1.76755300
N	1.87821000	1.61831900	-0.35409000	H	1.63367200	5.29918100	-1.92736700
N	2.26987000	-0.30539500	-1.29968100	C	4.83035100	-1.54328400	-0.46571300
Cl	3.59922000	3.32988700	-1.65631400	C	0.22506800	-1.77868100	-2.82343500
Cl	3.98696500	0.33114100	-3.35692400	C	6.13285800	-1.69442200	-1.28085100
C	1.73314800	2.73685300	1.83330300	H	6.90691800	-1.04011700	-0.86667300
C	1.33207400	2.67792200	0.47902100	H	6.51230300	-2.72050600	-1.23669900
C	0.45543800	3.62680000	-0.09894800	H	5.99135300	-1.43192500	-2.33151100
C	-0.09410000	4.58922900	0.75897500	C	0.51444900	-1.27283400	-4.25402400
C	0.23209300	4.63203400	2.10974800	H	1.34876700	-0.56677800	-4.28024600
C	1.15115700	3.72760900	2.63320200	H	0.76266200	-2.10872700	-4.91757100
H	-0.78446800	5.32271500	0.35501400	H	-0.36838900	-0.76837000	-4.66104600
H	-0.21342100	5.38580100	2.75230700	C	5.08427400	-1.96198500	0.99332600
H	1.42577900	3.79670300	3.67931200	H	5.33723900	-3.02469500	1.07007000
C	3.67440900	-2.31402800	-1.11247200	H	5.92240700	-1.39003200	1.40509000
C	3.84158000	-3.68416000	-1.35552800	H	4.21029900	-1.77428400	1.61893100
C	2.86309500	-4.42846700	-2.00534300	H	4.57830700	-0.48004800	-0.44649600
C	1.69655000	-3.81194400	-2.44865700	Cu	0.07251400	-0.38605400	0.90141900
C	1.46603600	-2.44698000	-2.23581000	H	-2.23578700	-0.99459200	-0.98899300
C	2.45719000	-1.72819000	-1.53446400	C	-1.01133000	-2.69385300	-2.83126000
H	4.75836700	-4.17052800	-1.03768900	H	-1.88758500	-2.12123900	-3.15030500
H	3.01615100	-5.48908800	-2.18202100	H	-0.90096400	-3.52635300	-3.53414800
H	0.95501400	-4.40057900	-2.97616900	H	-1.21255700	-3.10507200	-1.83857600
C	2.82935400	1.84224500	2.41245100	H	-0.02172600	-0.90961300	-2.20759200
H	2.83270200	0.89995500	1.85820700	C	-2.36547000	0.03250700	-0.64410400
C	2.61387600	1.49169500	3.89421100	C	-1.41325300	0.62083000	0.08925200
H	3.35109200	0.74438500	4.20419000	H	-1.56219700	1.63923900	0.45145000
H	2.74912000	2.36245500	4.54438500	C	0.06821700	-3.76158600	3.39848100
H	1.61516700	1.08116200	4.06399400	C	1.23758000	-3.07613800	2.65044200
C	4.21109500	2.50496700	2.21781900	H	-0.59342900	-3.02079900	3.85149000
H	5.00165300	1.85445100	2.60734500	H	-0.51662500	-4.38805200	2.71997300
H	4.42631700	2.70698000	1.16464600	H	0.48192100	-4.39634600	4.18943600
H	4.26067000	3.45711400	2.75750800	C	2.11131700	-4.15938400	1.97942300
C	0.12633000	3.72418100	-1.59256300	C	2.05187100	-2.21664600	3.62069600
H	0.66627700	2.93602600	-2.12452600	H	2.92652300	-3.72674300	1.39826000
C	-1.36963900	3.53096700	-1.90447400	H	2.54603700	-4.79581800	2.75703300

H	1.51279600	-4.78590100	1.31291800
H	2.51408500	-2.85749000	4.37878600
H	2.84873700	-1.67060600	3.11063900
H	1.41086800	-1.48832800	4.12005500
C	0.60580000	-2.23363700	1.51687700
O	-0.12428700	-2.71066900	0.67791600
Br	-0.98652700	-0.21288700	3.07268700

25

C	8.08656800	-0.62578600	-0.94436800
C	6.79194900	-0.08426300	-0.32484800
H	7.86067600	-1.06695100	-1.92576400
H	8.77333200	0.21048200	-1.13876300
C	6.07929800	0.94957600	-1.20618600
H	6.10742300	-0.92132100	-0.12557600
H	7.01684300	0.36436500	0.65334100
H	6.75930800	1.79073000	-1.40211800
H	5.85879500	0.50115700	-2.18525200
C	4.77793000	1.47982700	-0.59212100
C	4.06767800	2.51115900	-1.49414200
H	4.98935200	1.94019500	0.38211800
H	4.09606000	0.64157900	-0.39630500
H	4.72385900	3.37282000	-1.66676700
H	3.88686100	2.04419000	-2.47373700
C	8.79517500	-1.67008100	-0.07231100
C	10.08628700	-2.21568800	-0.69557600
H	8.10752000	-2.50543000	0.12430900
H	9.02518600	-1.22974000	0.90872900
C	10.78573200	-3.26134700	0.17918700
H	9.85634000	-2.65377800	-1.67648500
H	10.77437200	-1.38159500	-0.88989800
H	11.70175500	-3.63177200	-0.29305900
H	11.06012400	-2.84222100	1.15426500
H	10.13388800	-4.12338700	0.36272500
H	2.00247300	2.18864500	-0.76498600
C	2.75415100	2.95994100	-0.93341500
C	2.42956600	4.22626300	-0.62547000
H	3.14754200	5.02433800	-0.79372300
C	0.89692900	6.83728900	-1.17440300
C	0.78589900	6.07399400	0.16625100
H	0.19072600	6.44313700	-1.91263000
H	0.66341300	7.89589000	-1.01605900
H	1.90159500	6.78048100	-1.60320700
C	-0.63611800	6.22526600	0.72766300
C	1.80372500	6.64721400	1.18083500
H	-0.74483400	5.69605700	1.67846900
H	-0.85962300	7.28430400	0.89427600
H	-1.38017300	5.81958400	0.03681000
H	1.57657500	7.70160200	1.37234200
H	1.75335800	6.11368500	2.13598800
H	2.83333500	6.59252000	0.81548400
C	1.09516900	4.58023100	-0.07288300
O	0.26143800	3.71559700	0.18723800
C	-1.82041000	-0.78104000	-0.11144700
C	-3.42459000	-1.95227600	0.99000200
C	-2.21744600	-2.44177400	1.38603700
N	-1.24506100	-1.71377100	0.70607300
N	-3.16582500	-0.93638900	0.07508900
Cl	-1.87318500	-3.70826900	2.48331900
Cl	-4.99575800	-2.43248500	1.46647200
C	0.86450200	-1.19184500	1.85328800
C	0.18473300	-1.90399900	0.84405700
C	0.83287300	-2.79547200	-0.03464800
C	2.21644100	-2.95278300	0.11618400
C	2.91765700	-2.26000000	1.09949900
C	2.24712700	-1.39151600	1.95692400
H	2.74964700	-3.62857300	-0.54509300
H	3.98988400	-2.40066800	1.20109100
H	2.80438100	-0.86043400	2.72214700
C	-4.60969100	1.04975800	0.02854600
C	-5.56387500	1.81595500	-0.65281900
C	-6.06362900	1.41305400	-1.88837200
C	-5.62235900	0.22727900	-2.46945000
C	-4.66855700	-0.57945400	-1.83622500
C	-4.17347800	-0.13748600	-0.59305100
H	-5.91834800	2.74079500	-0.20857400
H	-6.80194200	2.02429500	-2.39918200
H	-6.02196400	-0.07782100	-3.43149800
C	0.16585800	-0.24822400	2.82839100
H	-0.89112700	-0.19023100	2.55361300
C	0.73253900	1.18256300	2.75123600
H	0.18758300	1.83463100	3.44234600
H	1.78935000	1.20967900	3.03823300

H	0.64102000	1.60507800	1.74692100
C	0.23718800	-0.78883300	4.27128300
H	-0.31657400	-0.12971200	4.94817600
H	-0.19155900	-1.79258600	4.34709700
H	1.27234500	-0.83690600	4.62621200
C	0.10051200	-3.57934300	-1.11948700
H	-0.96380600	-3.33513200	-1.06088900
C	0.58173900	-3.17383300	-2.52635700
H	0.44747000	-2.10070700	-2.69512600
H	1.64182100	-3.40864800	-2.66954400
H	0.01363200	-3.71503200	-3.29042600
C	0.23327600	-5.09972700	-0.90328800
H	-0.34917400	-5.63966500	-1.65718900
H	1.27454400	-5.42725400	-0.99103300
H	-0.13055000	-5.39597800	0.08537500
C	-4.09599200	1.51682600	1.38683500
C	-4.21253200	-1.87315300	-2.50367000
C	-5.24061800	1.61995500	2.41468100
H	-4.84052400	1.89255600	3.39691600
H	-5.96819400	2.38676200	2.12865300
H	-5.77460200	0.67010700	2.51615800
C	-5.38781600	-2.85012400	-2.70374600
H	-5.88438100	-3.07624600	-1.75508100
H	-6.13874600	-2.44055400	-3.38754600
H	-5.02645900	-3.79076900	-3.13255800
C	-3.33016600	2.84919500	1.27467000
H	-3.97900200	3.65075300	0.90545100
H	-2.95635500	3.15063300	2.25908400
H	-2.47389900	2.76738700	0.59920500
H	-3.39137500	0.76939000	1.76240200
Cu	-0.94267400	0.41598100	-1.36224300
H	-0.26845000	1.29724200	-2.40586000
C	-3.48922400	-1.59172200	-3.83515000
H	-3.13295500	-2.52819800	-4.27744600
H	-4.15718700	-1.11297900	-4.55909900
H	-2.62760600	-0.93350000	-3.68441700
H	-3.49271000	-2.36502400	-1.84329800

TS9

C	-9.24935900	0.12133200	-0.32031600
C	-7.97824200	-0.51506200	0.25672700
H	-9.12789100	1.21387500	-0.34689700
H	-9.36970100	-0.19544700	-1.36635200
C	-6.70903500	-0.16588400	-0.53069200
H	-7.85574500	-0.19824900	1.30239200
H	-8.09946900	-1.60743500	0.28298400
H	-6.83474800	-0.47864500	-1.57721900
H	-6.58460100	0.92639000	-0.55354200
C	-5.43702400	-0.80707500	0.03779300
C	-4.17195500	-0.45408300	-0.76875300
H	-5.55330200	-1.89895100	0.06141600
H	-5.30151900	-0.49072700	1.08143100
H	-4.29688700	-0.78033800	-1.80927600
H	-4.07164500	0.64176800	-0.79297900
C	-10.52164000	-0.22688500	0.46238300
C	-11.79224100	0.40726000	-0.11805200
H	-10.40393100	0.09162900	1.50829300
H	-10.64328900	-1.31940500	0.49053300
C	-13.05878500	0.05490700	0.66888900
H	-11.67054100	1.49883100	-0.14613900
H	-11.91002000	0.08842800	-1.16282800
H	-13.94678600	0.52228000	0.23024100
H	-13.22623700	-1.02832500	0.68467600
H	-12.98488000	0.39198400	1.70937200
H	-2.64363600	-0.73998200	0.81621300
C	-2.91666500	-1.04533200	-0.19295300
C	-2.11546900	-1.91272200	-0.82432400
H	-2.35414900	-2.23457400	-1.83488200
C	-0.83695100	-4.43149900	-1.91036600
C	-0.59941300	-4.00140900	-0.45259300
H	-0.23197100	-3.83611500	-2.60227100
H	-0.55483000	-5.48301200	-2.03478600
H	-1.88658300	-4.34120000	-2.20571100
C	0.83989200	-4.35147900	-0.04491100
C	-1.58649600	-4.76224700	0.46734500
H	1.03467300	-4.06308800	0.99011700
H	1.01017800	-5.42934700	-0.14433900
H	1.56062800	-3.83129900	-0.68558100
H	-1.45676900	-5.84339200	0.34664400
H	-1.41071800	-4.50893200	1.51673700
H	-2.62641600	-4.51759700	0.22606700
C	-0.87157000	-2.48405900	-0.19785900
O	-0.50503500	-2.01198700	0.95204600

C	1.98846400	0.42932800	-0.02267800
C	3.90703200	1.57784500	0.38706200
C	2.89634200	2.48506500	0.32036800
N	1.72650400	1.77017400	0.06990700
N	3.33920600	0.32333600	0.17491800
Cl	2.95623200	4.18638000	0.49415100
Cl	5.57445900	1.83339800	0.67316400
C	-0.37386500	2.48822100	1.11854200
C	0.40572700	2.34997000	-0.04824000
C	-0.04313800	2.75356800	-1.32199700
C	-1.32977200	3.30099100	-1.40555600
C	-2.12667500	3.44456500	-0.27265300
C	-1.65132700	3.04412800	0.97355800
H	-1.71077100	3.61884700	-2.37111600
H	-3.12030200	3.87457000	-0.36053100
H	-2.28119700	3.16493900	1.84951500
C	4.18398600	-1.63688800	1.38756000
C	4.87050300	-2.85740900	1.35269300
C	5.41535700	-3.34481600	0.16778900
C	5.28940600	-2.61681200	-1.01262400
C	4.61195400	-1.39112400	-1.03997200
C	4.06240500	-0.93020100	0.17384500
H	4.98072400	-3.43138800	2.26756300
H	5.94432600	-4.29349500	0.16505700
H	5.72473000	-3.00468800	-1.92836200
C	0.11677600	2.07524800	2.50298700
H	1.11961200	1.65157100	2.39841300
C	-0.77506300	0.97888400	3.11803300
H	-0.37867500	0.67988800	4.09460200
H	-1.79795000	1.33916700	3.27411300
H	-0.81528000	0.09342800	2.47689100
C	0.22982200	3.29333400	3.44138700
H	0.63831900	2.98645400	4.41006700
H	0.88672200	4.06208300	3.02265200
H	-0.74930400	3.74931900	3.62300600
C	0.80367300	2.62258200	-2.58431700
H	1.76724700	2.18631900	-2.30704800
C	0.15064600	1.66811400	-3.60285900
H	-0.00727300	0.67726300	-3.16644400
H	-0.81794200	2.04929300	-3.94367600
H	0.79422000	1.55727100	-4.48217500
C	1.08922500	3.99916800	-3.21656800
H	1.74408600	3.88515800	-4.08682600
H	0.16733900	4.48339400	-3.55566800
H	1.58049300	4.67099800	-2.50605500
C	3.62290700	-1.12527600	2.71132400
C	4.50745800	-0.61598200	-2.35034200
C	4.74816200	-0.88661000	3.73825500
H	4.33464800	-0.45841400	4.65742800
H	5.25137800	-1.82213300	4.00497100
H	5.50416300	-0.19638000	3.35102000
C	5.89853000	-0.18982400	-2.86127300
H	6.43235800	0.40918300	-2.11720500
H	6.51891300	-1.05976600	-3.10137400
H	5.79819100	0.40910500	-3.77260300
C	2.54521800	-2.07076500	3.27661300
H	2.95768200	-3.06293300	3.49052000
H	2.14918000	-1.66781700	4.21525200
H	1.71203000	-2.18760700	2.57776000
H	3.14053300	-0.16081300	2.52938400
Cu	0.76109700	-0.97556600	-0.39060700
H	0.15712200	-1.94676700	-1.50192900
C	3.74544500	-1.41553700	-3.42491400
H	3.65047000	-0.81996000	-4.33922000
H	4.27068200	-2.34098100	-3.68430200
H	2.74057200	-1.67773400	-3.08132500
H	3.93501300	0.29684300	-2.16358500

26

C	8.91131800	-0.28811100	-0.44047700
C	7.65058500	0.32606600	0.18157800
H	8.70258600	-1.32779300	-0.73142600
H	9.15159500	0.24450800	-1.37191600
C	6.43191800	0.30116700	-0.74988200
H	7.40768500	-0.20773100	1.11156300
H	7.86071700	1.36464900	0.47470000
H	6.67712700	0.83277500	-1.68067800
H	6.21842800	-0.73746700	-1.04141100
C	5.17321100	0.92155600	-0.13083000
C	3.95688000	0.91017000	-1.07725200
H	5.38250600	1.95796300	0.16721800
H	4.91726200	0.38435000	0.79325700
H	4.20365500	1.46549900	-1.99218500

H	3.76908800	-0.13026000	-1.38383900
C	10.13211100	-0.25813200	0.48777200
C	11.39360200	-0.86954700	-0.13533800
H	9.89400900	-0.79184600	1.41924100
H	10.34095700	0.78127100	0.77964300
C	12.60802500	-0.83483800	0.79830400
H	11.18564100	-1.90831800	-0.42671400
H	11.63191500	-0.33576700	-1.06559000
H	13.49088300	-1.27746800	0.32493500
H	12.86182100	0.19385100	1.07937600
H	12.41244300	-1.39025700	1.72289000
H	2.30728600	0.94904700	0.40942000
C	2.71328400	1.48239600	-0.44978000
C	2.08999500	2.59434600	-0.85343200
H	2.49146100	3.13284500	-1.71400000
C	1.72023600	5.55575400	-0.67876700
C	1.09544800	4.62177000	0.37615800
H	1.13204300	5.56309000	-1.60519100
H	1.75492100	6.58551200	-0.30348900
H	2.74463800	5.26531500	-0.93178700
C	-0.26173700	5.20895000	0.80658600
C	2.02470800	4.52793700	1.59770600
H	-0.75449900	4.55158300	1.52622400
H	-0.13297100	6.19729000	1.26446500
H	-0.92886500	5.32594300	-0.05694200
H	2.19352400	5.51965900	2.03495200
H	1.58614700	3.88371100	2.36441400
H	2.99841600	4.10899100	1.32217400
C	0.83607700	3.18675700	-0.22841100
O	0.25540200	2.36158900	0.73709100
C	-1.98186300	-0.51401300	0.06484400
C	-3.88233600	-1.71298700	-0.26007700
C	-2.84434100	-2.59327300	-0.22908600
N	-1.68646500	-1.84594300	-0.03111400
N	-3.34068600	-0.44409100	-0.07866800
Cl	-2.86710400	-4.29589200	-0.38794400
Cl	-5.55140800	-2.01518600	-0.47619300
C	0.16013900	-2.75391200	1.31126400
C	-0.34778300	-2.39452600	0.04694300
C	0.38413400	-2.55261800	-1.14736400
C	1.67581400	-3.08365800	-1.04118200
C	2.20989400	-3.43974200	0.19459300
C	1.45923400	-3.27571700	1.35560500
H	2.27057700	-3.21923500	-1.93917000
H	3.21456000	-3.84825200	0.25258600
H	1.88671800	-3.55697900	2.31296300
C	-4.60548800	1.25079800	1.17425600
C	-5.32541800	2.45230800	1.16202900
C	-5.53443900	3.15573500	-0.02106700
C	-5.02893800	2.66920800	-1.22367700
C	-4.30216200	1.47313600	-1.27380900
C	-4.10117000	0.78918300	-0.05798300
H	-5.72565600	2.84220500	2.09270300
H	-6.09505900	4.08581700	-0.00614800
H	-5.19978400	3.22644700	-2.13947200
C	-0.63460200	-2.59797900	2.60390000
H	-1.62150100	-2.19830400	2.35425600
C	0.03744300	-1.58998100	3.55666700
H	-0.56871800	-1.46139100	4.45962600
H	1.02958500	-1.93494700	3.86637300
H	0.15454800	-0.61162100	3.08018000
C	-0.85581900	-3.95643900	3.29776700
H	-1.47533800	-3.82609500	4.19122600
H	-1.35973100	-4.66583400	2.63402200
H	0.09196000	-4.40508200	3.61335900
C	-0.16748300	-2.17790600	-2.51960100
H	-1.17286200	-1.76874300	-2.38565800
C	0.68266400	-1.08129900	-3.18996700
H	0.76429900	-0.19512400	-2.55353800
H	1.69652600	-1.43670400	-3.40277300
H	0.22940700	-0.78294700	-4.14130600
C	-0.29488600	-3.41420800	-3.43167600
H	-0.74216500	-3.13110500	-4.39034700
H	0.68403100	-3.85885300	-3.63994400
H	-0.92458100	-4.18431000	-2.97589200
C	-4.39412200	0.51213600	2.49223100
C	-3.76102600	0.97544200	-2.61057200
C	-5.73402500	0.10973900	3.13878300
H	-5.55302600	-0.46534100	4.05288200
H	-6.32762400	0.98841200	3.41163200
H	-6.33529500	-0.50581900	2.46274300
C	-4.89209500	0.74301700	-3.63137200

H	-5.63902800	0.04155800	-3.24698700
H	-5.40503800	1.67722300	-3.88273400
H	-4.48258300	0.32996200	-4.55912800
C	-3.53438000	1.34268900	3.46533300
H	-4.03344300	2.27815300	3.73953400
H	-3.35349900	0.77803000	4.38618000
H	-2.56631200	1.59430800	3.02120800
H	-3.84484900	-0.41044400	2.28519400
Cu	-0.80848000	0.93065600	0.35278400
H	0.14041100	3.37220000	-1.07574500
C	-2.69388300	1.93618100	-3.17077700
H	-2.27932300	1.53986100	-4.10387400
H	-3.11869000	2.92265200	-3.38511100
H	-1.87216300	2.06948500	-2.45993300
H	-3.27163800	0.01137900	-2.44650300

27

C	8.25658100	-0.52216000	-0.80075500
C	6.95116000	-0.01053700	-0.17835000
H	8.02499800	-1.08988100	-1.71335500
H	8.86421300	0.33543000	-1.12344300
C	6.12759100	0.87154400	-1.12536500
H	6.34094100	-0.86764200	0.14115900
H	7.18213600	0.55535100	0.73548300
H	6.73891400	1.72663000	-1.44703500
H	5.89172600	0.30535800	-2.03751100
C	4.82514300	1.38671900	-0.50060200
C	4.01683800	2.28421300	-1.46116900
H	5.05267900	1.95289300	0.41234700
H	4.20293600	0.53632900	-0.19132900
H	4.62352500	3.14580800	-1.76528300
H	3.80010700	1.70739800	-2.37234100
C	9.08508100	-1.40072100	0.14515500
C	10.39049000	-1.91207200	-0.47748500
H	8.47843700	-2.25888000	0.46898100
H	9.31779400	-0.83294800	1.05769100
C	11.21284300	-2.78727300	0.47406000
H	10.15784600	-2.48036800	-1.38848400
H	10.99626100	-1.05473800	-0.80150500
H	12.13627100	-3.13681000	0.00034900
H	11.49156600	-2.23455300	1.37876300
H	10.64536800	-3.67062700	0.78924500
H	-0.46984800	1.43286400	-2.43514200
C	2.72100600	2.74575000	-0.86957700
C	2.37747700	4.02717700	-0.66088200
H	3.06467200	4.82056200	-0.94210600
C	-0.65435300	6.09942100	0.65422200
C	0.74614400	5.91309600	0.05180400
H	-0.72435600	5.63891100	1.64337800
H	-0.87782900	7.16690700	0.75282800
H	-1.42079000	5.64415200	0.02117200
C	1.79594700	6.57786500	0.97412400
C	0.79442000	6.56303300	-1.35082300
H	2.81191100	6.49465600	0.57734800
H	1.56826800	7.64408100	1.08049900
H	1.78415600	6.13023800	1.97365800
H	0.54751200	7.62737000	-1.27102400
H	1.78312000	6.48665400	-1.81220400
H	0.06848400	6.09814300	-2.02598000
C	1.06741400	4.40759100	-0.06998900
O	0.26639200	3.55786100	0.31395700
C	-1.86219500	-0.74876600	-0.13013100
C	-3.40589400	-1.94381100	1.03175400
C	-2.18784700	-2.49699600	1.28362800
N	-1.25236400	-1.75290500	0.57017300
N	-3.19094900	-0.87513200	0.16690100
Cl	-1.79591100	-3.84900800	2.25544800
Cl	-4.94577300	-2.41047400	1.61265600
C	0.96738900	-1.40994800	1.56767800
C	0.17500200	-2.00181800	0.56329100
C	0.70809000	-2.83036700	-0.44484300
C	2.09292200	-3.03970200	-0.43827400
C	2.90467100	-2.46038100	0.53327500
C	2.34557600	-1.65845600	1.52506600
H	2.53899900	-3.66765300	-1.20314400
H	3.97588700	-2.63968800	0.52183700
H	2.98783400	-1.21976700	2.28221800
C	-4.57952000	1.13902100	0.38406600
C	-5.57404000	1.96654000	-0.15257000
C	-6.18874400	1.66303900	-1.36424500
C	-5.82388500	0.51790500	-2.06717400
C	-4.83626300	-0.34786800	-1.58050700
C	-4.22656800	-0.00715400	-0.35615700

H	-5.86995400	2.86057300	0.38732100
H	-6.95676000	2.32034600	-1.76142400
H	-6.31222000	0.29134000	-3.00981700
C	0.39360000	-0.54642600	2.68768600
H	-0.68628700	-0.46083100	2.53742200
C	0.97038600	0.88237700	2.66593500
H	0.52456100	1.47453100	3.47253600
H	2.05454200	0.87617400	2.82284900
H	0.76538200	1.39347000	1.72124000
C	0.61455300	-1.20464900	4.06512800
H	0.14666900	-0.60081000	4.84977100
H	0.18295400	-2.20922300	4.10518500
H	1.68113700	-1.28660700	4.29998500
C	-0.14891100	-3.49864700	-1.51588800
H	-1.19522700	-3.24000700	-1.33037400
C	0.20432300	-2.97874400	-2.92283900
H	0.08160900	-1.89264700	-2.98372000
H	1.23942000	-3.21812100	-3.18932100
H	-0.44860300	-3.44012900	-3.67141000
C	-0.04153500	-5.03475300	-1.44616500
H	-0.70948400	-5.49228600	-2.18347300
H	0.97591000	-5.37707400	-1.66268800
H	-0.31897800	-5.40976700	-0.45612500
C	-3.94014700	1.49940400	1.72186100
C	-4.46822200	-1.59582700	-2.37673900
C	-4.98478600	1.51205200	2.85588300
H	-4.49637000	1.71427700	3.81494900
H	-5.73946100	2.28983100	2.69728300
H	-5.50311700	0.55136200	2.93379200
C	-5.67150900	-2.54830000	-2.52043300
H	-6.07562100	-2.83133100	-1.54359000
H	-6.47983500	-2.08844100	-3.09868800
H	-5.36858000	-3.46227800	-3.04218900
C	-3.18544800	2.84083500	1.64868100
H	-3.86242100	3.66565200	1.40136500
H	-2.72931800	3.06552000	2.61885400
H	-2.38861400	2.81749800	0.89996900
H	-3.20411500	0.72958800	1.96982000
Cu	-1.06712800	0.50064700	-1.38693800
H	2.00464600	1.97403500	-0.58806400
C	-3.87926400	-1.23154400	-3.75346900
H	-3.57634000	-2.13927000	-4.28617100
H	-4.61202600	-0.70792200	-4.37658200
H	-3.00166700	-0.58585500	-3.64817100
H	-3.69127200	-2.13593400	-1.82853100

TS10

C	8.14023100	-0.01955200	-1.17823800
C	6.89091200	0.40753200	-0.39658200
H	7.89118800	-0.87848800	-1.81789900
H	8.43533000	0.79066400	-1.86026700
C	5.69569800	0.75107800	-1.29469000
H	6.60360000	-0.39699400	0.29547600
H	7.13544500	1.27573100	0.23192000
H	5.98282800	1.54927600	-1.99367100
H	5.44509200	-0.12131300	-1.91488300
C	4.45066200	1.18792300	-0.51157100
C	3.24443800	1.49130600	-1.42661300
H	4.68569800	2.07657600	0.08857100
H	4.17008400	0.39871800	0.19945800
H	3.50868200	2.28377900	-2.13721700
H	3.01881300	0.59545700	-2.01477000
C	9.32965700	-0.38537500	-0.28155000
C	10.58022400	-0.80966500	-1.06256900
H	9.03531700	-1.19824000	0.39806600
H	9.57834000	0.47147900	0.36117000
C	11.76025300	-1.18144300	-0.15875200
H	10.33023100	-1.66273000	-1.70821200
H	10.87797300	0.00437100	-1.73753000
H	12.63604800	-1.48018800	-0.74447900
H	12.05545600	-0.33647900	0.47411900
H	11.50287800	-2.01557900	0.50433600
H	0.53513300	1.30848300	-1.73020900
C	2.02816300	1.89473300	-0.63429400
C	1.72671100	3.21938500	-0.35262200
H	2.33610000	3.99953400	-0.79606900
C	-1.07802400	5.43988700	-0.24404500
C	0.13435600	5.02034900	0.61722800
H	-1.92048400	4.76281200	-0.08369600
H	-1.39469300	6.45650700	0.01526600
H	-0.82688300	5.42665200	-1.31068900
C	-0.26030100	5.05933700	2.11129000
C	1.29366000	6.00428600	0.38074800

H	0.58863000	4.79143600	2.75062700
H	-0.58695700	6.06745600	2.38980100
H	-1.07453600	4.36025200	2.31494100
H	1.00373000	7.00457900	0.72035000
H	2.19204000	5.71125700	0.93392200
H	1.55515700	6.08147100	-0.67960400
C	0.49656800	3.56306400	0.26264200
O	-0.39762300	2.67997600	0.46550700
C	-1.64194500	-0.60415200	-0.02540500
C	-3.37712800	-2.04932800	0.26792400
C	-2.29206900	-2.58834300	0.88512400
N	-1.23742000	-1.69783100	0.69733600
N	-2.96783500	-0.83685500	-0.28342300
Cl	-2.16078200	-4.05956200	1.75130700
Cl	-4.96887800	-2.66818900	0.14478400
C	0.43763600	-1.35438300	2.45996000
C	0.10947900	-1.88050800	1.19342900
C	1.03868600	-2.57135100	0.38818600
C	2.34260900	-2.70459600	0.88264400
C	2.70170400	-2.17996700	2.12180200
C	1.75729500	-1.51687100	2.90110600
H	3.08469600	-3.22949100	0.28921700
H	3.71869000	-2.29621100	2.48520400
H	2.04614100	-1.12201000	3.87011900
C	-4.53143700	1.05602300	-0.30052700
C	-5.33698800	1.93286600	-1.03824100
C	-5.43672800	1.82816100	-2.42302200
C	-4.73260000	0.83756100	-3.10234400
C	-3.90900200	-0.06582700	-2.41861600
C	-3.82124200	0.07203400	-1.01820300
H	-5.89354300	2.70725200	-0.51959100
H	-6.06822600	2.51879000	-2.97444900
H	-4.82300200	0.76249900	-4.18156000
C	-0.57572900	-0.65253100	3.35931200
H	-1.53263200	-0.61443600	2.83132100
C	-0.16570700	0.80193100	3.66063500
H	-0.92239800	1.27911900	4.29293900
H	0.78831800	0.84582900	4.19745300
H	-0.07240600	1.38707700	2.74150800
C	-0.80296900	-1.44543700	4.66224800
H	-1.57915200	-0.96342900	5.26593900
H	-1.12009700	-2.47230300	4.45607400
H	0.10904800	-1.49014900	5.26716100
C	0.67919400	-3.18420900	-0.96259100
H	-0.36646800	-2.94816800	-1.17837900
C	1.52238300	-2.58875000	-2.10646500
H	1.39507000	-1.50398000	-2.16710900
H	2.58843600	-2.80236200	-1.97352700
H	1.21464300	-3.02207700	-3.06411700
C	0.80630100	-4.72065400	-0.92657800
H	0.48843300	-5.14819800	-1.88337400
H	1.84191700	-5.03099000	-0.75073900
H	0.18623300	-5.15475000	-0.13664100
C	-4.46486500	1.19081800	1.21803300
C	-3.17192200	-1.15091300	-3.19791000
C	-5.84858300	0.97044800	1.86084200
H	-5.76666800	1.00675800	2.95230600
H	-6.55990100	1.74530200	1.55568400
H	-6.26897600	-0.00088000	1.58256500
C	-4.16261800	-2.14219400	-3.84172600
H	-4.81963000	-2.59469200	-3.09265000
H	-4.79355900	-1.64610200	-4.58701000
H	-3.61813400	-2.94631500	-4.34798500
C	-3.86377900	2.54538400	1.64190000
H	-4.48244000	3.38072700	1.29526100
H	-3.81201500	2.60473900	2.73493100
H	-2.85325200	2.67580300	1.24370400
H	-3.80095800	0.41121000	1.60195300
Cu	-0.54346600	0.87091200	-0.62377300
H	1.66066800	1.13291000	0.04910500
C	-2.22429500	-0.55185800	-4.25496300
H	-1.67859600	-1.35231300	-4.76599200
H	-2.77471400	0.01225200	-5.01532000
H	-1.49393900	0.11964900	-3.79387000
H	-2.55263000	-1.71639400	-2.49617000

28

C	8.10852100	-0.31686300	0.06864100
C	6.65766300	0.14640700	0.25256300
H	8.11370300	-1.34923900	-0.31016400
H	8.58655000	0.29342200	-0.71118200
C	5.82433700	0.07212700	-1.03356100
H	6.17791500	-0.46255300	1.03244300

H	6.65170500	1.17929700	0.62918400	N	-1.53031500	-1.81718500	-0.06707100
H	6.31139600	0.67540500	-1.81353000	N	-3.07896500	-0.42113900	0.52998800
H	5.82808800	-0.96251100	-1.40715700	Cl	-2.69598500	-4.28207000	0.21936900
C	4.37552800	0.54546000	-0.86257000	Cl	-5.21702800	-2.01057100	1.17261800
C	3.54993700	0.46033100	-2.15224900	C	0.74619500	-2.61923400	0.39504600
H	4.36660600	1.58120800	-0.49816300	C	-0.27549400	-2.36385400	-0.54130200
H	3.88497200	-0.05575600	-0.08326900	C	-0.13608700	-2.62269500	-1.92011900
H	4.07097500	1.00979900	-2.95058100	C	1.09259100	-3.13536900	-2.35456500
H	3.50346100	-0.58656200	-2.48209700	C	2.12727000	-3.38548900	-1.45649000
C	8.94785000	-0.24505600	1.35060700	C	1.95288200	-3.13190100	-0.09838800
C	10.39852400	-0.70641000	1.16017600	H	1.23947900	-3.34194800	-3.41000800
H	8.47324600	-0.85707500	2.13132300	H	3.07152400	-3.78386300	-1.81592100
H	8.94376300	0.78668100	1.73085600	H	2.76518600	-3.33671000	0.59194800
C	11.23153000	-0.63345700	2.44412900	C	-3.73050200	1.31169200	2.14470100
H	10.40236500	-1.73692100	0.77915500	C	-4.39722400	2.51718800	2.39708600
H	10.87257500	-0.09372400	0.38112500	C	-5.08230400	3.18711400	1.38691500
H	12.25991500	-0.97009900	2.27516900	C	-5.12036100	2.66151600	0.09818800
H	11.27619600	0.39194800	2.82905800	C	-4.47303700	1.45945800	-0.21434900
H	10.80058900	-1.26238200	3.23184100	C	-3.77928900	0.81204900	0.82773900
H	1.56971300	0.75360300	-2.94079800	H	-4.37786800	2.93669300	3.39802500
C	2.11661800	1.01327700	-2.01864200	H	-5.59099500	4.12144600	1.60556300
C	2.07107500	2.49739600	-1.76870200	H	-5.66009600	3.19276200	-0.67934400
H	2.79582500	3.08380600	-2.32446800	C	0.58873500	-2.36809100	1.89155200
C	-0.07792000	5.28827500	-1.12821600	H	-0.42417400	-1.99824700	2.07304500
C	1.28367700	4.67980900	-0.72104700	C	1.56410600	-1.28199000	2.38516300
H	-0.89230200	4.82106500	-0.56960700	H	1.40332000	-1.08529800	3.45046200
H	-0.09642300	6.36723400	-0.93181500	H	2.60633400	-1.59300900	2.25679000
H	-0.26727900	5.13812500	-2.19770100	H	1.42131100	-0.34459900	1.83860400
C	1.52984900	4.95735100	0.77966400	C	0.74873400	-3.66915000	2.70246800
C	2.39141300	5.37214100	-1.53354600	H	0.57274500	-3.47352600	3.76539800
H	2.50206200	4.55973100	1.09366000	H	0.03800500	-4.43408100	2.37475900
H	1.52418300	6.03550100	0.98060700	H	1.75785900	-4.08271900	2.60399300
H	0.75699600	4.48555200	1.39056200	C	-1.25178300	-2.37365700	-2.93119200
H	2.37954700	6.44989500	-1.33374200	H	-2.13805100	-2.03411100	-2.38776200
H	3.38396400	4.99439600	-1.26736900	C	-0.87433700	-1.25846100	-3.92543400
H	2.25236400	5.23276800	-2.61068100	H	-0.64538700	-0.32351700	-3.40554500
C	1.22555200	3.14968900	-0.93311300	H	0.00171800	-1.53579300	-4.52141100
O	0.27142400	2.58042200	-0.18799400	H	-1.70310200	-1.07196700	-4.61681400
C	-1.78509700	-0.48293200	0.08876200	C	-1.64321600	-3.66678500	-3.67351000
C	-3.61981100	-1.69745100	0.64973300	H	-2.48954300	-3.47465400	-4.34111400
C	-2.64741100	-2.57407200	0.27744900	H	-0.81764100	-4.04477900	-4.28554300

H	-1.93343600	-4.45649200	-2.97403200
C	-2.98689600	0.60801800	3.27575100
C	-4.53507600	0.91721500	-1.63910500
C	-3.92686900	0.26129300	4.44685700
H	-3.38144900	-0.30093500	5.21195400
H	-4.32739300	1.16299400	4.92176200
H	-4.77221700	-0.34847000	4.11354400
C	-5.98735000	0.66975000	-2.09149600
H	-6.50580500	-0.01446000	-1.41272400
H	-6.56062300	1.60168400	-2.13344900
H	-5.99825100	0.22874300	-3.09368900
C	-1.78520200	1.44454700	3.75803400
H	-2.11042400	2.40308100	4.17619000
H	-1.23889700	0.90639200	4.54005600
H	-1.09179000	1.65310200	2.93736100
H	-2.59037000	-0.33598400	2.89117400
Cu	-0.64848600	0.99848200	-0.15874400
H	1.59942000	0.47514900	-1.21137200
C	-3.79657500	1.84751500	-2.62152800
H	-3.80938200	1.42006400	-3.62980000
H	-4.27064300	2.83361200	-2.66956400
H	-2.75334400	1.98885200	-2.32172200
H	-4.02225500	-0.04841900	-1.66274000

29

C	-8.90150900	-1.67469000	0.37226500
C	-7.64234600	-0.79831300	0.35320200
H	-8.69208600	-2.62135500	-0.14657900
H	-9.13965700	-1.94469700	1.41132400
C	-6.42042900	-1.45957000	1.00380900
H	-7.40070900	-0.53413800	-0.68644900
H	-7.85472000	0.15122500	0.86516600
H	-6.66027700	-1.71760400	2.04562600
H	-6.20825400	-2.41185300	0.49629700
C	-5.16396200	-0.58021900	0.97600600
C	-3.94098100	-1.22900800	1.65368100
H	-5.37536200	0.37835700	1.46919000
H	-4.91192100	-0.33721800	-0.06589100
H	-4.17958000	-1.44451300	2.70394200
H	-3.75082700	-2.19915100	1.16942700
C	-10.12404000	-1.00575400	-0.26868800
C	-11.38319700	-1.88199900	-0.25664300
H	-9.88559600	-0.73095600	-1.30644900
H	-10.33663600	-0.06143300	0.25306800
C	-12.59908100	-1.20306800	-0.89552400
H	-11.17231900	-2.82416500	-0.78087500
H	-11.62107000	-2.15823200	0.77978500
H	-13.48032500	-1.85280900	-0.87259700
H	-12.85574000	-0.27581500	-0.37026100
H	-12.40345900	-0.94486400	-1.94277700
H	-2.30281900	-0.18766300	0.57526000
C	-2.70502400	-0.37318300	1.57084200
C	-2.08661500	0.19484600	2.61158000
H	-2.47936500	0.01463400	3.61420700
O	-0.29918000	1.14009600	1.25063900
C	2.01645900	-1.39169300	-0.15379300
C	2.90701400	-3.16744400	-1.25383400
C	3.93568100	-2.48605000	-0.67938200
N	3.37717100	-1.40139400	-0.01014200
N	1.73738500	-2.48801300	-0.92342700
Cl	5.61190200	-2.82334100	-0.71807700
Cl	2.95213300	-4.58261000	-2.21327900
C	4.35104100	-0.66303300	2.11969900
C	4.12580200	-0.42086800	0.74948900
C	4.59906500	0.72842500	0.08570000
C	5.31219900	1.66147100	0.84897200
C	5.54298500	1.45644000	2.20656400
C	5.06786000	0.30652900	2.83204200
H	5.68923500	2.56089600	0.37217200
H	6.09657400	2.19489000	2.77924800
H	5.25491600	0.15872400	3.89109800
C	-0.30979900	-3.78123100	-0.50210800
C	-1.58745700	-4.16549100	-0.92885100
C	-2.12325800	-3.68792500	-2.12215100
C	-1.38907000	-2.81363700	-2.91880700
C	-0.10494700	-2.39673500	-2.54594200
C	0.40663800	-2.89289600	-1.32990800
H	-2.16845200	-4.84951900	-0.31821200
H	-3.11621600	-3.99966900	-2.43290900
H	-1.81805900	-2.44900200	-3.84701300
C	3.84218900	-1.90849500	2.83959300
H	3.37169600	-2.56400900	2.10137400
C	2.76380000	-1.54718100	3.88050200

H	2.37618000	-2.45492700	4.35550500
H	3.17181400	-0.90428900	4.66790200
H	1.92550000	-1.01903800	3.41431400
C	4.99318600	-2.70652700	3.48370600
H	4.60480900	-3.62495100	3.93648000
H	5.74924400	-2.98430500	2.74283100
H	5.48915900	-2.13198000	4.27300000
C	4.36820000	0.98797300	-1.39972900
H	3.80003400	0.14923100	-1.81180900
C	3.52709600	2.25944800	-1.62374500
H	2.56673900	2.20113600	-1.10282500
H	4.04867600	3.15220600	-1.26307600
H	3.32989900	2.39662000	-2.69241500
C	5.70013900	1.05980100	-2.17217100
H	5.50897700	1.19381500	-3.24209200
H	6.31314500	1.90257300	-1.83550500
H	6.28630800	0.14485800	-2.04271700
C	0.24604900	-4.33550300	0.80611700
C	0.67013800	-1.44341100	-3.45030500
C	0.46876500	-5.85883600	0.71905400
H	0.91199500	-6.22931100	1.64943900
H	-0.47687800	-6.38973800	0.56568200
H	1.13873900	-6.12011400	-0.10553100
C	0.92798700	-2.06462200	-4.83754900
H	1.46409400	-3.01530400	-4.75666000
H	-0.00856200	-2.25092300	-5.37396600
H	1.53088200	-1.38442400	-5.44840700
C	-0.65474900	-3.97935000	2.00447000
H	-1.62948300	-4.47384100	1.93312000
H	-0.18521100	-4.31009800	2.93713000
H	-0.82860700	-2.90120300	2.06839900
H	1.22003800	-3.87275100	0.98823700
Cu	0.81710000	-0.13509900	0.57533200
C	-0.04542700	-0.08389100	-3.57497900
H	0.54956600	0.60004900	-4.18965900
H	-1.02695000	-0.19112800	-4.04901400
H	-0.19372400	0.37797100	-2.59404500
H	1.64583300	-1.25339500	-2.99406500
Si	-0.06777600	4.87724700	-1.68387800
H	-0.02519700	3.41808900	-1.46490300
O	-1.56339600	5.33028900	-1.11041300
O	1.19568300	5.47610000	-0.77884200
C	1.68742900	6.81847000	-0.80446900
C	3.05142100	6.86738800	-0.13353200
H	0.98541200	7.47788100	-0.27583000
H	1.76336000	7.17895800	-1.84001900
H	3.43303200	7.89373800	-0.12246600
H	2.98423300	6.51138900	0.89891200
H	3.76793600	6.23721600	-0.66975900
C	-2.12317200	6.64562000	-1.14494900
C	-3.63583800	6.55304400	-1.01663100
H	-1.85699500	7.15688400	-2.08099100
H	-1.71004000	7.23812900	-0.31749200
H	-4.08016700	7.55385100	-1.01059700
H	-4.05960300	5.99029600	-1.85371400
H	-3.91094600	6.04612400	-0.08719800
C	0.12186700	5.33813100	-3.49576000
H	1.10382800	5.02923300	-3.87029900
H	-0.64201400	4.82680900	-4.09151900
H	0.01940400	6.41285600	-3.67856100
C	-1.12968400	2.53516800	3.07639200
C	-2.13423600	3.27416500	2.17624300
C	-1.67261200	2.47742900	4.51849500
C	0.20367800	3.30646300	3.08545700
H	-1.75011800	3.36818300	1.15744500
H	-3.09133500	2.74359900	2.13070100
H	-2.32643300	4.28361600	2.56063600
H	-1.02580800	1.87214000	5.16635000
H	-1.71798500	3.48516500	4.94870900
H	-2.68231000	2.05752000	4.56390000
H	0.05988100	4.32363900	3.47058500
H	0.94179000	2.80841500	3.72736300
H	0.61916800	3.37232100	2.07749800
C	-0.85118100	1.07903700	2.53155900
H	-0.13108800	0.65333200	3.26452800

TS11

C	8.91877600	-1.35358300	-0.79918000
C	7.69565400	-0.53769800	-0.36141000
H	8.64912900	-2.41898600	-0.83621100
H	9.19257700	-1.07470700	-1.82694000
C	6.47398900	-0.72563200	-1.26999800
H	7.42589900	-0.81338600	0.66822600

H	7.96318800	0.52816900	-0.32907200
H	6.74036800	-0.44526000	-2.29932500
H	6.20908100	-1.79238400	-1.30532200
C	5.24961400	0.08319800	-0.82365000
C	4.02334700	-0.11435900	-1.73366700
H	5.50692600	1.15019200	-0.79281700
H	4.98394100	-0.19685900	0.20536600
H	4.26456900	0.21482300	-2.75311800
H	3.81876800	-1.19454700	-1.79865500
C	10.13668300	-1.17250400	0.11561300
C	11.35904100	-1.99160400	-0.31819600
H	9.86246300	-1.44952400	1.14388200
H	10.40915400	-0.10777600	0.15176300
C	12.56880100	-1.80827100	0.60407900
H	11.08583700	-3.05511400	-0.35634000
H	11.63539800	-1.71279900	-1.34435300
H	13.42330000	-2.40568100	0.26891500
H	12.88746600	-0.75985600	0.63513400
H	12.33279400	-2.11129600	1.63080100
H	2.44209100	0.32519500	-0.24686300
C	2.78322400	0.58788900	-1.24631300
C	2.09175400	1.49079600	-1.94680100
H	2.44137300	1.74028100	-2.94824700
O	0.37908400	1.83703300	-0.20859700
C	-2.20835400	-0.98307300	0.03947700
C	-3.25299100	-3.00308700	0.07688100
C	-4.19079300	-2.06608300	-0.22558300
N	-3.53968600	-0.83534000	-0.25206500
N	-2.04480400	-2.32967700	0.23819600
Cl	-5.86470300	-2.26928100	-0.51553000
Cl	-3.43427000	-4.69605700	0.24405700
C	-4.28069200	0.80862400	-1.91949000
C	-4.17235200	0.42903300	-0.56557400
C	-4.66199600	1.22026300	0.49327700
C	-5.24980000	2.44701400	0.15846700
C	-5.35313700	2.85914200	-1.16708200
C	-4.87880400	2.04523800	-2.19264700
H	-5.63429200	3.08494300	0.94806100
H	-5.81206400	3.81487800	-1.40281900
H	-4.97753900	2.37291000	-3.22280500
C	0.05657600	-3.37971800	-0.47904500
C	1.27520100	-3.97406300	-0.12752500
C	1.63337400	-4.14961900	1.20650700
C	0.77321800	-3.74028000	2.22206500
C	-0.45867100	-3.13951600	1.93227900
C	-0.78494700	-2.96065400	0.57209000
H	1.94941000	-4.30705600	-0.91041200
H	2.58349400	-4.61309000	1.45587000
H	1.06009600	-3.89248400	3.25786100
C	-3.80098400	-0.06759100	-3.07373500
H	-3.36272600	-0.97769000	-2.65456600
C	-2.70184800	0.62576100	-3.90030000
H	-2.34449800	-0.04354600	-4.69018200
H	-3.07518100	1.53668600	-4.38006700
H	-1.84828200	0.90056200	-3.27386500
C	-4.97533100	-0.49696100	-3.97636800
H	-4.61944800	-1.17152200	-4.76215000
H	-5.74983200	-1.01734300	-3.40549600
H	-5.43911200	0.36688100	-4.46414100
C	-4.60615900	0.78515600	1.95456500
H	-4.07494800	-0.16897000	2.00806800
C	-3.82544000	1.78798700	2.82501000
H	-2.81068700	1.93999100	2.44607800
H	-4.32373200	2.76274800	2.85958600
H	-3.75574400	1.41568100	3.85278600
C	-6.02439400	0.55225500	2.51424200
H	-5.96868300	0.19127900	3.54671000
H	-6.60822100	1.47897200	2.51549800
H	-6.57128300	-0.18878700	1.92300000
C	-0.31671800	-3.23981800	-1.95190100
C	-1.38588700	-2.73433100	3.07450900
C	-0.52700100	-4.62192300	-2.60394700
H	-0.84234000	-4.50379700	-3.64609900
H	0.39885400	-5.20724600	-2.59984700
H	-1.29326100	-5.20115200	-2.08000500
C	-1.86545200	-3.96791700	3.86611600
H	-2.36603400	-4.69195800	3.21634800
H	-1.02785200	-4.47662800	4.35521900
H	-2.57193500	-3.66414100	4.64579200
C	0.72355000	-2.41766500	-2.73542700
H	1.69167700	-2.92876000	-2.77317300
H	0.38700400	-2.27560300	-3.76806800

H	0.88214500	-1.43247600	-2.28724800
H	-1.26664800	-2.70197800	-2.01446600
Cu	-0.92011300	0.38490700	0.29593200
C	-0.72628400	-1.70257700	4.00893200
H	-1.43291000	-1.39769800	4.78832000
H	0.15628500	-2.11802300	4.50694100
H	-0.41770700	-0.80968400	3.45824500
H	-2.27153900	-2.25796500	2.64478800
Si	0.79798700	2.32987400	1.53660700
H	-0.18792900	1.07483000	1.73070000
O	2.33922400	2.82396400	0.99137800
O	-0.24975700	3.66104000	1.63725200
C	0.02027100	4.80273500	2.43881400
C	-1.20983100	5.70031400	2.47850700
H	0.87300500	5.36334500	2.02560700
H	0.29402100	4.50815400	3.46235500
H	-1.01748100	6.58983900	3.08848600
H	-1.48429600	6.02645600	1.47032900
H	-2.06279900	5.16480300	2.90779300
C	3.42731400	3.25708300	1.78919500
C	4.48732400	3.90354300	0.90382300
H	3.86995800	2.40771700	2.33110200
H	3.10743600	3.98329600	2.55076300
H	5.35833100	4.19543500	1.50147200
H	4.81651800	3.20759100	0.12691000
H	4.09158300	4.79644800	0.41091900
C	1.27663900	1.94554700	3.38088200
H	0.35251300	1.78516300	3.94954700
H	1.83662700	1.00055700	3.41708900
H	1.87682300	2.69421300	3.90995300
C	0.55969100	3.59640900	-2.05027900
C	1.60041200	4.58461900	-1.49932100
C	0.63951400	3.61486000	-3.59549600
C	-0.85562200	4.05218400	-1.64400800
H	1.55435500	4.64523300	-0.41255800
H	2.61647700	4.28052300	-1.77071200
H	1.42256900	5.58296000	-1.91816900
H	-0.03918300	2.88072800	-4.04606300
H	0.34894300	4.60383800	-3.96688200
H	1.64913200	3.41545200	-3.96831800
H	-1.05298400	5.05671900	-2.03775100
H	-1.62102800	3.38055700	-2.05220700
H	-0.96097700	4.07270500	-0.55842600
C	0.76642300	2.11717100	-1.56477800
H	0.01722600	1.56429700	-2.15685600

30

C	-8.61854300	4.92198900	-1.15320700
C	-7.69840600	3.84085100	-0.57254900
H	-8.08092600	5.47122500	-1.93954900
H	-9.47301200	4.44064100	-1.65038700
C	-7.18995500	2.84504800	-1.62319700
H	-6.84031900	4.32020200	-0.07994000
H	-8.23405000	3.29326800	0.21604400
H	-8.04958100	2.36779800	-2.11514200
H	-6.65422300	3.39207600	-2.41229600
C	-6.27168800	1.75950200	-1.04901800
C	-5.78906200	0.75559900	-2.11438500
H	-6.79758200	1.21113000	-0.25600100
H	-5.40110300	2.23043100	-0.57147700
H	-6.65557800	0.26445100	-2.57467700
H	-5.28361800	1.31536000	-2.91558000
C	-9.13765700	5.91697100	-0.10721700
C	-10.05676800	6.99692900	-0.69161300
H	-8.28449900	6.39948200	0.39131000
H	-9.67732400	5.36920600	0.67883100
C	-10.57356300	7.98625700	0.35820200
H	-9.51664700	7.54517300	-1.47577900
H	-10.90851900	6.51486100	-1.19088800
H	-11.22389600	8.74431100	-0.09106500
H	-11.14964900	7.47275900	1.13667500
H	-9.74550400	8.50846900	0.85142200
H	-3.91095200	0.09028000	-1.15259800
C	-4.84945100	-0.28380700	-1.56802300
C	-5.08366100	-1.60020600	-1.54904200
H	-6.02311500	-1.98601500	-1.94365000
O	-4.80959300	-3.40095400	0.02604300
C	4.12693700	0.39228400	0.24284000
C	5.83602400	1.52598800	-0.73227600
C	5.83049400	0.26805800	-1.25353200
N	4.77929200	-0.41389600	-0.64721500
N	4.78807300	1.58693500	0.18164800
Cl	6.86703300	-0.42273100	-2.42514200

Cl	6.88312700	2.83409200	-1.07441400	C	3.16603900	4.69363800	-1.87000100
C	3.48915300	-2.05535500	-1.94159200	H	2.74914000	4.51041000	-2.86582800
C	4.41894200	-1.79141100	-0.91607000	H	2.71975900	5.61835200	-1.48962700
C	5.01800300	-2.80634100	-0.14348700	H	4.24270700	4.85796000	-1.97628200
C	4.64357500	-4.12729100	-0.42011000	C	7.39066200	2.59258600	3.10794300
C	3.72248300	-4.42061300	-1.42221100	H	7.80927800	3.05233100	2.20740600
C	3.15408500	-3.39534200	-2.17338000	H	7.30212500	3.37059700	3.87344900
H	5.07887800	-4.93592500	0.15856300	H	8.10500000	1.84751900	3.47351200
H	3.44671400	-5.45256300	-1.61869900	C	1.35183600	3.25483900	-0.81963600
H	2.43698400	-3.63704200	-2.95160500	H	0.84564700	4.11750500	-0.37345800
C	3.51318600	3.67230900	0.42734900	H	0.91361500	3.08408200	-1.80875500
C	3.18161700	4.78287300	1.21368300	H	1.14153400	2.38053700	-0.19539900
C	3.74750000	4.96978100	2.47204700	H	3.29976500	2.61058100	-1.41612900
C	4.66198300	4.04728400	2.97307400	Cu	2.59875100	-0.05674800	1.35180600
C	5.03130200	2.91696400	2.23289500	C	5.46600500	1.24387500	4.07986800
C	4.43581300	2.75325900	0.96609400	H	6.17568500	0.50142600	4.46013600
H	2.46982100	5.50999200	0.83536000	H	5.28280300	1.97108800	4.87804000
H	3.47502800	5.83831100	3.06449800	H	4.52088200	0.73565700	3.86373100
H	5.09529900	4.20481700	3.95589900	H	6.20988700	1.13921600	2.07956400
C	2.84067700	-0.95884400	-2.78074700	Si	-5.23270500	-2.89771500	1.54596200
H	3.26186100	0.00287300	-2.47477700	H	1.40152100	-0.40931200	2.22641700
C	1.32178800	-0.89046800	-2.52699900	O	-6.79754500	-2.34537800	1.42372000
H	0.87900400	-0.06737700	-3.09791700	O	-5.17066200	-4.22128800	2.54393000
H	0.82501700	-1.81674000	-2.83491200	C	-5.87286200	-5.44401500	2.28762300
H	1.10551000	-0.72814500	-1.46622900	C	-5.59582600	-6.42404700	3.41602700
C	3.14726300	-1.13263000	-4.28097900	H	-5.54427700	-5.86219100	1.32756900
H	2.71751100	-0.30227500	-4.85098200	H	-6.95034500	-5.24554400	2.21011900
H	4.22531900	-1.15221200	-4.46808300	H	-6.12371400	-7.36684700	3.23892200
H	2.72011700	-2.06086800	-4.67462100	H	-4.52465400	-6.63591000	3.48858200
C	6.02621600	-2.52272800	0.96556200	H	-5.93112000	-6.01506100	4.37424900
H	6.22664400	-1.44767100	0.98037200	C	-7.56448400	-1.89707900	2.54686300
C	5.45288100	-2.89849600	2.34637300	C	-8.94382400	-1.47094200	2.07021900
H	4.51981500	-2.36237500	2.54733700	H	-7.05722500	-1.05361700	3.03546700
H	5.24526100	-3.97184000	2.41181900	H	-7.65055100	-2.70336900	3.28775500
H	6.16945700	-2.64695900	3.13553200	H	-9.54801400	-1.12391700	2.91482700
C	7.37042700	-3.23110100	0.70947800	H	-8.86563600	-0.65683000	1.34301000
H	8.09293400	-2.95828800	1.48569800	H	-9.46294500	-2.30850700	1.59420400
H	7.26146400	-4.32048400	0.72710300	C	-4.07247800	-1.62934200	2.26648200
H	7.79053300	-2.94980000	-0.26108900	H	-4.36630400	-1.36776500	3.28797700
C	2.86885700	3.49810500	-0.94423000	H	-3.04817100	-2.01361300	2.30299300
C	6.03190300	1.92547400	2.81862400	H	-4.07174000	-0.71113700	1.67147800

C	-3.54615200	-3.61739800	-2.03592300
C	-4.66264900	-4.41950800	-2.73179600
C	-2.75005900	-2.81690700	-3.08356500
C	-2.59070900	-4.58917800	-1.31615900
H	-5.28207400	-4.94526500	-1.99960400
H	-5.31367700	-3.77380100	-3.33030700
H	-4.22786100	-5.16459200	-3.40705700
H	-1.94523500	-2.23817700	-2.61471600
H	-2.29169300	-3.49789300	-3.80903600
H	-3.38973100	-2.11857700	-3.63093600
H	-2.13039000	-5.27426400	-2.03696000
H	-1.78387000	-4.04731500	-0.80832500
H	-3.12063500	-5.18454600	-0.56887900
C	-4.13581800	-2.62672400	-0.98551400
H	-3.28255700	-2.10365100	-0.52931600

31

C	-6.25060100	0.35878300	0.24927000
C	-4.76162300	0.11245900	-0.02343100
H	-6.46388500	0.15508900	1.30848200
H	-6.47642600	1.42361300	0.09427600
C	-3.82838900	0.95322000	0.85630100
H	-4.53730300	-0.95336300	0.12687000
H	-4.54751000	0.32052900	-1.08145500
H	-4.05108500	2.01944900	0.70720100
H	-4.04071100	0.74413200	1.91463500
C	-2.34100200	0.70317800	0.58022400
C	-1.40629800	1.54054000	1.47343500
H	-2.11902500	0.92049500	-0.47309000
H	-2.11897100	-0.36347800	0.72512000
H	-1.60818300	2.60808100	1.31805300
H	-1.65187100	1.32741200	2.52497800
C	-7.18202700	-0.48851200	-0.62592100
C	-8.67168200	-0.24366300	-0.35588400
H	-6.95689900	-1.55355800	-0.47027400
H	-6.96876700	-0.28611600	-1.68546800
C	-9.59357700	-1.09649000	-1.23278300
H	-8.88463700	-0.44465300	0.70297800
H	-8.89729900	0.81988600	-0.51368100
H	10.64874200	-0.89802300	-1.01761500
H	-9.42687700	-0.89301600	-2.29686200
H	-9.41619000	-2.16589000	-1.07026600
H	0.37450400	0.23208800	1.41034800
C	0.05226300	1.25563700	1.23646900
C	0.94671800	2.15711200	0.82783600
H	0.61381300	3.18174500	0.66882800
C	2.42870200	1.95242400	0.60855900
O	2.87254100	0.68478000	1.08757800
Si	3.01902000	-0.91501500	0.77537600
O	1.70142100	-1.58040600	0.01375200
O	4.29932300	-1.09916500	-0.27068000
C	4.58214200	-2.33096300	-0.94500300
C	5.83941900	-2.16507000	-1.78205800
H	3.72956800	-2.60689200	-1.57756300
H	4.72456600	-3.13836500	-0.21231400
H	6.06976800	-3.09626100	-2.30979200
H	5.70749900	-1.37139200	-2.52347900
H	6.69380800	-1.90622300	-1.14938100
C	0.76643500	-2.51642400	0.55800400
C	-0.14256200	-3.01287900	-0.55421500
H	0.16875100	-2.03806000	1.34573400
H	1.29766700	-3.35968900	1.01829700
H	-0.86489500	-3.73528700	-0.16043900
H	-0.69360900	-2.18016200	-1.00110100
H	0.44167900	-3.50071300	-1.34030500
C	3.35978700	-1.74048900	2.41605000
H	4.22385100	-1.27224100	2.89700400
H	2.50733900	-1.65082700	3.09670300
H	3.58037700	-2.80607900	2.29255000
C	2.91503200	2.29485800	-0.84171100
C	4.45451100	2.22954500	-0.87959400
H	4.89380800	2.93052400	-0.15961800
H	4.81801300	1.22582900	-0.65419500
H	4.81729700	2.50697900	-1.87568900
C	2.31921000	1.33838600	-1.88986400
H	2.59396800	1.67226900	-2.89669300
H	2.69556600	0.32018000	-1.77001000
H	1.22669000	1.31146600	-1.82903900
C	2.48696400	3.74028900	-1.17850800
H	1.40621900	3.83203000	-1.31921900
H	2.79052000	4.44507000	-0.39521400
H	2.96685500	4.05734600	-2.11020200
H	2.93765500	2.68296100	1.25737200

32

Si	-0.12606700	-1.66140900	-0.01480500
O	0.25645600	-1.65465300	-1.68733100
O	-1.71768000	-2.16449400	0.37954500
C	-2.12850200	-3.44899400	0.79792000
C	-3.63638500	-3.44841300	1.02687600
H	-1.61652400	-3.74519800	1.72249500
H	-1.87492100	-4.20718000	0.04449900
H	-3.97768600	-4.43663500	1.35564800
H	-3.91516700	-2.71769000	1.79347700
H	-4.16958900	-3.19313300	0.10464200
C	0.66399500	-2.72322700	-2.51843800
C	-0.52383800	-3.50699000	-3.07325000
H	1.33493400	-3.40490600	-1.98875600
H	1.22647200	-2.28474900	-3.35732400
H	-0.18739000	-4.27780600	-3.77738400
H	-1.07079200	-3.99873400	-2.26278300
H	-1.21789200	-2.84256600	-3.59959000
C	0.79518600	-0.70656400	1.36566500
H	1.38311900	-1.30556000	2.06238500
H	1.47193400	0.03039900	0.91853000
H	0.05165200	-0.13914500	1.93622300
N	-3.43514500	1.90695600	-0.59917800
C	-2.10986700	2.68791900	-0.63117100
C	-2.00148800	3.99776200	0.14873800
H	-1.94740300	2.91054900	-1.68878400
H	-1.35477600	1.95958600	-0.33073300
C	-0.58418100	4.57386800	-0.01880800
H	-2.72303200	4.73202100	-0.22608100
H	-2.20254900	3.85951200	1.21325100
C	-0.40578400	5.90906500	0.70918900
H	0.14831500	3.84860100	0.35637500
H	-0.36790400	4.70552900	-1.08677900
H	0.60883800	6.29620700	0.57512500
H	-1.10418600	6.66408600	0.33144900
H	-0.58195500	5.80065800	1.78502700
C	-3.35584100	0.99375900	-1.84724700
C	-4.43140800	-0.08195500	-1.98862600
H	-2.37190300	0.52531000	-1.77943900
H	-3.38475300	1.67570000	-2.70134500
C	-4.29577600	-0.77477300	-3.35621800
H	-4.32253800	-0.83366500	-1.20191400
H	-5.44297800	0.33228500	-1.90632700
C	-5.32947200	-1.88713700	-3.55175400
H	-4.40154100	-0.02949800	-4.15528000
H	-3.28546800	-1.19099300	-3.45058500
H	-5.21304800	-2.36364900	-4.52997400
H	-5.22325700	-2.66446700	-2.78741000
H	-6.35104400	-1.49537000	-3.49023600
C	-3.53102700	0.97372700	0.61745200
C	-3.09976500	1.50576200	1.98361200
H	-2.88220800	0.13202100	0.37131200
H	-4.56912000	0.63575000	0.64702500
C	-3.31296700	0.41039000	3.04304900
H	-2.03592000	1.76171500	1.96187000
H	-3.64950700	2.40260400	2.28003300
C	-2.84872300	0.84604700	4.43569400
H	-4.37680100	0.14031900	3.07877800
H	-2.77241800	-0.49242500	2.73512900
H	-3.01496100	0.05323000	5.17151000
H	-1.77954500	1.08483600	4.43917700
H	-3.39032700	1.73616100	4.77517300
C	-7.13918500	5.03384500	1.21773000
C	-6.45598600	4.35828400	0.02532800
H	-7.98231500	5.64923000	0.88969400
H	-7.52241000	4.29237200	1.92713800
H	-6.44189800	5.68316800	1.75828400
C	-5.26459900	3.48238900	0.45063600
H	-7.18613600	3.74318300	-0.51619000
H	-6.11148400	5.12308300	-0.68249200
C	-4.64515800	2.82116900	-0.78068100
H	-4.54165200	4.10176600	0.98608800
H	-5.62152400	2.71966800	1.15018600
H	-5.41209200	2.20912000	-1.25518000
H	-4.33577700	3.57437000	-1.51004100
F	-0.87237700	-0.08556900	-0.39244700
C	7.63551800	2.55834000	-0.43260600
C	6.23910400	1.95930000	-0.22335200
H	8.33844900	2.09426100	0.27409600
H	7.99716500	2.29410900	-1.43668100
C	6.19306300	0.43475700	-0.38339100
H	5.87626700	2.22840700	0.77894300

H	5.53687900	2.41975800	-0.93296000
H	6.55229100	0.16337100	-1.38650800
H	6.89731400	-0.02484700	0.32505900
C	4.79658200	-0.16072600	-0.16652400
C	4.75677500	-1.69467300	-0.30616900
H	4.09353600	0.28665700	-0.88285600
H	4.43066800	0.11510600	0.83163400
H	5.14765200	-1.95962600	-1.30066400
H	5.44231200	-2.14368200	0.42499600
C	7.68131000	4.08174600	-0.26337900
C	9.07704400	4.68234600	-0.47244900
H	7.32070700	4.34625500	0.74112400
H	6.97832500	4.54717200	-0.96929900
C	9.11365400	6.20391700	-0.30016500
H	9.77964500	4.21729800	0.23252200
H	9.43656300	4.41884300	-1.47652700
H	10.12204600	6.60132700	-0.45611300
H	8.44650800	6.69922400	-1.01505600
H	8.79284300	6.49590800	0.70642300
H	2.62804300	-1.96369500	-0.86103400
C	3.37634300	-2.27257600	-0.13544600
C	3.01592400	-3.08806100	0.85872100
H	3.77189000	-3.35248600	1.59902500
C	2.79744500	-5.75188500	2.11559300
C	1.72778100	-5.27303000	1.11037500
H	2.64963600	-5.30045200	3.10453300
H	2.73581400	-6.83919900	2.23856300
H	3.81435000	-5.51937800	1.78703600
C	0.37539200	-5.85981100	1.54953500
C	2.07098700	-5.80387900	-0.29180100
H	-0.41365800	-5.59447700	0.84643000
H	0.43390100	-6.95347700	1.60515600
H	0.08585200	-5.49197000	2.54150800
H	2.13927300	-6.89845100	-0.28399500
H	1.30082900	-5.51500300	-1.01153100
H	3.02906800	-5.40861900	-0.64448000
C	1.64405100	-3.69452100	1.10890400
O	0.64404200	-3.25954900	0.22921900
H	1.38354100	-3.43434300	2.15557200

TS12

Si	-0.37634700	0.04413100	1.28805300
O	-1.49158500	1.19380100	1.70948400
O	-0.29183000	-0.17652900	-0.35437800
C	0.94516000	-0.30891600	-1.07389500
C	0.69106500	-0.10151700	-2.55737300
H	1.35216500	-1.31676000	-0.90602600
H	1.65119400	0.42874600	-0.68579400
H	1.62595900	-0.21224700	-3.11730500
H	-0.02533000	-0.83453500	-2.94475500
H	0.29908100	0.90308400	-2.74292000
C	-1.21472700	2.37857500	2.47848000
C	-1.41020200	2.12536400	3.96760600
H	-1.92412000	3.14236000	2.13764200
H	-0.20461000	2.71908300	2.23176000
H	-1.25667100	3.05289700	4.53076100
H	-2.42144100	1.76086700	4.17803800
H	-0.69628100	1.38329200	4.33941700
C	1.14273700	-0.14796000	2.34026400
H	1.81609200	-0.88788600	1.89430200
H	1.65882800	0.81218500	2.37289300
H	0.87584200	-0.49724800	3.34309500
N	-4.48410600	-0.46850100	-0.40743200
C	-4.46969500	-0.54860400	1.12894500
C	-5.29297900	-1.63274300	1.82349000
H	-4.83577600	0.42532200	1.46195300
H	-3.41724100	-0.61771000	1.40511300
C	-5.08209200	-1.53032900	3.34486500
H	-6.35955000	-1.50974100	1.60636000
H	-5.00583900	-2.63412800	1.49635800
C	-5.90118300	-2.56671500	4.11901100
H	-4.01613800	-1.65854900	3.56949800
H	-5.35055100	-0.52166500	3.68439600
H	-5.73157700	-2.47473100	5.19602900
H	-6.97437100	-2.44104700	3.93772900
H	-5.63009900	-3.58646200	3.82445700
C	-4.03820300	0.98085500	-0.71375600
C	-3.67919700	1.30717700	-2.16281100
H	-3.18007300	1.16726200	-0.06319700
H	-4.86869800	1.60778200	-0.37862900
C	-3.45503600	2.82217700	-2.31444600
H	-2.76408600	0.78501600	-2.45640700
H	-4.46756200	0.99729300	-2.85858900

C	-3.03683700	3.20818900	-3.73582400
H	-4.37527400	3.35523500	-2.04269800
H	-2.68427100	3.14707700	-1.60559000
H	-2.88800600	4.28890600	-3.81999300
H	-2.09804600	2.71930600	-4.01729700
H	-3.79840000	2.91730700	-4.46812100
C	-3.45152700	-1.40390300	-1.05095200
C	-3.30133500	-2.82345000	-0.50358600
H	-2.49004300	-0.89942600	-0.93492200
H	-3.69866600	-1.42361400	-2.11433300
C	-2.25246600	-3.57753800	-1.33978900
H	-2.95248000	-2.78197400	0.53131700
H	-4.24129600	-3.37980600	-0.52545400
C	-2.00557500	-4.99736600	-0.82204000
H	-2.57962900	-3.62014600	-2.38704900
H	-1.31238100	-3.01279200	-1.32844300
H	-1.25782400	-5.51322400	-1.43215800
H	-1.64180200	-4.98319900	0.21097700
H	-2.92433300	-5.59408300	-0.84442300
C	-8.44481600	-3.32928800	-2.11901400
C	-7.86375400	-1.95130500	-1.79035500
H	-9.46697000	-3.24241100	-2.49942500
H	-7.84673000	-3.84025100	-2.88132200
H	-8.47230500	-3.97050000	-1.23126400
C	-6.42360000	-2.03461700	-1.25565900
H	-7.88420600	-1.32047100	-2.68833200
H	-8.49916300	-1.45218000	-1.04752500
C	-5.89518200	-0.62772700	-0.97759000
H	-6.41301000	-2.65588700	-0.35753700
H	-5.79790300	-2.53231700	-2.00386000
H	-5.90056300	-0.07060800	-1.91461600
H	-6.54961800	-0.09791100	-0.28076700
F	-1.28480000	-1.29688100	1.66697800
C	9.26000600	-1.73138700	-0.21186200
C	7.75457600	-1.44977800	-0.12907200
H	9.68588600	-1.18160900	-1.06353000
H	9.75352800	-1.32976600	0.68484200
C	7.41212900	0.03839500	0.01249400
H	7.26114400	-1.85134600	-1.02583300
H	7.32969300	-2.00105200	0.72211600
H	7.90833300	0.44118800	0.90735100
H	7.83299500	0.59002100	-0.84062500
C	5.90649500	0.31471800	0.10234900
C	5.55843400	1.80892700	0.24430500
H	5.48651400	-0.23464900	0.95688500
H	5.40483400	-0.08418500	-0.79006500
H	6.09678500	2.20168900	1.12182900
H	5.94859600	2.35640200	-0.62471200
C	9.59895800	-3.22040900	-0.35093900
C	11.10407800	-3.50478100	-0.42856000
H	9.10831900	-3.62240800	-1.24920800
H	9.17096100	-3.77092100	0.49930400
C	11.43269900	-4.99465700	-0.56426900
H	11.53215400	-2.95646600	-1.27888300
H	11.59395600	-3.10252600	0.46874500
H	12.51333900	-5.16436300	-0.61491100
H	11.04600200	-5.56404000	0.28881200
H	10.98664100	-5.41761100	-1.47180800
H	3.58535000	1.62070100	1.25708300
C	4.08161700	2.06265000	0.39341500
C	3.31768700	2.76044300	-0.45251900
H	3.78793500	3.19750900	-1.33737300
C	2.10745100	5.28991300	-1.41940400
C	1.45293600	4.51568500	-0.25977400
H	1.90964000	4.80150900	-2.38278600
H	1.70772500	6.31058900	-1.48293200
H	3.19279400	5.37231300	-1.30242600
C	-0.07343200	4.64588500	-0.39783800
C	1.90381500	5.11136000	1.08223000
H	-0.57036100	4.02100100	0.34542200
H	-0.40339800	5.68552500	-0.27199300
H	-0.40094000	4.31099400	-1.39112500
H	1.58764700	6.15751100	1.18728800
H	1.47964100	4.53043700	1.90537600
H	2.99508800	5.07845300	1.17978400
C	1.80391900	2.95846300	-0.29681400
O	1.26106700	2.25564000	0.73198900
H	1.40102200	2.65116900	-1.30613400

33

N	-3.03416400	-0.99481100	-0.13487400
C	-2.86293100	-0.59883000	1.34106600
C	-2.55614000	-1.69395800	2.36236400

H	-3.81860600	-0.14391300	1.61581400
H	-2.11571800	0.20286000	1.32205800
C	-2.40133300	-1.06468600	3.75818600
H	-3.36978400	-2.42730100	2.39968600
H	-1.64192200	-2.24023000	2.11962200
C	-2.14022800	-2.10989800	4.84646000
H	-1.57958800	-0.33826500	3.73811200
H	-3.30772100	-0.49659700	4.00501000
H	-2.03127500	-1.63785800	5.82773400
H	-2.96430800	-2.82915400	4.91133400
H	-1.22251900	-2.67292700	4.64336700
C	-3.79377900	0.20933400	-0.74765000
C	-3.93309000	0.23544200	-2.26943700
H	-3.20456100	1.07896300	-0.41507300
H	-4.77988900	0.19090900	-0.27486000
C	-4.89711100	1.36130000	-2.68315000
H	-2.95890100	0.42005900	-2.73266900
H	-4.30763000	-0.71144500	-2.67779100
C	-5.02166300	1.49820000	-4.20315900
H	-5.88700600	1.17051100	-2.24823000
H	-4.54934600	2.30972200	-2.25583000
H	-5.71731600	2.29959400	-4.47089500
H	-4.05331900	1.73049200	-4.65967500
H	-5.38978100	0.57105300	-4.65693400
C	-1.68417700	-1.05137200	-0.86049100
C	-0.53338100	-1.83421700	-0.22776600
H	-1.38576900	0.00611800	-0.90554000
H	-1.90246600	-1.43752500	-1.85851500
C	0.67392800	-1.81865200	-1.18158000
H	-0.23603100	-1.36180000	0.71356400
H	-0.79340400	-2.87204500	-0.00591700
C	1.86461300	-2.60867900	-0.63116300
H	0.37782900	-2.23633500	-2.15305800
H	0.97256400	-0.77981800	-1.36823500
H	2.71543900	-2.57020700	-1.31846400
H	2.19651300	-2.20665100	0.33243400
H	1.60535900	-3.66260100	-0.47894700
C	-3.80504300	-6.10868200	-0.44376900
C	-4.37633900	-4.68797100	-0.43546100
H	-4.60054700	-6.85115000	-0.55897600
H	-3.09739900	-6.24663100	-1.26856600
H	-3.27546400	-6.32848900	0.48967100
C	-3.28665500	-3.61589900	-0.26514900
H	-4.92350400	-4.50721100	-1.36980200
H	-5.11047400	-4.59200900	0.37496000
C	-3.91925100	-2.22485800	-0.30676200
H	-2.75668700	-3.79247000	0.67382600
H	-2.55833000	-3.72110500	-1.07595900
H	-4.40815300	-2.10885400	-1.27407300
H	-4.69523400	-2.13186800	0.45800300
C	7.41403400	0.04904300	-0.00664600
C	5.90670700	0.02544600	-0.28890200
H	7.82516200	1.02149400	-0.31355400
H	7.58098500	-0.02158000	1.07783600
C	5.12933000	1.14232900	0.41863200
H	5.74016000	0.09893000	-1.37318600
H	5.49686000	-0.94870000	0.01467900
H	5.29761500	1.07054000	1.50299500
H	5.53642100	2.11708200	0.11334500
C	3.62197400	1.11257400	0.13834400
C	2.83894000	2.23006200	0.85263900
H	3.21598600	0.13792900	0.44385000
H	3.44712500	1.18921200	-0.94355600
H	3.05059500	2.15620200	1.93151800
H	3.22741400	3.20638400	0.53176700
C	8.18777600	-1.07205700	-0.71107500
C	9.69543500	-1.05003600	-0.43081400
H	8.02102100	-1.00254200	-1.79574900
H	7.77744100	-2.04491400	-0.40370700
C	10.45863600	-2.17461800	-1.13732000
H	10.10585900	-0.07893500	-0.73965100
H	9.86238500	-1.11888500	0.65282500
H	11.53088600	-2.13086300	-0.91943500
H	10.09471100	-3.15909400	-0.82120900
H	10.33722500	-2.11242800	-2.22494100
H	0.82827700	1.27231000	0.95040400
C	1.35230200	2.16964800	0.62057800
C	0.61528600	3.11906100	0.03772200
H	1.11723500	4.02299000	-0.31628200
C	-1.05015700	5.60861200	0.09621700
C	-1.62941500	4.24918700	0.52996500
H	-1.01524800	5.69322700	-0.99791400

H	-1.66868600	6.43557300	0.46839300
H	-0.03587500	5.76691600	0.47632700
C	-3.11407400	4.20608000	0.13207700
C	-1.51231300	4.09099200	2.05327500
H	-3.55578500	3.24969900	0.42143200
H	-3.67969400	5.01437400	0.61347900
H	-3.23190000	4.31876800	-0.95391800
H	-2.11085000	4.84163200	2.58532600
H	-1.86035900	3.09573900	2.34345200
H	-0.47272000	4.19257700	2.38342700
C	-0.89581700	3.02941100	-0.19441400
O	-1.43886500	1.82224400	0.11851600
H	-1.01361300	3.29241300	-1.28605200

3a

C	4.80882900	0.38228300	0.30828800
C	3.49586800	-0.32037100	-0.05864700
H	4.74253600	1.44250200	0.02474000
H	4.93560200	0.36829400	1.40034400
C	2.26143900	0.30538100	0.60213200
H	3.36948200	-0.30348000	-1.15058900
H	3.56001400	-1.38117200	0.22264200
H	2.37735400	0.27205100	1.69492100
H	2.20901500	1.37057100	0.33508900
C	0.94521000	-0.37681600	0.21070500
C	-0.28897600	0.26396600	0.87392000
H	0.98943500	-1.44145100	0.47924900
H	0.82337100	-0.34173700	-0.88013100
H	-0.15703600	0.22142800	1.96553400
H	-0.33765900	1.32754700	0.60774700
C	6.04472000	-0.24046800	-0.35227000
C	7.35557200	0.47196100	0.00300100
H	5.91468900	-0.23436300	-1.44412800
H	6.11797200	-1.29853300	-0.06220100
C	8.58539700	-0.15654600	-0.65931400
H	7.28260200	1.52849300	-0.28911000
H	7.48498600	0.46750900	1.09395500
H	9.50321200	0.37528100	-0.38753400
H	8.70580400	-1.20343900	-0.35778500
H	8.50017600	-0.13618000	-1.75190800
H	-1.66261300	-1.46815900	0.76266700
C	-1.57870800	-0.41379900	0.49892800
C	-2.58877500	0.17208300	-0.15072100
H	-2.48649700	1.21599000	-0.44237400
C	-5.10859000	1.69012800	-0.96015100
C	-5.16850100	0.33021600	-0.23659700
H	-4.90701700	1.56433200	-2.03045600
H	-6.06891300	2.20805500	-0.86378700
H	-4.34108400	2.35028600	-0.54576600
C	-6.39031300	-0.45130600	-0.75628700
C	-5.30838800	0.55832900	1.28014100
H	-6.44379700	-1.44293600	-0.30093400
H	-7.31643200	0.08716100	-0.52789500
H	-6.33914300	-0.58348900	-1.84351000
H	-6.20482100	1.14857300	1.49738500
H	-5.40787400	-0.38878000	1.82266200
H	-4.44478100	1.09425800	1.68719100
C	-3.88042300	-0.50444200	-0.55450000
O	-3.96853200	-1.83357100	-0.03602600
H	-3.86708800	-0.64175700	-1.64629100
H	-3.88939300	-1.77188100	0.92670800

35

C	-10.13728200	-0.01241900	-2.28841700
C	-9.20014100	-0.00490100	-1.07367300
H	-9.90329200	0.84866000	-2.93070500
H	-9.93524400	-0.90669700	-2.89518800
C	-7.71443600	-0.03616800	-1.45353100
H	-9.40107300	0.88855500	-0.46543300
H	-9.42991500	-0.86765600	-0.43222000
H	-7.51445600	-0.92841900	-2.06355400
H	-7.48580600	0.82713700	-2.09437500
C	-6.77096800	-0.03028600	-0.24348300
C	-5.29504200	-0.05597800	-0.65233900
H	-6.99092400	-0.89691200	0.39411700
H	-6.96714800	0.86113500	0.36711900
H	-5.09810400	-0.93718200	-1.28270200
H	-5.07571000	0.79977900	-1.30969200
C	-11.62555200	0.02233100	-1.91883700
C	-12.55874800	0.01355200	-3.13667900
H	-11.82954700	0.91738900	-1.31354200
H	-11.86150500	-0.83834900	-1.27642200
C	-14.04393300	0.04955000	-2.76190000
H	-12.32198500	0.87312700	-3.77853200

H	-12.35481700	-0.88119800	-3.74059200
H	-14.68262600	0.04171100	-3.65149200
H	-14.31829900	-0.81603000	-2.14775000
H	-14.28530800	0.95117200	-2.18700900
H	-3.23814000	-0.06470100	0.13320000
C	-4.28041200	-0.05168100	0.45064900
C	-4.51757100	-0.03373700	1.77292500
H	-5.53448700	-0.02098700	2.14999400
C	-4.61254000	-1.27416200	4.58762200
C	-3.77513600	-0.01530600	4.25850200
H	-4.05345500	-2.18959300	4.36698100
H	-4.86052300	-1.28047700	5.65450700
H	-5.55226100	-1.30789600	4.02911400
C	-2.49677200	-0.01374500	5.11022100
C	-4.60000500	1.25747800	4.56487400
H	-1.88094600	0.86485900	4.89946700
H	-2.75828200	-0.00412100	6.17339600
H	-1.88801100	-0.90041400	4.91344400
H	-4.84736200	1.28553900	5.63155100
H	-4.03206000	2.16323700	4.32757900
H	-5.53969600	1.29038800	4.00632200
C	-3.40580100	-0.03109400	2.76014100
O	-2.22829700	-0.04113200	2.40258800
C	2.97084000	0.00654600	-0.74993300
C	3.98538900	0.68769100	1.16383700
C	3.99858200	-0.67382100	1.15708700
N	3.37438100	-1.07601200	-0.01996500
N	3.35343500	1.08947000	-0.00927800
Cl	4.63539700	-1.75566000	2.31847200
Cl	4.60259300	1.77009400	2.33520900
C	4.12789300	-3.12279800	-1.15373100
C	3.13920500	-2.45273100	-0.40620600
C	1.92974700	-3.06045400	-0.01243000
C	1.72391500	-4.38909300	-0.40510900
C	2.67848300	-5.07696700	-1.14954700
C	3.86559400	-4.44938100	-1.51836000
H	0.80203200	-4.88870200	-0.12432700
H	2.49688000	-6.10664800	-1.44361600
H	4.60113400	-4.99638500	-2.09978600
C	4.07355500	3.15911500	-1.12222600
C	3.78912400	4.48375700	-1.47690400
C	2.59041900	5.08763500	-1.10592200
C	1.64625100	4.37708300	-0.36968800
C	1.87365000	3.04857700	0.01177500
C	3.09444600	2.46522500	-0.38373700
H	4.51654300	5.04813800	-2.05187900
H	2.39175300	6.11647600	-1.39178300
H	0.71537400	4.85843400	-0.08658900
C	5.43677900	-2.46535300	-1.57966400
H	5.47122300	-1.46051100	-1.14939900
C	5.50651300	-2.30716600	-3.11134800
H	6.43152500	-1.79547100	-3.39772500
H	5.49306900	-3.28072000	-3.61298600
H	4.66074700	-1.72266400	-3.48762700
C	6.66081400	-3.23221300	-1.04256900
H	7.58236000	-2.70520600	-1.31110700
H	6.62644200	-3.32460800	0.04736800
H	6.72130600	-4.24086900	-1.46459200
C	0.85730700	-2.33496000	0.79363200
H	1.22478900	-1.33324200	1.03210200
C	-0.43635100	-2.15827400	-0.02526300
H	-0.24017200	-1.62682300	-0.96242800
H	-0.88416100	-3.12675000	-0.27430400
H	-1.16449100	-1.58214900	0.55392800
C	0.56976500	-3.03873100	2.13416900
H	-0.16396900	-2.45979900	2.70430300
H	0.15861200	-4.04249900	1.98253400
H	1.47704100	-3.13420700	2.73902000
C	5.39476400	2.52780500	-1.54968600
C	0.81276200	2.30016800	0.81230100
C	6.60480100	3.31948700	-1.01700900
H	7.53555900	2.80873200	-1.28515800
H	6.64631700	4.32761000	-1.44255900
H	6.57040700	3.41486600	0.07267400
C	0.54064900	2.97305500	2.17200700
H	1.45511300	3.05757100	2.76756000
H	0.12591800	3.97909200	2.04705800
H	-0.18456800	2.37988600	2.73832300
C	5.46391200	2.36852000	-3.08133700
H	5.43051100	3.34112800	-3.58393300
H	6.39786600	1.87425100	-3.36935400
H	4.62856200	1.76745200	-3.45485300

H	5.45061400	1.52477800	-1.11744700
Cu	2.06953300	0.00595400	-2.46910700
H	1.37255700	0.00545600	-3.82501600
C	-0.49124700	2.13835900	0.00694100
H	-1.21020600	1.54712300	0.58250200
H	-0.94562600	3.11056400	-0.21397000
H	-0.30600400	1.62903100	-0.94461400
H	1.18597900	1.29432100	1.02271200

TS13

C	-9.24942800	-0.12131100	-0.32045800
C	-7.97822100	0.51443100	0.25710600
H	-9.36959500	0.19614200	-1.36630900
H	-9.12820600	-1.21386600	-0.34770200
C	-6.70904900	0.16563300	-0.53053800
H	-8.09925600	1.60680700	0.28421000
H	-7.85581200	0.19678700	1.30252800
H	-6.58451200	-0.92662200	-0.55374900
H	-6.83488400	0.47871900	-1.57695300
C	-5.43704400	0.80675500	0.03804100
C	-4.17192500	0.45356800	-0.76833900
H	-5.30168700	0.49047900	1.08172100
H	-5.55322100	1.89864300	0.06156500
H	-4.07154800	-0.64228400	-0.79219000
H	-4.29684800	0.77945900	-1.80897800
C	-10.52170600	0.22671300	0.46233000
C	-11.79231400	-0.40725700	-0.11828100
H	-10.64333300	1.31922700	0.49078000
H	-10.40401000	-0.09209000	1.50815400
C	-13.05892600	-0.05469100	0.66845500
H	-11.90988700	-0.08844200	-1.16308600
H	-11.67077200	-1.49884600	-0.14631400
H	-13.94688700	-0.52218900	0.22986100
H	-12.98510700	-0.39148400	1.70903700
H	-13.22638400	1.02854400	0.68393300
H	-2.64366800	0.74010200	0.81657100
C	-2.91668000	1.04508600	-0.19271100
C	-2.11552000	1.91232100	-0.82434000
H	-2.35418000	2.23383400	-1.83501200
C	-1.58728400	4.76206500	0.46688800
C	-0.59995700	4.00139500	-0.45292600
H	-1.41145500	4.50893400	1.51631600
H	-1.45786100	5.84323200	0.34605600
H	-2.62712500	4.51708400	0.22561400
C	0.83924200	4.35190000	-0.04523600
C	-0.83754400	4.43125300	-1.91075200
H	1.56012600	3.83185200	-0.68584900
H	1.00924600	5.42980100	-0.14478600
H	1.03409000	4.06366400	0.98982000
H	-0.55551000	5.48277100	-2.03532900
H	-0.23250800	3.83582500	-2.60256300
H	-1.88716900	4.34082100	-2.20608500
C	-0.87171500	2.48400500	-0.19798300
O	-0.50506000	2.01219800	0.95198700
C	1.98856100	-0.42921800	-0.02247200
C	3.90718100	-1.57774300	0.38702500
C	2.89649900	-2.48497200	0.32035200
N	1.72663100	-1.77007800	0.07004800
N	3.33932700	-0.32322900	0.17497200
Cl	2.95639400	-4.18628200	0.49418800
Cl	5.57462600	-1.83329600	0.67301900
C	-0.04285700	-2.75356700	-1.32198700
C	0.40588300	-2.34992200	-0.04819900
C	-0.37381000	-2.48817400	1.11851800
C	-1.65123700	-3.04413700	0.97343200
C	-2.12646700	-3.44460500	-0.27281300
C	-1.32947000	-3.30102600	-1.40564900
H	-2.28117300	-3.16497600	1.84933900
H	-3.12007700	-3.87463100	-0.36077100
H	-1.71038500	-3.61889800	-2.37123900
C	4.61212500	1.39122700	-1.03984800
C	5.28963100	2.61688400	-1.01245500
C	5.41554900	3.34487500	0.16797000
C	4.87059300	2.85749500	1.35283800
C	4.18404400	1.63699300	1.38766700
C	4.06253000	0.93030300	0.17394900
H	5.72501800	3.00475000	-1.92816800
H	5.94456900	4.29352600	0.16527400
H	4.98074800	3.43148900	2.26770700
C	0.80406400	-2.62261000	-2.58423900
H	1.76762600	-2.18635900	-2.30691000
C	0.15112600	-1.66815700	-3.60285700
H	0.79477800	-1.55733600	-4.48211900

H	-0.81743000	-2.04934800	-3.94374900
H	-0.00683000	-0.67729400	-3.16648400
C	1.08963600	-3.99921200	-3.21644800
H	1.74454000	-3.88522400	-4.08667700
H	1.58085900	-4.67103400	-2.50589800
H	0.16775900	-4.48342900	-3.55558300
C	0.11668700	-2.07517100	2.50300600
H	1.11947800	-1.65137000	2.39850700
C	-0.77532800	-0.97894900	3.11804700
H	-0.81543900	-0.09337700	2.47706300
H	-1.79823900	-1.33929200	3.27382200
H	-0.37917900	-0.68012300	4.09476400
C	0.22981600	-3.29328200	3.44136800
H	0.63849600	-2.98644400	4.40998400
H	-0.74931100	-3.74920300	3.62314100
H	0.88659600	-4.06206600	3.02251000
C	4.50763100	0.61611000	-2.35023800
C	3.62271700	1.12547800	2.71136200
C	5.89869700	0.18976700	-2.86104000
H	5.79838400	-0.40886500	-3.77256700
H	6.51932600	1.05963600	-3.10076200
H	6.43224600	-0.40958700	-2.11705300
C	4.74774400	0.88693900	3.73856600
H	5.50368100	0.19644000	3.35168400
H	5.25108900	1.82245100	4.00507200
H	4.33398900	0.45911600	4.65780500
C	3.74584100	1.41576100	-3.42489100
H	4.27125800	2.34109900	-3.68429100
H	3.65082700	0.82015600	-4.33917400
H	2.74098700	1.67813900	-3.08139100
H	3.93503600	-0.29663100	-2.16353200
Cu	0.76103000	0.97550900	-0.39055900
H	0.15698400	1.94662000	-1.50192000
C	2.54487700	2.07100000	3.27631600
H	2.14840300	1.66796600	4.21473500
H	2.95735500	3.06309900	3.49052600
H	1.71198700	2.18801500	2.57713600
H	3.14041300	0.16098200	2.52940700

36

C	-8.73467000	-0.32236100	-0.22617800
C	-7.46551800	0.35217100	0.31086100
H	-9.03102200	0.16241500	-1.16752500
H	-8.50893200	-1.36774800	-0.48204200
C	-6.28989200	0.31831000	-0.67392900
H	-7.69201200	1.39663700	0.56879300
H	-7.16632800	-0.13376400	1.25065700
H	-6.06162400	-0.72630800	-0.93111600
H	-6.59085300	0.80279300	-1.61403000
C	-5.02109100	0.99523700	-0.14027000
C	-3.84707800	0.96564300	-1.13792400
H	-4.71267900	0.50603900	0.79438600
H	-5.24252200	2.03912800	0.12073800
H	-3.65189600	-0.08345600	-1.40741200
H	-4.14245200	1.47693200	-2.06403400
C	-9.91355600	-0.28509200	0.75431800
C	-11.18295200	-0.95651700	0.21406600
H	-10.13931300	0.75990700	1.01160700
H	-9.61990500	-0.77182200	1.69561800
C	-12.35696700	-0.91264700	1.19756500
H	-11.47506400	-0.47066100	-0.72697800
H	-10.95815100	-2.00126300	-0.04124300
H	-13.24541300	-1.40172000	0.78417900
H	-12.10534800	-1.41858000	2.13694600
H	-12.62954500	0.12042300	1.44267800
H	-2.15424800	1.10811400	0.29010800
C	-2.58852800	1.58401400	-0.58896800
C	-1.98166500	2.66708100	-1.08538200
H	-2.41234900	3.14596800	-1.96680600
C	-1.88998700	4.78917400	1.18020600
C	-0.95981000	4.78227100	-0.04453100
H	-1.46331900	4.19300700	1.99142100
H	-2.04110200	5.81147400	1.54777000
H	-2.87116000	4.36980900	0.93377700
C	0.40051000	5.39311800	0.34087300
C	-1.57794900	5.63899700	-1.16724100
H	1.07407200	5.42654800	-0.52492500
H	0.27736000	6.42011000	0.70582800
H	0.88409700	4.80102000	1.12098600
H	-1.61145200	6.69335100	-0.86779600
H	-0.98549200	5.57721500	-2.08881000
H	-2.60219200	5.33438700	-1.40373900
C	-0.71107900	3.30444200	-0.54372500

O	-0.09705800	2.55818700	0.46332100
C	1.93242300	-0.51470500	0.05875400
C	3.73791500	-1.89161700	0.02598600
C	2.63019000	-2.66675700	-0.13134900
N	1.53193300	-1.81155800	-0.11058100
N	3.29675500	-0.57685600	0.14082800
Cl	2.51638100	-4.36286300	-0.31690200
Cl	5.38238200	-2.35663500	0.08534400
C	-0.38363600	-2.32380000	-1.55910900
C	0.15481400	-2.23617600	-0.25958600
C	-0.58069800	-2.55564500	0.89916600
C	-1.90685100	-2.97004200	0.72206300
C	-2.46783400	-3.06894500	-0.54833900
C	-1.71314600	-2.74948600	-1.67423100
H	-2.50653400	-3.22021900	1.59150300
H	-3.49683300	-3.39744900	-0.66175600
H	-2.16232000	-2.83127400	-2.65905000
C	4.62811400	1.23246300	-0.84888200
C	5.44729200	2.35258300	-0.66111800
C	5.78635200	2.79102500	0.61629500
C	5.31209300	2.11570600	1.73767600
C	4.48682700	0.99090400	1.61232500
C	4.15719500	0.57686400	0.30650800
H	5.82390500	2.88728200	-1.52751800
H	6.42350900	3.66207100	0.73830400
H	5.58553300	2.46710200	2.72763400
C	0.40826300	-1.97541300	-2.81579500
H	1.41115300	-1.66065300	-2.51388000
C	-0.22970400	-0.79262400	-3.57043100
H	0.39394300	-0.50984600	-4.42525300
H	-1.22169700	-1.05281600	-3.95463400
H	-0.33976600	0.08062700	-2.92048200
C	0.57098000	-3.19864400	-3.73961200
H	1.18584700	-2.93726500	-4.60724800
H	1.05292400	-4.03186700	-3.21927000
H	-0.39745700	-3.54905600	-4.11205700
C	-0.00076100	-2.46472400	2.30713600
H	1.04144800	-2.14279600	2.22989700
C	-0.73989800	-1.40602300	3.14887700
H	-0.70912300	-0.42462600	2.66523800
H	-1.79061200	-1.67632100	3.29853900
H	-0.27467500	-1.31658800	4.13628900
C	-0.00333000	-3.83623500	3.01040900
H	0.46970900	-3.75573400	3.99473300
H	-1.02223500	-4.20800900	3.16124900
H	0.54489200	-4.58391200	2.42897000
C	4.27699200	0.78145800	-2.26356400
C	3.98590800	0.27817500	2.86489000
C	5.53836700	0.44623000	-3.08288900
H	5.25586600	0.06747100	-4.07068000
H	6.16604500	1.33047300	-3.23419000
H	6.14542200	-0.31687000	-2.58609000
C	5.15316500	-0.28339100	3.70026700
H	5.77250700	-0.96778000	3.11243300
H	5.79901500	0.51759300	4.07478600
H	4.76692900	-0.83117800	4.56621600
C	3.40885700	1.83189600	-2.98401700
H	3.94508200	2.77983400	-3.09930900
H	3.13645500	1.47679500	-3.98366200
H	2.48727900	2.03082800	-2.42791700
H	3.68359100	-0.13474600	-2.19471800
Cu	0.86716800	1.03302500	0.19335500
H	-0.04002100	3.42579900	-1.42200300
C	3.08794300	1.19995200	3.71312000
H	2.70229500	0.65556300	4.58160200
H	3.64246000	2.06879200	4.08302200
H	2.23634400	1.56605900	3.13141900
H	3.37119000	-0.57132800	2.55395300

37

C	-8.67767300	-0.90856500	-1.41671100
C	-7.54831300	-0.40494000	-0.50867500
H	-8.84211600	-0.18305100	-2.22634500
H	-8.36057500	-1.84107200	-1.90560900
C	-6.22557700	-0.17049400	-1.24941800
H	-7.86289000	0.52979500	-0.02283800
H	-7.38581200	-1.12859300	0.30302600
H	-5.91319300	-1.10604900	-1.73556000
H	-6.38800500	0.55303200	-2.06119700
C	-5.09422000	0.33082200	-0.34245700
C	-3.77650400	0.54691700	-1.09464900
H	-4.93612600	-0.38910100	0.47224700
H	-5.40279300	1.27031900	0.13563700

H	-3.49670000	-0.39077000	-1.59918100
H	-3.94536500	1.26288700	-1.91460000
C	-10.00008500	-1.15021100	-0.67798600
C	-11.12869300	-1.65228300	-1.58790000
H	-10.31839600	-0.21866600	-0.18804900
H	-9.83728800	-1.87724100	0.13081600
C	-12.44615300	-1.89123000	-0.84306400
H	-11.29118600	-0.92542000	-2.39552400
H	-10.81091100	-2.58318800	-2.07736300
H	-13.23056800	-2.24770000	-1.51910200
H	-12.32331700	-2.63988900	-0.05178600
H	-12.80676100	-0.96974100	-0.37142900
H	-1.67164000	1.16335700	-0.83331400
C	-2.59775100	1.02518100	-0.28165900
C	-2.59882400	1.33138200	1.01878800
H	-3.52725300	1.24218500	1.57976900
C	-1.27976200	-0.37768600	3.09524700
C	-1.31427900	1.15404100	3.22739700
H	-0.44426800	-0.70762800	2.46770000
H	-1.15474100	-0.84690100	4.07797800
H	-2.20159900	-0.76630100	2.65130000
C	-0.04164600	1.63174000	3.94912500
C	-2.52828500	1.55575600	4.09455700
H	-0.01673800	2.72167600	4.02369100
H	0.00004300	1.20765300	4.95982700
H	0.85748100	1.32211700	3.41082400
H	-2.42701600	1.13527600	5.10172900
H	-2.60056900	2.64501100	4.19580600
H	-3.47681800	1.19163000	3.68775400
C	-1.42634000	1.86103100	1.82212800
O	-0.19948500	1.86621700	1.10211300
C	1.91889300	-0.99841200	-0.23126100
C	3.38796600	-2.11075900	-1.56365800
C	2.88928800	-3.00712800	-0.67152300
N	1.99174200	-2.31605000	0.13786200
N	2.79136200	-0.88498600	-1.28258600
Cl	3.24633900	-4.67097200	-0.50359100
Cl	4.52469600	-2.36046300	-2.81643300
C	0.02723300	-3.51882700	0.99796700
C	1.27885000	-2.92003300	1.24517700
C	1.89300300	-2.92205300	2.51466600
C	1.18963400	-3.52423900	3.56535700
C	-0.05676700	-4.10871100	3.35714700
C	-0.62680300	-4.10864600	2.08710700
H	1.62820000	-3.54048400	4.55816900
H	-0.58245000	-4.57275700	4.18657400
H	-1.59395700	-4.57780600	1.93600700
C	2.32893600	0.70673900	-3.10093600
C	2.69856800	1.86925600	-3.78958400
C	3.79436200	2.62817500	-3.38811100
C	4.54483400	2.24246100	-2.28064800
C	4.22544500	1.08939900	-1.55364700
C	3.11124200	0.34128700	-1.98743600
H	2.12212400	2.18098000	-4.65473700
H	4.06447200	3.52374400	-3.94003000
H	5.39382800	2.84581300	-1.97506500
C	-0.61610100	-3.57051900	-0.38446500
H	0.02358700	-3.02275500	-1.08232800
C	-1.99502800	-2.88483300	-0.39863500
H	-2.40655600	-2.89562100	-1.41363000
H	-2.70740100	-3.40401000	0.25131500
H	-1.92984100	-1.84508200	-0.06570000
C	-0.71955900	-5.02144800	-0.89712300
H	-1.13664300	-5.03398600	-1.90958900
H	0.25982200	-5.50796800	-0.92531200
H	-1.37579000	-5.62237600	-0.25856300
C	3.27561200	-2.33038700	2.77579000
H	3.65667700	-1.91822900	1.83730000
C	3.21996000	-1.17171400	3.78906400
H	2.54829700	-0.37854100	3.44880000
H	2.87009600	-1.51256300	4.76917200
H	4.21757400	-0.74042800	3.92314300
C	4.27011400	-3.41617500	3.23437500
H	5.26853700	-2.98384600	3.35824900
H	3.97332100	-3.84882000	4.19558700
H	4.33880000	-4.22990500	2.50612200
C	1.13260300	-0.10714600	-3.58532700
C	5.07990000	0.69857800	-0.35100500
C	1.43724700	-0.80510000	-4.92648100
H	0.57904500	-1.40724100	-5.24343500
H	1.64107700	-0.07180600	-5.71426200
H	2.30638500	-1.46526500	-4.84953400

C	6.53403000	0.39476400	-0.76377800
H	6.58056900	-0.39322800	-1.52117800
H	7.02597400	1.28401500	-1.17192400
H	7.11143500	0.06616500	0.10679000
C	-0.13816900	0.75735800	-3.69438100
H	-0.05319400	1.49743000	-4.49728500
H	-1.00293000	0.12511800	-3.92188400
H	-0.33722000	1.29526800	-2.76310700
H	0.92871700	-0.88793900	-2.84692500
Cu	0.83922500	0.39806600	0.47678500
H	-1.63848700	2.91484500	2.05441500
C	5.03598300	1.77776400	0.74874500
H	5.59693400	1.44149100	1.62735800
H	5.48662900	2.71515200	0.40577700
H	4.00801700	1.99197800	1.05405900
H	4.66639000	-0.21703100	0.08169200
Si	0.65657600	3.52125200	0.31634400
H	1.72024200	2.46360400	0.14420300
O	-0.66155500	3.52803300	-0.75184400
O	0.38611200	4.20656400	1.85073000
C	0.52753200	5.58358100	2.16469100
C	0.08006900	5.82464200	3.60133100
H	-0.07608300	6.20590700	1.48706000
H	1.57092600	5.90759000	2.04548400
H	0.17525500	6.88534600	3.85923800
H	-0.96547200	5.52983500	3.73701000
H	0.69127300	5.24510800	4.30074300
C	-0.96362400	4.47260700	-1.76444200
C	-1.92961800	5.54828200	-1.27443200
H	-1.42811300	3.91964400	-2.59285700
H	-0.05754500	4.94343200	-2.16469700
H	-2.21092400	6.21787500	-2.09573400
H	-2.84060700	5.09255700	-0.87328200
H	-1.47455100	6.15282800	-0.48253200
C	1.79183000	4.88812700	-0.46741500
H	2.70380600	4.96663300	0.14050300
H	2.11498100	4.56492700	-1.46552600
H	1.38023800	5.90035000	-0.56309100

TS14

C	-8.62380500	-0.82070200	-1.22096200
C	-7.48656900	-0.14841800	-0.44129600
H	-8.75195600	-0.31104300	-2.18682100
H	-8.33751400	-1.85511300	-1.46006600
C	-6.15137200	-0.12891700	-1.19633300
H	-7.77673100	0.88274000	-0.19377400
H	-7.35213500	-0.66429000	0.52039500
H	-5.86438600	-1.15893400	-1.45296100
H	-6.28445900	0.39614800	-2.15313500
C	-5.01414700	0.53334400	-0.40786100
C	-3.69101400	0.57072800	-1.18002800
H	-4.87130100	-0.00313700	0.54008400
H	-5.30778500	1.55694800	-0.13864700
H	-3.41552300	-0.45480500	-1.47102200
H	-3.84800600	1.09774800	-2.13407400
C	-9.96208200	-0.82637200	-0.47140100
C	-11.09853800	-1.50464600	-1.24708900
H	-10.25139200	0.20840200	-0.23749900
H	-9.83428600	-1.33100300	0.49730100
C	-12.43271800	-1.49982300	-0.49372700
H	-11.22384200	-1.00281300	-2.21640700
H	-10.81135900	-2.53996600	-1.47675800
H	-13.22240000	-1.99026600	-1.07273600
H	-12.34800900	-2.02477000	0.46493900
H	-12.76292400	-0.47646300	-0.28070400
H	-1.59615400	1.25802200	-1.05488800
C	-2.51652500	1.20609300	-0.47614000
C	-2.51003300	1.72339300	0.75569800
H	-3.42930300	1.70701400	1.33651900
C	-1.18550800	0.58049100	3.21888200
C	-1.23533800	2.09379600	2.95578400
H	-0.34327400	0.11260900	2.69989400
H	-1.06533200	0.37981700	4.28958900
H	-2.10129200	0.08143000	2.88625400
C	0.02946700	2.75321700	3.53431200
C	-2.45864700	2.69598900	3.68233200
H	0.05298300	3.82626000	3.32254800
H	0.06246100	2.61246600	4.62139800
H	0.93440000	2.31846100	3.10507000
H	-2.36449800	2.54448800	4.76364800
H	-2.53526800	3.77485600	3.50379300
H	-3.40233400	2.23569400	3.37349100
C	-1.34436300	2.42026600	1.42425500

O	-0.11326800	2.20664700	0.72540100	H	4.44926300	0.32295300	3.34453300
C	1.69219800	-1.11642900	-0.15928900	C	4.37040900	-2.41510800	3.66066700
C	2.86303200	-2.74648200	-1.23506800	H	5.38468400	-2.02989600	3.51280500
C	2.45820500	-3.25699800	-0.04268900	H	4.18347800	-2.45033100	4.73895300
N	1.73995700	-2.25474700	0.60395800	H	4.33629100	-3.44027300	3.27940600
N	2.39370200	-1.43746700	-1.29538500	C	0.47806100	-1.32058600	-3.52733400
Cl	2.74992700	-4.80791700	0.61703800	C	4.90294900	0.09328700	-1.26284400
Cl	3.77107600	-3.50220800	-2.47179100	C	0.59367600	-2.40802300	-4.61548400
C	-0.13460400	-2.97166700	2.02382000	H	-0.30470400	-3.03439900	-4.62140800
C	1.15780600	-2.41814600	1.92048000	H	0.69633200	-1.95996200	-5.60965500
C	1.93494400	-2.06843300	3.04387400	H	1.45962800	-3.05490300	-4.44773900
C	1.36155600	-2.26556400	4.30630400	C	6.22696100	-0.50931400	-1.77595500
C	0.08356800	-2.80111300	4.44154900	H	6.07253200	-1.49187300	-2.23107300
C	-0.65223500	-3.15149500	3.31280300	H	6.69298500	0.13958600	-2.52514300
H	1.92704600	-2.00193700	5.19457000	H	6.93442300	-0.62346500	-0.94790600
H	-0.33888100	-2.95036500	5.43095100	C	-0.78047100	-0.46191100	-3.75016900
H	-1.64450900	-3.57469900	3.43287600	H	-0.77141900	0.02275500	-4.73195500
C	1.74606600	-0.47375900	-3.46515500	H	-1.67632500	-1.08955800	-3.70141000
C	2.05172500	0.38916700	-4.52568400	H	-0.86905900	0.31945100	-2.99074300
C	3.22377500	1.13999400	-4.53070000	H	0.35667100	-1.82853700	-2.56626400
C	4.12363600	1.03841600	-3.47344100	Cu	0.91287200	0.58547700	0.23146300
C	3.87179200	0.19534800	-2.38417400	H	-1.54284900	3.49728400	1.36114000
C	2.66702300	-0.53837100	-2.39959700	C	5.15078400	1.45455400	-0.58533900
H	1.36568200	0.46666400	-5.36306800	H	5.84595400	1.33468600	0.25267900
H	3.44026300	1.80065300	-5.36506700	H	5.59496400	2.17293900	-1.28258900
H	5.03925400	1.62094000	-3.49367500	H	4.22006600	1.88332500	-0.20497700
C	-0.96213700	-3.39503000	0.81337500	H	4.51249200	-0.58173900	-0.49582900
H	-0.40354900	-3.13752400	-0.09115500	Si	0.86106300	3.49789400	-0.26514800
C	-2.30520300	-2.64305500	0.74637000	H	1.75698800	2.19776500	-0.34051900
H	-2.85256800	-2.93688000	-0.15577400	O	-0.66659900	4.17681300	-0.62033200
H	-2.93915200	-2.87967400	1.60764000	O	1.48784200	4.44252900	0.99796100
H	-2.15911700	-1.55959600	0.72060800	C	2.78919500	4.25002500	1.52333500
C	-1.18908200	-4.92046900	0.79777000	C	3.08451500	5.32454100	2.56259900
H	-1.73344100	-5.21126800	-0.10685100	H	3.54442600	4.29680900	0.72292300
H	-0.24221200	-5.46777500	0.81658100	H	2.87465200	3.25381400	1.98501600
H	-1.78150300	-5.24247300	1.66084500	H	4.08936900	5.19353600	2.97909600
C	3.35182900	-1.51187600	2.93760700	H	3.02437600	6.32115500	2.11334700
H	3.63439500	-1.48944200	1.88159000	H	2.36135500	5.27636100	3.38286700
C	3.43032400	-0.06286400	3.45550100	C	-0.97297700	5.29619600	-1.42707300
H	2.75458400	0.59245500	2.89737500	C	-0.75126300	6.62421800	-0.70561700
H	3.16250600	-0.00071100	4.51566300	H	-2.03303300	5.20938300	-1.70503000

H	-0.40122800	5.28384300	-2.36434800
H	-1.07031300	7.46349000	-1.33492900
H	-1.32716200	6.65335200	0.22533200
H	0.30434300	6.76067800	-0.45319200
C	1.81867000	4.11729800	-1.83314900
H	2.88255400	3.88974500	-1.69390100
H	1.50141700	3.56691900	-2.72997200
H	1.73381100	5.18783900	-2.05419200
38			
C	-10.58570100	-3.91432300	0.29139800
C	-9.92319800	-2.55073300	0.52625700
H	-10.48671100	-4.18675100	-0.76925700
H	-10.03841000	-4.68434400	0.85405300
C	-8.44256700	-2.51586500	0.12696000
H	-10.46933600	-1.78019100	-0.03656000
H	-10.02006300	-2.27769300	1.58684700
H	-7.89741800	-3.28651300	0.69069600
H	-8.34745300	-2.79197200	-0.93301000
C	-7.77437400	-1.15397200	0.35596000
C	-6.29793500	-1.14340900	-0.05363400
H	-7.86399700	-0.87828900	1.41556100
H	-8.31672200	-0.38349400	-0.20863300
H	-5.76337800	-1.93009200	0.50140200
H	-6.21480500	-1.44599500	-1.10923000
C	-12.06694400	-3.95612300	0.68741400
C	-12.72705100	-5.32050700	0.45014500
H	-12.61559000	-3.18658200	0.12527400
H	-12.16759600	-3.68542500	1.74846300
C	-14.20631700	-5.35454900	0.84789400
H	-12.62677800	-5.59056600	-0.61002700
H	-12.17901400	-6.08930500	1.01199800
H	-14.64781300	-6.34053000	0.66822000
H	-14.33549500	-5.12060500	1.91106800
H	-14.78665800	-4.62085200	0.27641300
H	-4.50645600	0.13604800	-0.18340600
C	-5.55027200	0.15355200	0.12559100
C	-6.03673700	1.29925300	0.61030700
H	-7.07703100	1.36012700	0.92163800
C	-4.18521700	2.08946800	3.01265400
C	-5.07921500	3.06803500	2.23161700
H	-3.19060800	2.02384400	2.56284000
H	-4.06915400	2.42411000	4.04957600
H	-4.61735300	1.08378700	3.02697700
C	-4.43440500	4.46718600	2.21958000
C	-6.45848200	3.16902200	2.91375100
H	-5.07972500	5.19339000	1.71060200
H	-4.27298400	4.82444300	3.24269600
H	-3.47071600	4.45682700	1.70511900
H	-6.35514000	3.63569500	3.89938600
H	-7.15284700	3.78413400	2.32852000
H	-6.91636800	2.18636200	3.06097800
C	-5.25886300	2.58916500	0.75263200
O	-3.97358700	2.46180900	0.13506800
C	4.19985600	-0.51835800	-0.03036100
C	5.26506700	-2.47465200	-0.47099200
C	5.76900700	-1.98945900	0.69725700
N	5.10738500	-0.79212300	0.95412900
N	4.30586000	-1.56399900	-0.90414700
Cl	6.97613200	-2.65154100	1.71187700
Cl	5.67100100	-3.90771700	-1.31144800
C	4.55702200	-0.17787600	3.26761300
C	5.33091000	0.05011600	2.11183900
C	6.31219400	1.05820800	2.03211800
C	6.49819400	1.86247400	3.16364900
C	5.74532100	1.66701100	4.31842800
C	4.78727600	0.65780900	4.36765900
H	7.24179400	2.65279500	3.13745900
H	5.90608700	2.30340300	5.18371200
H	4.20668700	0.51582500	5.27376300
C	2.27544700	-2.36971200	-2.02683300
C	1.52286000	-2.47195400	-3.20357700
C	1.98429000	-1.93676600	-4.40324300
C	3.21536400	-1.28831900	-4.45339500
C	4.01246800	-1.15615700	-3.30924200
C	3.51287000	-1.69979800	-2.10913500
H	0.56195700	-2.97647800	-3.17837800
H	1.38270000	-2.02675600	-5.30300200
H	3.56410700	-0.87593100	-5.39498700
C	3.49817600	-1.27208500	3.35855200
H	3.49450800	-1.82599100	2.41555500
C	2.08928100	-0.67349100	3.53839800
H	1.33868500	-1.47083900	3.55255200

H	2.00762100	-0.12082600	4.48041400
H	1.84374300	0.01308600	2.72197100
C	3.82061200	-2.28189500	4.47763800
H	3.07990100	-3.08838100	4.48173200
H	4.80992200	-2.72875900	4.33886700
H	3.80015700	-1.80821400	5.46474200
C	7.15212100	1.30601800	0.78325900
H	6.88778300	0.55274100	0.03589300
C	6.84006800	2.68452200	0.16825800
H	5.77632700	2.77702200	-0.07326300
H	7.10188200	3.49594300	0.85569900
H	7.41521700	2.82727800	-0.75270700
C	8.65829800	1.15193200	1.07066600
H	9.23229100	1.27791300	0.14666500
H	9.01084600	1.90339200	1.78486100
H	8.88651700	0.16355600	1.48136600
C	1.73642400	-2.96925900	-0.73176100
C	5.35590100	-0.43975800	-3.40461800
C	1.52348500	-4.49058900	-0.85727400
H	1.19523500	-4.90511800	0.10162500
H	0.75643800	-4.72875400	-1.60158500
H	2.44657900	-5.00013700	-1.15034600
C	6.30101000	-1.13881700	-4.40126200
H	6.45223200	-2.18998400	-4.13701000
H	5.90737100	-1.10124300	-5.42238100
H	7.27776900	-0.64386300	-4.40404700
C	0.44249800	-2.26140000	-0.28445000
H	-0.36110400	-2.39944100	-1.01559600
H	0.09800600	-2.67014100	0.67143400
H	0.60303300	-1.18597900	-0.15907700
H	2.47883100	-2.81115400	0.05561600
Cu	3.02654900	1.02071900	-0.16420900
H	-5.82922400	3.37572800	0.23647000
C	5.17059600	1.04785800	-3.76264000
H	6.14046100	1.55620600	-3.78233700
H	4.71078600	1.16544000	-4.74961600
H	4.53274600	1.55424300	-3.03119200
H	5.83660100	-0.47834800	-2.42312200
Si	-3.42764100	3.17039600	-1.25459700
H	2.10907000	2.23224400	-0.26902300
O	-4.76074900	3.72842000	-2.06392500
O	-2.49769900	4.51218700	-0.94682500
C	-1.18254500	4.48610500	-0.37727200
C	-0.62967700	5.90147100	-0.33425900
H	-0.52476300	3.84088600	-0.97431900
H	-1.22620800	4.06475800	0.63588300
H	0.37441400	5.90161700	0.10197800
H	-0.56865700	6.32281400	-1.34254600
H	-1.27119900	6.54904600	0.27150400
C	-4.71541300	4.59796600	-3.20148900
C	-6.13394700	4.97575800	-3.59621300
H	-4.21309000	4.09027600	-4.03671700
H	-4.13202500	5.49454100	-2.95910300
H	-6.12130300	5.63775900	-4.46823000
H	-6.71632100	4.08398900	-3.84763900
H	-6.63695000	5.49557500	-2.77500500
C	-2.45935200	1.88799800	-2.20373800
H	-2.03786200	2.30539000	-3.12402900
H	-1.63011500	1.49451800	-1.60650100
H	-3.10491800	1.04670400	-2.47413400

39

C	-5.92524800	0.28273100	-0.57347400
C	-4.47199600	0.20280900	-0.08977800
H	-6.10629700	1.27393000	-1.01356100
H	-6.07680500	-0.44169700	-1.38651500
C	-3.44347800	0.48097100	-1.19285700
H	-4.32351000	0.91804100	0.73175000
H	-4.28613100	-0.79279900	0.33785700
H	-3.59464000	-0.22878000	-2.01879200
H	-3.62680300	1.47983400	-1.61419800
C	-1.99004100	0.39404900	-0.71226400
C	-0.96580400	0.71003800	-1.81912700
H	-1.79574100	-0.61163500	-0.31461500
H	-1.83508000	1.08824200	0.12439600
H	-1.14743300	0.02824800	-2.66359800
H	-1.13796500	1.72628000	-2.19655100
C	-6.95648000	0.02581700	0.53199800
C	-8.40937600	0.10151400	0.04666300
H	-6.80814800	0.75347700	1.34290500
H	-6.77499400	-0.96350200	0.97631800
C	-9.43309700	-0.14602300	1.15882700
H	-8.58888100	1.08782600	-0.40268400

H	-8.55968700	-0.63023900	-0.75879800
H	-10.45895100	-0.08721700	0.78035300
H	-9.29980000	-1.13784400	1.60604400
H	-9.33159000	0.59349100	1.96145800
H	0.76429400	-0.43588200	-1.06649100
C	0.46209200	0.56609500	-1.36276300
C	1.33469800	1.57500300	-1.30521400
H	1.00219300	2.55891700	-1.63401200
C	2.31793500	2.47798600	1.45971400
C	3.16110900	2.62741500	0.18188600
H	2.43748300	1.48834600	1.90647100
H	2.61831500	3.22868900	2.19940900
H	1.25310100	2.62156200	1.24921600
C	4.65750800	2.48842500	0.52196000
C	2.93517700	4.03047300	-0.42094800
H	5.27847000	2.58202900	-0.37681600
H	4.95953700	3.27574800	1.22092700
H	4.87723800	1.52283800	0.98258500
H	3.31238200	4.79374300	0.26775800
H	3.46727900	4.15172000	-1.37179400
H	1.87658900	4.24502900	-0.59311500
C	2.78574100	1.54297600	-0.88943900
O	3.26920000	0.25700600	-0.51756400
H	3.37330500	1.80872900	-1.78322900
Si	3.05473100	-1.14519400	0.29352000
O	2.18246800	-0.89871000	1.68052300
O	2.17356600	-2.25370500	-0.58327800
C	2.50893100	-2.66119000	-1.91494100
C	1.56297100	-3.76649100	-2.35366500
H	3.54765800	-3.01762400	-1.95107400
H	2.43084200	-1.79951400	-2.59052400
H	1.80056800	-4.08712000	-3.37309400
H	1.64718900	-4.63291800	-1.69064000
H	0.52585100	-3.41806300	-2.33429400
C	1.59607300	-1.95346700	2.45589300
C	0.86365100	-1.35147700	3.64315800
H	2.37977600	-2.64060200	2.80374800
H	0.90586300	-2.52850600	1.82753900
H	0.40483500	-2.14237500	4.24529500
H	1.55365400	-0.78927300	4.27967700
H	0.07527500	-0.67230700	3.30524400
C	4.76320800	-1.81323000	0.64676200
H	4.71001400	-2.76244500	1.18988000
H	5.32093700	-1.98844000	-0.27874000
H	5.34027300	-1.10849200	1.25324300

40

C	-8.70452000	-2.60274900	0.35173900
C	-7.76442900	-1.44167800	0.00507500
H	-8.27620300	-3.54175900	-0.02735300
H	-8.75751100	-2.71335200	1.44438000
C	-6.34517400	-1.60889700	0.56169200
H	-7.71333700	-1.33158600	-1.08764700
H	-8.19351400	-0.50293100	0.38380000
H	-6.39407800	-1.71453000	1.65500500
H	-5.91642300	-2.54874400	0.18524300
C	-5.41131400	-0.44604800	0.20405900
C	-3.99325300	-0.61747400	0.75753900
H	-5.83990400	0.49241800	0.58140300
H	-5.36583500	-0.34215400	-0.88849300
H	-4.04670200	-0.74047500	1.85080400
H	-3.57886600	-1.57101800	0.39345700
C	-10.12163400	-2.43067100	-0.20858800
C	-11.06474800	-3.59063300	0.13362700
H	-10.06866000	-2.31858800	-1.30116400
H	-10.55073500	-1.49217900	0.17115100
C	-12.47707300	-3.40858100	-0.43078500
H	-10.63653600	-4.52828000	-0.24634300
H	-11.11839800	-3.70257100	1.22522300
H	-13.12542000	-4.25164900	-0.16997000
H	-12.94401600	-2.49662300	-0.04126400
H	-12.45895000	-3.32837000	-1.52377200
H	-2.00402000	0.33029800	0.83429900
C	-3.00775900	0.48285900	0.44453300
C	-3.24578500	1.58136100	-0.27672700
H	-4.23697000	1.72762900	-0.70176800
C	-2.79108400	4.05603700	1.49497800
C	-2.75127400	4.07334800	-0.04239000
H	-1.79785900	3.85364200	1.90315000
H	-3.13263400	5.02312400	1.88348300
H	-3.47212800	3.28295100	1.86500600
C	-1.79265100	5.18307700	-0.50657700
C	-4.15758700	4.39946800	-0.58815300

H	-1.74725300	5.23555900	-1.60125400	H	4.40150700	-4.22960900	-5.11516100
H	-2.13126000	6.15987200	-0.14064400	H	5.80850600	-4.22721500	-4.04295500
H	-0.78336000	5.00401700	-0.13485500	H	4.28535200	-4.94833100	-3.50352000
H	-4.43193900	5.42890100	-0.33010300	C	4.46944800	0.77101800	-0.15306900
H	-4.19355600	4.31433100	-1.68136400	C	4.49417100	1.50744300	1.18489200
H	-4.92911300	3.74472200	-0.17272800	H	3.52705300	0.97712000	-0.66447800
C	-2.25191700	2.68472600	-0.60647700	H	5.30440400	1.09734900	-0.77934300
O	-0.94277500	2.43727400	-0.17891600	C	4.48602600	3.02543200	0.93164800
H	-2.28681500	2.80737400	-1.70893800	H	3.61272500	1.24805300	1.77779900
Si	0.27867600	1.22145700	-0.65245200	H	5.37700700	1.25203600	1.78291400
O	1.45103900	2.34935000	-1.18913000	C	4.46637200	3.83567000	2.23062600
O	0.49645500	0.74476900	0.99389300	H	5.36908700	3.30146900	0.34019200
C	0.13638900	1.50174800	2.13630000	H	3.60848100	3.27258600	0.32396000
C	0.66008600	0.80525900	3.38838400	H	4.46218600	4.91021900	2.02307200
H	-0.95075400	1.61841800	2.20737100	H	3.57470500	3.60797800	2.82483900
H	0.55213500	2.51814900	2.07672900	H	5.34440200	3.61873800	2.84967700
H	0.38137700	1.36899800	4.28625800	C	3.50644500	-1.25799900	0.88037300
H	0.24209000	-0.20356200	3.47586800	C	2.96852000	-2.68006900	0.73256800
H	1.75176500	0.71624200	3.36809800	H	2.66671200	-0.57639100	0.74236500
C	1.20033000	3.64348900	-1.70028700	H	3.93915200	-1.10825500	1.87176700
C	2.23662200	3.98058200	-2.76859000	C	1.93867100	-2.94988900	1.84385800
H	1.25214800	4.39007100	-0.89384800	H	2.46627800	-2.78257600	-0.23404500
H	0.19333800	3.71557800	-2.12685300	H	3.75590000	-3.43672600	0.78184200
H	2.07569000	4.99185000	-3.15966000	C	1.30455300	-4.33883200	1.72852600
H	3.25118800	3.93128900	-2.35862300	H	2.42423600	-2.84815000	2.82356800
H	2.17560900	3.27509500	-3.60412400	H	1.15960400	-2.17997200	1.80068300
C	-0.73639700	0.34833000	-2.02273400	H	0.58127100	-4.50921300	2.53205100
H	-1.02485800	-0.65404200	-1.68617400	H	0.77683800	-4.45424100	0.77549100
H	-1.64627400	0.85317500	-2.35077700	H	2.06176100	-5.12891700	1.78789000
H	-0.08194600	0.20529300	-2.88934000	C	8.11923600	-4.01133000	1.81232000
N	4.57441500	-0.77173800	-0.11224500	C	7.77591400	-2.64516700	1.21194400
C	4.26848100	-1.19389500	-1.56003700	H	9.18607600	-4.08048100	2.04530800
C	4.70946700	-2.57582400	-2.04078800	H	7.56266300	-4.18865200	2.73909500
H	4.77335900	-0.44627100	-2.17687600	H	7.87574100	-4.82225400	1.11719800
H	3.19396800	-1.03944700	-1.66968300	C	6.28227900	-2.51321400	0.86854900
C	4.27886700	-2.76659200	-3.50622900	H	8.05996900	-1.85242600	1.91598400
H	5.79864500	-2.67703400	-1.98279900	H	8.37369800	-2.48154700	0.30599200
H	4.27566700	-3.37720100	-1.43894100	C	6.00211900	-1.12235700	0.29886500
C	4.71856200	-4.11915400	-4.07369400	H	6.00847700	-3.30156200	0.16375800
H	3.18823000	-2.67325700	-3.57902400	H	5.69538600	-2.67292200	1.77893600
H	4.69861100	-1.95765600	-4.11805500	H	6.28480700	-0.38500000	1.05070500

H	6.61674000	-0.93490300	-0.58557800
F	1.49615600	-0.03045300	-0.95743000
TS15			
C	-10.35909100	-1.15426000	0.62292300
C	-9.06504100	-0.54228600	0.07258800
H	-10.26628200	-2.24982600	0.63424800
H	-10.48602300	-0.85043400	1.67201100
C	-7.81115200	-0.93860900	0.86190400
H	-8.94077800	-0.84167100	-0.97803400
H	-9.15731100	0.55329800	0.06579400
H	-7.93942100	-0.64819600	1.91471600
H	-7.71388500	-2.03393100	0.86010600
C	-6.52165000	-0.31247800	0.31671700
C	-5.27053300	-0.72316700	1.10061400
H	-6.61680100	0.78175700	0.32924600
H	-6.39853800	-0.59349200	-0.73811000
H	-5.41549800	-0.46492000	2.16233600
H	-5.19365700	-1.82267600	1.09522400
C	-11.61050700	-0.76154300	-0.17175700
C	-12.90636400	-1.36794000	0.38049600
H	-11.48612000	-1.06879200	-1.22022500
H	-11.70219500	0.33413800	-0.18667500
C	-14.15006300	-0.97154500	-0.42102200
H	-12.81485000	-2.46263200	0.39621300
H	-13.03217000	-1.05933700	1.42734800
H	-15.05714000	-1.42044700	-0.00283900
H	-14.28834300	0.11581400	-0.42496600
H	-14.06856100	-1.29678700	-1.46460500
H	-3.07336100	-0.44806500	1.18606300
C	-3.95931200	-0.13875300	0.63230300
C	-3.76121600	0.70841600	-0.38232600
H	-4.61446300	1.03955700	-0.97595400
C	-2.47012400	3.28459900	0.75037600
C	-2.37909300	2.84391500	-0.71816100
H	-1.66195900	2.82676900	1.32778000
H	-2.39222600	4.37549200	0.84737500
H	-3.42045200	2.97270500	1.19771300
C	-1.03902900	3.31661900	-1.30432900
C	-3.52628600	3.47992500	-1.52430900
H	-0.99011900	3.11688700	-2.38263200
H	-0.89015900	4.39434600	-1.15712300
H	-0.22978700	2.76335200	-0.82171600
H	-3.39670200	4.56762700	-1.59947000
H	-3.55868500	3.08296300	-2.54746800
H	-4.50426800	3.30164100	-1.06513400
C	-2.38993700	1.24699800	-0.80949400
O	-1.33175600	0.68043300	-0.17704600
H	-2.38180200	1.07517300	-1.92827500
Si	0.66779600	-1.14471900	-0.12726400
O	1.18918400	-0.35094200	-1.48839000
O	0.99791400	-0.34172300	1.28298500
C	0.06177500	0.08989700	2.28750900
C	0.71948400	1.14439500	3.16171900
H	-0.21710600	-0.77952300	2.90081200
H	-0.82139100	0.48140800	1.77476200
H	0.03073100	1.45971300	3.95332400
H	1.63072200	0.76384700	3.63660300
H	0.98183100	2.02669000	2.56851100
C	0.36733500	0.04366400	-2.59429300
C	0.59273800	-0.87793800	-3.78569600
H	0.64290700	1.07203800	-2.85498400
H	-0.67517200	0.06210800	-2.27739000
H	-0.00301500	-0.54154900	-4.64174500
H	1.64602600	-0.88822300	-4.08571200
H	0.29732100	-1.90555100	-3.54899900
C	-0.79489900	-2.29038900	-0.24472200
H	-0.81153300	-2.96212700	0.62130600
H	-1.71715100	-1.71505300	-0.28282200
H	-0.70360100	-2.91444000	-1.14087100
N	4.91848600	0.29204100	-0.25020300
C	4.64203400	-0.80814000	-1.28961500
C	5.67185300	-1.92025100	-1.48467700
H	4.53192000	-0.27570900	-2.23712600
H	3.66642600	-1.21664400	-1.02457700
C	5.14245400	-2.91440100	-2.53371700
H	6.62497700	-1.50902400	-1.83454400
H	5.87001500	-2.46138200	-0.55721200
C	6.13273700	-4.04621700	-2.82188700
H	4.19232900	-3.33418900	-2.18130800
H	4.91704600	-2.37813800	-3.46460000
H	5.72928100	-4.73931200	-3.56628200
H	7.08090600	-3.65611600	-3.20819400

H	6.35280900	-4.62125300	-1.91576600	41			
C	4.01877700	1.46859500	-0.69664100	C	-7.84979100	-1.00645100	0.25880400
C	3.85252900	2.62643900	0.28700400	C	-6.62527700	-0.15492400	-0.09832800
H	3.04683200	1.02341000	-0.92479700	H	-7.70725800	-2.02642800	-0.12642900
H	4.46361500	1.82480000	-1.62970600	H	-7.91745100	-1.10268600	1.35205800
C	3.12945500	3.79731400	-0.40141100	C	-5.30430800	-0.72072700	0.43732500
H	3.26608500	2.30870800	1.15393500	H	-6.55961900	-0.05500500	-1.19131300
H	4.81803400	2.98349400	0.66375900	H	-6.76701600	0.86374300	0.29028800
C	2.88879400	4.97258800	0.55003700	H	-5.37305300	-0.82814400	1.52956300
H	3.72211000	4.13411700	-1.26172000	H	-5.15954700	-1.73673300	0.04222900
H	2.16965600	3.44811700	-0.80016500	C	-4.08318000	0.13911400	0.08864300
H	2.38058000	5.79414200	0.03632700	C	-2.76573300	-0.43732700	0.61789300
H	2.26377400	4.67259500	1.39787700	H	-4.22518000	1.15124200	0.49110300
H	3.83235800	5.36043100	0.95028900	H	-4.01833300	0.25337000	-1.00198300
C	4.46488200	-0.11277900	1.15858600	H	-2.85100500	-0.57562700	1.70819000
C	4.76599600	-1.52856400	1.65017900	H	-2.64062800	-1.45848400	0.22178500
H	3.38058900	0.01596200	1.16202700	C	-9.16944200	-0.44229600	-0.28131700
H	4.89783400	0.63133700	1.83034800	C	-10.39526100	-1.29003700	0.08041300
C	4.27291800	-1.67300500	3.10038100	H	-9.10436300	-0.34963900	-1.37511200
H	4.23121500	-2.25240100	1.02978400	H	-9.31133800	0.57905000	0.10059400
H	5.83175200	-1.76582300	1.60961000	C	-11.70829000	-0.71890700	-0.46367000
C	4.49188000	-3.08412700	3.65353800	H	-10.25409500	-2.31056000	-0.30109500
H	4.79039200	-0.94414000	3.73813700	H	-10.46112400	-1.38159900	1.17322000
H	3.20606000	-1.42270100	3.14007400	H	-12.56331100	-1.34517100	-0.18821400
H	4.13108200	-3.16210600	4.68373500	H	-11.89358400	0.28814200	-0.07256300
H	3.95761100	-3.83016000	3.05545400	H	-11.68605000	-0.64843200	-1.55730200
H	5.55425800	-3.35254400	3.65081900	H	-0.57997600	-0.05481600	0.69547000
C	9.92286200	0.04233900	1.05397100	C	-1.51776100	0.35946500	0.32507700
C	8.80473900	0.71676200	0.25409700	C	-1.42289900	1.51948100	-0.33132100
H	10.88475600	0.53021800	0.87023200	H	-2.32164000	1.98580600	-0.73660000
H	9.72425200	0.08931500	2.13019900	C	-0.20329100	3.65275500	1.54489700
H	10.02555800	-1.01311000	0.77945400	C	-0.14208700	3.71921500	0.01104700
C	7.43540000	0.05499000	0.48849300	H	0.60655900	3.01821900	1.91658700
H	8.74855000	1.77887600	0.52496900	H	-0.10470700	4.64793800	1.99735500
H	9.04692300	0.68315200	-0.81586300	H	-1.15019600	3.21974700	1.88587800
C	6.36282500	0.79229000	-0.31247000	C	1.15570100	4.42727000	-0.41162100
H	7.49717300	-0.99856100	0.20776200	C	-1.33930100	4.52335600	-0.52745500
H	7.20376600	0.09528200	1.55786400	H	1.20982700	4.52718300	-1.50382600
H	6.33345800	1.82661200	0.03072700	H	1.22390200	5.43451700	0.01896900
H	6.61571400	0.80933200	-1.37571000	H	2.01665100	3.83954200	-0.08476900
F	1.93744400	-2.21963800	-0.04225300	H	-1.26381000	5.58046000	-0.24125500

H	-1.38192600	4.48361100	-1.62386400
H	-2.29387700	4.15121300	-0.14157500
C	-0.09561500	2.24214100	-0.59249000
O	1.00482800	1.54602300	-0.20057300
H	-0.11583800	2.43666600	-1.70472900
N	3.54228300	-0.44438300	-0.46350900
C	2.38332900	-0.90012500	-1.36653600
C	2.05440500	-2.39011600	-1.44542500
H	2.67071600	-0.56779600	-2.36823300
H	1.54294600	-0.26943900	-1.03712000
C	0.84167700	-2.59345900	-2.37105400
H	2.90173800	-2.95610200	-1.85018600
H	1.82394500	-2.81460600	-0.46582800
C	0.46322400	-4.06871400	-2.52921300
H	-0.01276400	-2.03168900	-1.97381500
H	1.05977800	-2.16292300	-3.35714500
H	-0.40072800	-4.18493200	-3.19089800
H	1.29025900	-4.64775100	-2.95538800
H	0.20620100	-4.51775900	-1.56340200
C	3.86579400	0.97652700	-0.98785700
C	4.83783300	1.81351500	-0.15715900
H	2.88059200	1.46506900	-1.02141400
H	4.26209600	0.82480900	-1.99584300
C	5.21262300	3.09261900	-0.92609100
H	4.37617300	2.09720800	0.79370800
H	5.75984900	1.27085600	0.08490700
C	6.13514500	4.01189700	-0.12083800
H	5.69901100	2.81896700	-1.87147600
H	4.29722100	3.63387900	-1.19456800
H	6.39299300	4.90941300	-0.69161400
H	5.65702400	4.33467400	0.81043000
H	7.06976200	3.50426100	0.14332800
C	3.08877200	-0.26135400	0.99202000
C	2.26904700	-1.36504800	1.66030400
H	2.45917300	0.63377700	0.95521600
H	4.00076100	-0.06697600	1.56110900
C	1.98657400	-0.96955500	3.12010300
H	1.31192700	-1.47703700	1.14291900
H	2.76944400	-2.33641800	1.64608400
C	1.13480500	-2.00876300	3.85467100
H	2.93675500	-0.83118400	3.65300800
H	1.47701900	0.00184300	3.13639500
H	0.94618800	-1.70421800	4.88884600
H	0.16429500	-2.14243600	3.36442600
H	1.63245200	-2.98484400	3.87944300
C	6.51365200	-4.53622300	0.64708800
C	6.26325900	-3.27925400	-0.19066700
H	7.44574100	-5.02672900	0.35059100
H	6.58784000	-4.29365500	1.71278100
H	5.70142100	-5.26138300	0.52653000
C	4.95619700	-2.56587100	0.19447300
H	7.10645200	-2.58615800	-0.07330200
H	6.23071200	-3.54699800	-1.25464400
C	4.79150600	-1.29853600	-0.64478200
H	4.12004800	-3.25565800	0.05608800
H	4.99376200	-2.30887500	1.25833400
H	5.63771900	-0.64455300	-0.43314600
H	4.82702200	-1.53727000	-1.71123600

3a’

C	-4.80884300	0.38193600	0.30878600
C	-3.49575400	-0.32010400	-0.05883700
H	-4.93580300	0.36653000	1.40079900
H	-4.74262300	1.44253000	0.02661600
C	-2.26147800	0.30492800	0.60289700
H	-3.55982000	-1.38126600	0.22112500
H	-3.36921900	-0.30184500	-1.15074000
H	-2.20901100	1.37043400	0.33712400
H	-2.37758800	0.27030700	1.69562500
C	-0.94517900	-0.37682700	0.21091900
C	0.28895500	0.26335200	0.87481600
H	-0.82323400	-0.34074200	-0.87987400
H	-0.98939200	-1.44171100	0.47848000
H	0.33772800	1.32714700	0.60953900
H	0.15689700	0.21979900	1.96637500
C	-6.04455000	-0.24012500	-0.35276600
C	-7.35552700	0.47176000	0.00310400
H	-6.11776000	-1.29854200	-0.06396300
H	-5.91431100	-0.23271900	-1.44459100
C	-8.58519100	-0.15607000	-0.66015200
H	-7.48514200	0.46601800	1.09402900
H	-7.28260700	1.52864200	-0.28775500
H	-9.50307400	0.37543700	-0.38796800

H	-8.49975500	-0.13450200	-1.75270500
H	-8.70564300	-1.20329700	-0.35979600
H	1.66251900	-1.46873800	0.76217000
C	1.57863600	-0.41416500	0.49927800
C	2.58869000	0.17218500	-0.14997500
H	2.48647300	1.21633300	-0.44076200
C	5.30916900	0.55750400	1.27997900
C	5.16843100	0.33035200	-0.23683800
H	5.40908500	-0.38995200	1.82180600
H	6.20564100	1.14773700	1.49707900
H	4.44571800	1.09306700	1.68785200
C	6.38995800	-0.45078900	-0.75776700
C	5.10809800	1.69072000	-0.95948500
H	6.33819800	-0.58207000	-1.84507400
H	7.31622000	0.08745400	-0.52943900
H	6.44363800	-1.44279500	-0.30325000
H	6.06849300	2.20855500	-0.86335500
H	4.90588200	1.56559700	-2.02974700
H	4.34085400	2.35063200	-0.54422400
C	3.88021400	-0.50416600	-0.55448800
O	3.96852500	-1.83346900	-0.03651300
H	3.86639700	-0.64108100	-1.64633000
H	3.88924800	-1.77215400	0.92622200

43

C	-8.25322400	0.71051900	0.41128900
C	-6.79995100	0.23163000	0.30263300
H	-8.26520300	1.78302600	0.65389300
H	-8.73990500	0.61671600	-0.57032000
C	-5.97593400	0.99214800	-0.74445300
H	-6.31324300	0.32518500	1.28427000
H	-6.78917000	-0.84089900	0.06088400
H	-6.46716800	0.90397500	-1.72451300
H	-5.98071000	2.06450000	-0.49962000
C	-4.52756800	0.50061100	-0.85990800
C	-3.69997600	1.26114000	-1.90257900
H	-4.52176300	-0.56834300	-1.11029500
H	-4.03604200	0.58565300	0.12044300
H	-4.21596600	1.22022400	-2.87330500
H	-3.65478100	2.32385300	-1.62572500
C	-9.07473900	-0.05360600	1.45734300
C	-10.52970600	0.42050200	1.56443700
H	-8.59038600	0.04161700	2.44006900
H	-9.06113900	-1.12640800	1.21626600
C	-11.34150100	-0.34926500	2.61142900
H	-10.54386500	1.49229500	1.80578100
H	-11.01411500	0.32440500	0.58296500
H	-12.37481700	0.01010400	2.66213200
H	-11.37258400	-1.42004400	2.37874200
H	-10.90240900	-0.24194500	3.61013800
H	-1.74997200	0.74953600	-1.10615500
C	-2.26165200	0.72534900	-2.07557800
C	-2.20460600	-0.66262200	-2.65711100
H	-2.71623400	-0.78909200	-3.60632800
C	-0.23721000	-3.70850300	-2.87297100
C	-1.67190300	-3.15298700	-2.73093600
H	0.27000600	-3.72929300	-1.90593200
H	-0.25882500	-4.72848000	-3.27466600
H	0.35613500	-3.09087600	-3.55747000
C	-2.47939000	-4.08220900	-1.79265400
C	-2.33961100	-3.16873500	-4.11786300
H	-3.51546400	-3.73530100	-1.70570200
H	-2.49900100	-5.10403500	-2.19032000
H	-2.04645800	-4.11406200	-0.79007200
H	-2.33559600	-4.18907700	-4.51783500
H	-3.38174200	-2.83681200	-4.07159700
H	-1.80921100	-2.52825900	-4.83040500
C	-1.61140800	-1.74446100	-2.10311500
O	-0.95202900	-1.71803500	-0.91973100
C	1.94789400	0.34199900	0.20331000
C	3.96899700	0.86712800	1.08984600
C	3.37917800	2.03050400	0.70052900
N	2.14193900	1.69457900	0.15934100
N	3.08120100	-0.15936200	0.78181200
Cl	3.96920800	3.63096300	0.81404100
Cl	5.50276900	0.62374500	1.80415000
C	0.22834300	3.19565600	0.49618500
C	1.19025500	2.64724900	-0.37550400
C	1.27762500	2.99269900	-1.73905100
C	0.34469700	3.91739100	-2.22571600
C	-0.62335800	4.47177000	-1.39220700
C	-0.67910400	4.11363200	-0.04774800
H	0.37815200	4.20705800	-3.27130900

H	-1.33573500	5.18765500	-1.79163800
H	-1.43703900	4.55498500	0.59196300
C	2.91430900	-2.12236500	2.25601000
C	3.16863200	-3.48482600	2.45802600
C	3.80055400	-4.25427500	1.48487100
C	4.19922800	-3.67491700	0.28345400
C	3.97628200	-2.31666800	0.02503300
C	3.32568700	-1.56753000	1.02635900
H	2.86571100	-3.94801800	3.39137800
H	3.98467900	-5.30944100	1.66454500
H	4.69276900	-4.28479300	-0.46673400
C	0.14258200	2.83426200	1.97583400
H	0.95346800	2.13796300	2.20725500
C	-1.18008600	2.11347300	2.30083600
H	-1.20325700	1.82460100	3.35687300
H	-2.04385900	2.75948700	2.11126100
H	-1.29515600	1.20864300	1.69601800
C	0.33671600	4.07250900	2.87287200
H	0.33035400	3.77773500	3.92742400
H	1.28812800	4.57146900	2.66454900
H	-0.46556000	4.80357000	2.72785600
C	2.32585900	2.40947400	-2.68163400
H	2.96117800	1.72730900	-2.10971200
C	1.67289000	1.58350800	-3.80727700
H	1.04531400	0.78377300	-3.40192800
H	1.04618200	2.21051400	-4.45029500
H	2.44448500	1.12776000	-4.43674300
C	3.24074900	3.50762300	-3.25858900
H	4.01691500	3.05886300	-3.88726900
H	2.67805900	4.21340700	-3.87848300
H	3.73261600	4.07586100	-2.46324500
C	2.24385200	-1.30845000	3.35929600
C	4.43815200	-1.71670000	-1.29987200
C	3.20541200	-1.09360800	4.54684000
H	2.72730700	-0.47403800	5.31304300
H	3.47578400	-2.04893900	5.00960100
H	4.12979600	-0.59800000	4.23604500
C	5.96632800	-1.82884200	-1.46772500
H	6.49530900	-1.35158700	-0.63726800
H	6.28798400	-2.87441400	-1.51554200
H	6.27980500	-1.34187200	-2.39706100
C	0.92476600	-1.94645300	3.83592900
H	1.10429200	-2.89491800	4.35408800
H	0.43004000	-1.27736900	4.54863500
H	0.23729100	-2.14057800	3.00717500
H	1.99662600	-0.32288600	2.95417100
Cu	0.45947200	-0.63990100	-0.40574000
H	-1.71822200	1.43043600	-2.72302200
C	3.70126400	-2.35376700	-2.49386500
H	4.01749700	-1.87914500	-3.42889300
H	3.91860900	-3.42423000	-2.57285100
H	2.61754900	-2.23703200	-2.39914600
H	4.18998600	-0.65170900	-1.30084900
O	-1.52982200	-2.93447900	1.41649300
C	-2.83060300	-2.57248500	1.84181800
H	-3.61385300	-2.96602900	1.17625000
H	-2.99394100	-2.99675200	2.83814900
H	-2.96606600	-1.48265900	1.91400800
H	-1.37134700	-2.51917200	0.53449500

TS16

C	-8.77510800	0.50306500	0.39692100
C	-7.29759800	0.09440900	0.33884800
H	-8.85991500	1.58242400	0.20424100
H	-9.32101000	0.00658100	-0.41834200
C	-6.61840300	0.43074000	-0.99502100
H	-6.75281100	0.58795600	1.15671300
H	-7.21218300	-0.98548300	0.52718200
H	-7.16308200	-0.06360500	-1.81272500
H	-6.70799800	1.51087800	-1.18301000
C	-5.14015200	0.02555900	-1.05393200
C	-4.45925600	0.37865500	-2.38157500
H	-5.04760200	-1.05447800	-0.87944500
H	-4.59676300	0.51405900	-0.23167500
H	-5.01280500	-0.09351500	-3.20717500
H	-4.53631300	1.46325600	-2.54682500
C	-9.45331100	0.17395600	1.73276700
C	-10.92998700	0.58565000	1.79041300
H	-8.90773600	0.66962900	2.54888200
H	-9.37143200	-0.90546500	1.92610600
C	-11.59938500	0.25528100	3.12848000
H	-11.01199800	1.66407100	1.59662700
H	-11.47537600	0.08930100	0.97598300

H	-12.65048700	0.56279200	3.13821800
H	-11.56581100	-0.82116600	3.33279800
H	-11.09597800	0.76401300	3.95883800
H	-2.42387700	0.40715200	-1.62610000
C	-2.97420100	-0.03778500	-2.46171800
C	-2.75400800	-1.52704200	-2.46231600
H	-3.26982400	-2.08303600	-3.23916900
C	-0.36439300	-4.12402100	-1.68090200
C	-1.85758700	-3.74302300	-1.58525600
H	0.20419500	-3.68552100	-0.85702200
H	-0.23898700	-5.21277700	-1.64226300
H	0.06946700	-3.76752700	-2.62205900
C	-2.43439100	-4.31497300	-0.26755600
C	-2.60291700	-4.40305600	-2.75957400
H	-3.49083800	-4.04656900	-0.15559000
H	-2.36067800	-5.40910900	-0.26126800
H	-1.89162800	-3.94119800	0.60462200
H	-2.45872600	-5.48918000	-2.72774600
H	-3.67951900	-4.20953900	-2.71601700
H	-2.23218900	-4.04461200	-3.72538300
C	-1.99048000	-2.20260600	-1.56893000
O	-1.30707400	-1.57704600	-0.59569400
C	2.05282900	0.38601700	0.20590800
C	4.17818600	1.18961400	0.26583000
C	3.38211700	2.17811000	-0.22322100
N	2.08473700	1.67326500	-0.25774700
N	3.35454800	0.09741200	0.52261600
Cl	3.80654300	3.75821200	-0.72097400
Cl	5.86555300	1.20122500	0.54475000
C	0.17567700	3.17158900	0.13610700
C	0.93828800	2.39995300	-0.76299400
C	0.65276900	2.32103000	-2.14125400
C	-0.45186300	3.04407800	-2.60830700
C	-1.23091400	3.80878200	-1.74400400
C	-0.91892100	3.87041400	-0.38856200
H	-0.70544100	3.00425900	-3.66292600
H	-2.08333100	4.36097800	-2.12880500
H	-1.53077100	4.47432200	0.27422700
C	3.82092400	-1.39205900	2.42288000
C	4.25282000	-2.64438000	2.87815200
C	4.66606600	-3.63209100	1.98817000
C	4.66823200	-3.38379500	0.61826200
C	4.24808700	-2.15065200	0.10400800
C	3.81286300	-1.18000400	1.02955300
H	4.26817400	-2.84609100	3.94461300
H	4.99561100	-4.59623000	2.36427400
H	5.00554800	-4.15723200	-0.06454300
C	0.49785000	3.28034700	1.62325900
H	1.37809400	2.66498000	1.82958500
C	-0.65159900	2.73317300	2.49124700
H	-0.37645200	2.77204600	3.55066800
H	-1.56618900	3.32165500	2.36311600
H	-0.88134600	1.69471200	2.23453300
C	0.84773500	4.72878800	2.01827200
H	1.12592000	4.77500200	3.07643000
H	1.68589900	5.11184700	1.42833600
H	-0.00429400	5.40032100	1.86810700
C	1.49070300	1.50451200	-3.12119100
H	2.29346700	1.01575800	-2.56219000
C	0.66188500	0.39066100	-3.78989300
H	0.20057700	-0.26946600	-3.05009800
H	-0.13778800	0.80888000	-4.41036900
H	1.30420400	-0.21316200	-4.44020200
C	2.15570300	2.40871700	-4.17833000
H	2.79469700	1.81139600	-4.83718300
H	1.40771300	2.90754900	-4.80367300
H	2.77455000	3.18178600	-3.71267600
C	3.40295800	-0.32637600	3.43109500
C	4.29653800	-1.90692600	-1.40154000
C	4.58736300	0.09312800	4.32432300
H	4.28031200	0.89199200	5.00757200
H	4.94485700	-0.74544300	4.93111300
H	5.42844900	0.45951900	3.72787200
C	5.74052500	-1.99679300	-1.93496900
H	6.40307700	-1.29881900	-1.41440200
H	6.14923800	-3.00536800	-1.81212900
H	5.76300200	-1.75670300	-3.00312600
C	2.20566200	-0.79094600	4.28159200
H	2.46788100	-1.64957200	4.90882000
H	1.87791300	0.01675500	4.94469500
H	1.36381200	-1.08175700	3.64707700
H	3.08167000	0.56069000	2.87797100

Cu	0.54761200	-0.71816700	0.51657100
H	-2.55479400	0.40864300	-3.37736200
C	3.36574800	-2.86772600	-2.16452400
H	3.38740000	-2.64110400	-3.23583500
H	3.67630900	-3.91041900	-2.03871400
H	2.33266000	-2.77908100	-1.81814300
H	3.94138700	-0.89148100	-1.59836600
O	-0.66141400	-1.87889600	1.64549000
C	-1.53147100	-1.38585200	2.65923000
H	-2.19200600	-2.18696300	3.01523300
H	-0.93991800	-1.02810500	3.50745100
H	-2.15515700	-0.55850700	2.29597400
H	-1.17001100	-1.94443300	0.67898000

44

C	-8.77510800	0.50306500	0.39692100
C	-7.29759800	0.09440900	0.33884800
H	-8.85991500	1.58242400	0.20424100
H	-9.32101000	0.00658100	-0.41834200
C	-6.61840300	0.43074000	-0.99502100
H	-6.75281100	0.58795600	1.15671300
H	-7.21218300	-0.98548300	0.52718200
H	-7.16308200	-0.06360500	-1.81272500
H	-6.70799800	1.51087800	-1.18301000
C	-5.14015200	0.02555900	-1.05393200
C	-4.45925600	0.37865500	-2.38157500
H	-5.04760200	-1.05447800	-0.87944500
H	-4.59676300	0.51405900	-0.23167500
H	-5.01280500	-0.09351500	-3.20717500
H	-4.53631300	1.46325600	-2.54682500
C	-9.45331100	0.17395600	1.73276700
C	-10.92998700	0.58565000	1.79041300
H	-8.90773600	0.66962900	2.54888200
H	-9.37143200	-0.90546500	1.92610600
C	-11.59938500	0.25528100	3.12848000
H	-11.01199800	1.66407100	1.59662700
H	-11.47537600	0.08930100	0.97598300
H	-12.65048700	0.56279200	3.13821800
H	-11.56581100	-0.82116600	3.33279800
H	-11.09597800	0.76401300	3.95883800
H	-2.42387700	0.40715200	-1.62610000
C	-2.97420100	-0.03778500	-2.46171800
C	-2.75400800	-1.52704200	-2.46231600
H	-3.26982400	-2.08303600	-3.23916900
C	-0.36439300	-4.12402100	-1.68090200
C	-1.85758700	-3.74302300	-1.58525600
H	0.20419500	-3.68552100	-0.85702200
H	-0.23898700	-5.21277700	-1.64226300
H	0.06946700	-3.76752700	-2.62205900
C	-2.43439100	-4.31497300	-0.26755600
C	-2.60291700	-4.40305600	-2.75957400
H	-3.49083800	-4.04656900	-0.15559000
H	-2.36067800	-5.40910900	-0.26126800
H	-1.89162800	-3.94119800	0.60462200
H	-2.45872600	-5.48918000	-2.72774600
H	-3.67951900	-4.20953900	-2.71601700
H	-2.23218900	-4.04461200	-3.72538300
C	-1.99048000	-2.20260600	-1.56893000
O	-1.30707400	-1.57704600	-0.59569400
C	2.05282900	0.38601700	0.20590800
C	4.17818600	1.18961400	0.26583000
C	3.38211700	2.17811000	-0.22322100
N	2.08473700	1.67326500	-0.25774700
N	3.35454800	0.09741200	0.52261600
Cl	3.80654300	3.75821200	-0.72097400
Cl	5.86555300	1.20122500	0.54475000
C	0.17567700	3.17158900	0.13610700
C	0.93828800	2.39995300	-0.76299400
C	0.65276900	2.32103000	-2.14125400
C	-0.45186300	3.04407800	-2.60830700
C	-1.23091400	3.80878200	-1.74400400
C	-0.91892100	3.87041400	-0.38856200
H	-0.70544100	3.00425900	-3.66292600
H	-2.08333100	4.36097800	-2.12880500
H	-1.53077100	4.47432200	0.27422700
C	3.82092400	-1.39205900	2.42288000
C	4.25282000	-2.64438000	2.87815200
C	4.66606600	-3.63209100	1.98817000
C	4.66823200	-3.38379500	0.61826200
C	4.24808700	-2.15065200	0.10400800
C	3.81286300	-1.18000400	1.02955300
H	4.26817400	-2.84609100	3.94461300
H	4.99561100	-4.59623000	2.36427400

H	5.00554800	-4.15723200	-0.06454300
C	0.49785000	3.28034700	1.62325900
H	1.37809400	2.66498000	1.82958500
C	-0.65159900	2.73317300	2.49124700
H	-0.37645200	2.77204600	3.55066800
H	-1.56618900	3.32165500	2.36311600
H	-0.88134600	1.69471200	2.23453300
C	0.84773500	4.72878800	2.01827200
H	1.12592000	4.77500200	3.07643000
H	1.68589900	5.11184700	1.42833600
H	-0.00429400	5.40032100	1.86810700
C	1.49070300	1.50451200	-3.12119100
H	2.29346700	1.01575800	-2.56219000
C	0.66188500	0.39066100	-3.78989300
H	0.20057700	-0.26946600	-3.05009800
H	-0.13778800	0.80888000	-4.41036900
H	1.30420400	-0.21316200	-4.44020200
C	2.15570300	2.40871700	-4.17833000
H	2.79469700	1.81139600	-4.83718300
H	1.40771300	2.90754900	-4.80367300
H	2.77455000	3.18178600	-3.71267600
C	3.40295800	-0.32637600	3.43109500
C	4.29653800	-1.90692600	-1.40154000
C	4.58736300	0.09312800	4.32432300
H	4.28031200	0.89199200	5.00757200
H	4.94485700	-0.74544300	4.93111300
H	5.42844900	0.45951900	3.72787200
C	5.74052500	-1.99679300	-1.93496900
H	6.40307700	-1.29881900	-1.41440200
H	6.14923800	-3.00536800	-1.81212900
H	5.76300200	-1.75670300	-3.00312600
C	2.20566200	-0.79094600	4.28159200
H	2.46788100	-1.64957200	4.90882000
H	1.87791300	0.01675500	4.94469500
H	1.36381200	-1.08175700	3.64707700
H	3.08167000	0.56069000	2.87797100
Cu	0.54761200	-0.71816700	0.51657100
H	-2.55479400	0.40864300	-3.37736200
C	3.36574800	-2.86772600	-2.16452400
H	3.38740000	-2.64110400	-3.23583500
H	3.67630900	-3.91041900	-2.03871400
H	2.33266000	-2.77908100	-1.81814300
H	3.94138700	-0.89148100	-1.59836600
O	-0.66141400	-1.87889600	1.64549000
C	-1.53147100	-1.38585200	2.65923000
H	-2.19200600	-2.18696300	3.01523300
H	-0.93991800	-1.02810500	3.50745100
H	-2.15515700	-0.55850700	2.29597400
H	-1.17001100	-1.94443300	0.67898000

45

C	4.18153000	0.43208000	0.27985000
C	2.72753400	0.27926300	-0.18333300
H	4.57483500	1.39595100	-0.07393100
H	4.20983900	0.47852600	1.37804200
C	1.80573800	1.40547400	0.30088400
H	2.70008300	0.23626500	-1.28163800
H	2.33463100	-0.68603100	0.16691300
H	1.82635900	1.44254100	1.39972000
H	2.20419200	2.37154700	-0.04132000
C	0.35527600	1.25797200	-0.17444000
C	-0.56532700	2.38274600	0.31336300
H	-0.04379600	0.29173500	0.16168500
H	0.33447900	1.22814100	-1.27348800
H	-0.54957500	2.41450300	1.41239700
H	-0.16617400	3.34890900	-0.02440800
C	5.10155200	-0.69634500	-0.20176300
C	6.55764000	-0.54001700	0.25367600
H	5.07003200	-0.74667700	-1.29977700
H	4.71219200	-1.66034600	0.15637400
C	7.46848400	-1.67210200	-0.23107200
H	6.94703800	0.42228700	-0.10580100
H	6.58990200	-0.48900000	1.35064400
H	8.50008700	-1.53021100	0.10771200
H	7.12596000	-2.64354400	0.14365900
H	7.48236700	-1.72766300	-1.32568600
H	-2.04578100	2.21859100	-1.26406900
C	-2.02461000	2.25422200	-0.16995800
C	-2.74501900	1.05825300	0.39606400
H	-2.76581500	0.97372300	1.47718400
C	-5.57977200	-1.05870000	-0.21643600
C	-4.09789600	-1.11326700	0.23138300
H	-5.68701600	-1.03755900	-1.30601000

H	-6.11849200	-1.93920300	0.14853400
H	-6.07151000	-0.16591700	0.18237200
C	-3.43997500	-2.40532700	-0.31584100
C	-4.05265000	-1.16286200	1.76772500
H	-2.39351000	-2.47127800	-0.00258000
H	-3.96894200	-3.28590200	0.06244200
H	-3.46352600	-2.46582300	-1.41013900
H	-4.58750000	-2.04972300	2.12183900
H	-3.02450100	-1.22050200	2.13713000
H	-4.52933500	-0.28424800	2.21228400
C	-3.35921400	0.10642300	-0.32230900
O	-3.36313800	0.22714900	-1.70031300
H	-2.56073200	3.17037500	0.12000600
H	-3.73042200	-0.57352600	-2.09435000

46

C	-4.89822700	-0.49114500	-0.02129300
C	-3.62890100	0.36812500	0.02963700
H	-4.89348500	-1.09069100	-0.94294100
H	-4.88162100	-1.21182600	0.80884600
C	-2.33162800	-0.44602800	-0.05123900
H	-3.65075700	1.09572700	-0.79423800
H	-3.62881400	0.95998600	0.95615300
H	-2.31187300	-1.18020900	0.76686300
H	-2.32841100	-1.03010800	-0.98273000
C	-1.06389600	0.41474400	0.01095300
C	0.23427100	-0.39463300	-0.09880700
H	-1.05803600	0.98440700	0.95112000
H	-1.09229000	1.16130600	-0.79539100
H	0.25890200	-1.15208700	0.69768800
H	0.23402300	-0.95174600	-1.04669800
C	-6.19482200	0.32520800	0.04340000
C	-7.46507600	-0.53297900	-0.00381300
H	-6.21316900	1.04349900	-0.78890500
H	-6.19964700	0.92782600	0.96313200
C	-8.75478400	0.29123900	0.05648400
H	-7.45893400	-1.13663200	-0.92169500
H	-7.44872300	-1.24850400	0.82958900
H	-9.64238100	-0.34900800	0.01990400
H	-8.80605800	0.87873400	0.98041600
H	-8.81555400	0.99266400	-0.78359100
H	1.51322200	1.01127600	0.93847900
C	1.49565600	0.47305300	-0.01753100
C	6.54842900	0.75910100	-0.32903100
C	5.41538200	-0.21181300	0.04207100
H	6.51541500	1.65882600	0.28919200
H	7.51874300	0.27271200	-0.18641000
H	6.47406400	1.07177600	-1.37540900
C	5.56142900	-0.62638100	1.52813500
C	5.48804700	-1.46680500	-0.85239800
H	4.78494800	-1.33359200	1.83561100
H	6.53166800	-1.11125800	1.67923200
H	5.51223800	0.24553400	2.18816800
H	6.47310600	-1.93384500	-0.74970800
H	4.73967600	-2.21581300	-0.57857900
H	5.34856500	-1.21399500	-1.90895100
C	4.05478600	0.50657300	-0.10169200
O	3.99308300	1.72612700	-0.14212100
H	1.46787100	1.24466100	-0.79535700
C	2.78592200	-0.33590800	-0.16478700
H	2.84061400	-1.12906200	0.59203700
H	2.79251000	-0.86368100	-1.12940200

47

C	8.84888200	-0.41382900	-0.41269900
C	7.68979800	0.23756800	0.35264300
H	8.44264100	-1.07745300	-1.18958700
H	9.41511900	0.36406000	-0.94498100
C	6.73647200	1.04190000	-0.54030100
H	7.12081900	-0.54166800	0.88002600
H	8.09619200	0.89613400	1.13376000
H	7.30357800	1.82685900	-1.06117200
H	6.33474100	0.38610800	-1.32599100
C	5.57278900	1.68128300	0.22797300
C	4.62209300	2.49631600	-0.65804200
H	5.97394600	2.32955900	1.02032600
H	5.00134000	0.89423500	0.74057900
H	5.18891400	3.29358100	-1.16039900
H	4.22895300	1.85243900	-1.45763900
C	9.80502200	-1.21033300	0.48391700
C	10.96225600	-1.86682700	-0.27988900
H	9.23921400	-1.98638100	1.01962100
H	10.21451300	-0.54588300	1.25857300
C	11.91528800	-2.65433000	0.62522000

H	10.55364000	-2.53454300	-1.05071100	H	-6.19619800	2.13670000	-1.77583700
H	11.52549900	-1.09201400	-0.81791700	C	-0.29729700	-3.39029700	-1.39028100
H	12.72831100	-3.11127200	0.05116100	C	0.93529800	-3.97029600	-1.71589700
H	12.36747500	-2.00456700	1.38355200	C	2.02411300	-3.88164400	-0.85271800
H	11.38745100	-3.45763400	1.15237500	C	1.90242200	-3.21066300	0.36116900
H	3.83731900	3.74391000	0.92833200	C	0.69507300	-2.61046600	0.74046800
C	3.45120100	3.10807100	0.12062500	C	-0.38504000	-2.71024600	-0.15893400
C	2.50951600	3.93094600	-0.76152900	H	1.04208700	-4.49814800	-2.65841500
H	3.04791900	4.74982400	-1.25436300	H	2.97062100	-4.33867000	-1.12633900
C	-0.89279600	5.72970700	-0.01651500	H	2.75814800	-3.14959500	1.02619100
C	0.49504700	5.63364300	-0.67107200	C	-4.95590600	-0.27154100	-1.94632500
H	-0.81034000	5.85912500	1.06502300	H	-4.31989300	-1.12447100	-1.69307700
H	-1.44249000	6.58172700	-0.43022300	C	-4.45588400	0.28272100	-3.29446000
H	-1.47861100	4.82357100	-0.20058100	H	-4.50821600	-0.49385200	-4.06495500
C	1.28290300	6.94044100	-0.39798700	H	-5.06628900	1.12763700	-3.63040500
C	0.34281100	5.42907900	-2.19280300	H	-3.41822300	0.62366100	-3.22153600
H	2.28129300	6.92019400	-0.84624300	C	-6.39981100	-0.79887100	-2.06209800
H	0.74277900	7.79119400	-0.82721200	H	-6.45530700	-1.58081500	-2.82673500
H	1.39348900	7.11658100	0.67700300	H	-6.74629200	-1.22336700	-1.11470800
H	-0.25289300	6.24607300	-2.61416900	H	-7.09552500	-0.00341900	-2.34941700
H	1.30692300	5.42541700	-2.70946900	C	-3.03139400	1.34177000	2.56436000
H	-0.16913600	4.48796100	-2.41899100	H	-2.47885400	0.40505500	2.44713300
C	1.29609500	4.48248300	-0.02286100	C	-1.99028200	2.46600000	2.72357200
O	0.97787400	4.03605700	1.06992000	H	-1.35240000	2.56135500	1.84071900
H	2.87617400	2.31429100	0.60955300	H	-2.47057100	3.43481700	2.89732700
H	2.11795300	3.30687100	-1.57836900	H	-1.34746300	2.25863100	3.58561400
C	-1.98506700	-0.80421500	-0.11919600	C	-3.89502100	1.21197500	3.83590700
C	-2.66938900	-2.71256100	0.90413500	H	-3.25841100	1.02117300	4.70634100
C	-3.67218400	-1.80011600	1.02917800	H	-4.45626500	2.13261800	4.02872400
N	-3.23803600	-0.63648800	0.40108100	H	-4.61388900	0.39137900	3.75295500
N	-1.64376300	-2.08906100	0.19970100	C	-1.46691100	-3.50922900	-2.36258400
Cl	-5.19989100	-1.97130600	1.77896200	C	0.60069200	-1.88557100	2.07932200
Cl	-2.59990900	-4.32714100	1.46436300	C	-1.83597400	-4.98160500	-2.62940000
C	-4.82914800	0.76658900	-0.83575600	H	-2.71403200	-5.03747100	-3.28134000
C	-4.00661000	0.58748000	0.29486800	H	-1.01990100	-5.51686300	-3.12598400
C	-3.90169500	1.54167900	1.32703600	H	-2.06851400	-5.50992000	-1.69955900
C	-4.65449700	2.71522400	1.19185300	C	0.88260900	-2.83752700	3.25844300
C	-5.47046800	2.92566400	0.08350900	H	0.20507400	-3.69693000	3.24828900
C	-5.55532000	1.96142700	-0.91733700	H	1.90926800	-3.21777300	3.23134100
H	-4.59975900	3.47380400	1.96630200	H	0.74962000	-2.30952900	4.20847600
H	-6.04380800	3.84435800	0.00011800	C	-1.17500000	-2.76088700	-3.67792400

H	-0.31885700	-3.19793200	-4.20274800
H	-2.04109900	-2.81638000	-4.34603400
H	-0.95313400	-1.70550200	-3.49019400
H	-2.34153800	-3.03482200	-1.90858500
Cu	-0.95058400	0.47309500	-1.15148700
H	-0.15789100	1.45831700	-2.00220700
C	1.53285700	-0.65904900	2.11875600
H	1.41717600	-0.12648200	3.06852300
H	2.58371100	-0.95368000	2.02599400
H	1.30370100	0.03788800	1.30667700
H	-0.42190600	-1.51700900	2.19916400

TS17

C	8.62338400	0.80079900	-0.16357600
C	7.14847700	0.53109000	0.16076200
H	8.72612000	1.01164400	-1.23782000
H	8.94796100	1.71340500	0.35671400
C	6.21097300	1.68411000	-0.22038000
H	6.82552800	-0.38354800	-0.35741300
H	7.04665100	0.32221100	1.23551300
H	6.53517200	2.59994200	0.29459700
H	6.30912100	1.89034200	-1.29600100
C	4.73845900	1.40974200	0.11090400
C	3.79556100	2.55719800	-0.27177700
H	4.64124200	1.20694900	1.18723400
H	4.41544400	0.49185500	-0.39930900
H	4.11680400	3.47473600	0.24253300
H	3.89407900	2.76315000	-1.34751100
C	9.55609400	-0.35632600	0.21604600
C	11.03230500	-0.08857300	-0.10395200
H	9.23316900	-1.26893000	-0.30569300
H	9.45220600	-0.56893400	1.28998200
C	11.95474900	-1.25081400	0.27825200
H	11.13680300	0.12388600	-1.17679000
H	11.35574300	0.82223200	0.41837200
H	12.99994700	-1.02965700	0.03738500
H	11.89863000	-1.46390900	1.35211800
H	11.67728700	-2.16781000	-0.25450700
H	2.22152100	2.05375500	1.12943000
C	2.32365100	2.27739000	0.06207200
C	1.40657600	3.44498300	-0.30066200
H	1.73040900	4.33599400	0.25927400
C	-2.50070800	3.94536500	-0.26838300
C	-1.03879700	4.41082900	-0.34615800
H	-2.72861100	3.52455300	0.71305500
H	-3.17593400	4.78957500	-0.44822700
H	-2.70644200	3.18049400	-1.02487500
C	-0.82588600	5.52409200	0.71228600
C	-0.75946800	4.98294700	-1.74626000
H	0.19249200	5.92507100	0.68832100
H	-1.51252200	6.35555300	0.51878000
H	-1.02242400	5.14422300	1.71886700
H	-1.51161300	5.74031600	-1.99417800
H	0.22109500	5.46407100	-1.81067800
H	-0.80693800	4.19767400	-2.50797700
C	-0.07691800	3.24018200	0.04450900
O	-0.35435700	2.59093900	1.11954900
H	1.98974900	1.37785300	-0.47466300
H	1.51370700	3.68957300	-1.36111400
C	-1.63108100	-0.60158600	-0.04805300
C	-1.88143800	-2.84619000	0.22709600
C	-3.11917600	-2.28877500	0.29342000
N	-2.95408600	-0.91576400	0.12316200
N	-0.97928600	-1.80477700	0.01935000
Cl	-4.63430000	-3.04619100	0.53478900
Cl	-1.42752300	-4.49062500	0.36023800
C	-4.67751200	0.35653800	-1.07905800
C	-4.03210900	0.05003700	0.13650000
C	-4.39920100	0.63207100	1.36710700
C	-5.44449400	1.56454400	1.34865200
C	-6.09389800	1.89705400	0.16274700
C	-5.71377100	1.29788600	-1.03543000
H	-5.75311300	2.03405400	2.27750200
H	-6.90201100	2.62274400	0.17282600
H	-6.23213800	1.56031700	-1.95237600
C	1.01074100	-2.17675700	-1.37186000
C	2.39923700	-2.34525400	-1.44665900
C	3.19132700	-2.31747900	-0.30175500
C	2.61014900	-2.11944000	0.94813600
C	1.22732000	-1.94477800	1.08525200
C	0.45369200	-1.97222700	-0.09302500
H	2.86451700	-2.50496300	-2.41442900
H	4.26567400	-2.45482600	-0.38321900

H	3.23918800	-2.10169900	1.83249700
C	-4.30643700	-0.29514000	-2.40832500
H	-3.49201800	-1.00222800	-2.22829300
C	-3.78823700	0.74154700	-3.42360900
H	-3.50027200	0.24416300	-4.35600900
H	-4.55627600	1.48393300	-3.66533800
H	-2.91258000	1.26896500	-3.03375700
C	-5.48885500	-1.09629700	-2.98943700
H	-5.18441400	-1.60079900	-3.91248100
H	-5.84125300	-1.85659900	-2.28574200
H	-6.33455300	-0.44360100	-3.23077400
C	-3.72512500	0.28144200	2.69051300
H	-2.94586800	-0.45960600	2.49151300
C	-3.03393200	1.50712700	3.32022100
H	-2.28270900	1.93194000	2.64794500
H	-3.76043400	2.28948800	3.56636300
H	-2.53627200	1.21572600	4.25184300
C	-4.72588700	-0.35830800	3.67393500
H	-4.21158000	-0.65583600	4.59384700
H	-5.51967100	0.34430500	3.94948400
H	-5.19816100	-1.24751700	3.24483900
C	0.17394800	-2.23809000	-2.64609800
C	0.62589300	-1.74373700	2.47343200
C	0.26106100	-3.62832900	-3.30696500
H	-0.38780000	-3.66826700	-4.18827900
H	1.28188800	-3.85162900	-3.63490600
H	-0.05108600	-4.41912500	-2.61790000
C	0.92257800	-2.94305000	3.39536700
H	0.56973800	-3.88151800	2.95672800
H	1.99541000	-3.04452100	3.59037700
H	0.42222200	-2.80806000	4.35998700
C	0.56854400	-1.12659100	-3.63781900
H	1.60376400	-1.23959700	-3.97720500
H	-0.07706100	-1.16489100	-4.52177800
H	0.46462400	-0.13804100	-3.18056000
H	-0.87237400	-2.07013500	-2.37679100
Cu	-0.88268400	1.12347500	-0.38091900
H	-0.39848000	2.25470100	-1.39113400
C	1.10200700	-0.42260900	3.10923600
H	0.64496300	-0.29625100	4.09687300
H	2.18931000	-0.41651000	3.24340200
H	0.82767800	0.43861900	2.49312900
H	-0.46075000	-1.67738400	2.37040400

48

C	-8.72073100	0.52710200	0.04240500
C	-7.22390200	0.39256100	0.35080200
H	-9.10964100	1.43471100	0.52613900
H	-8.85531000	0.67893800	-1.03823100
C	-6.39379100	1.59979900	-0.10405200
H	-7.08828700	0.24498700	1.43199200
H	-6.83524100	-0.51672100	-0.13032200
H	-6.52988600	1.74492100	-1.18544700
H	-6.78533400	2.50913800	0.37451400
C	-4.89606400	1.47231900	0.20302100
C	-4.07074900	2.67974400	-0.26071800
H	-4.50309900	0.56161200	-0.27147500
H	-4.75865200	1.33298300	1.28531800
H	-4.21938100	2.82353500	-1.34085700
H	-4.45979100	3.58921900	0.22073000
C	-9.55347600	-0.68075300	0.49010700
C	-11.04986600	-0.54353000	0.18079000
H	-9.42038700	-0.83397400	1.57088800
H	-9.16637100	-1.58897900	0.00566000
C	-11.87450300	-1.75477200	0.62852100
H	-11.43722600	0.36271100	0.66624400
H	-11.18263400	-0.38921500	-0.89885200
H	-12.93627100	-1.62685900	0.39253100
H	-11.53190100	-2.67131900	0.13422600
H	-11.79078000	-1.91268900	1.71004000
H	-2.17857000	1.64976900	-0.46038800
C	-2.56927200	2.55072300	0.02682200
C	-1.75280700	3.76293000	-0.43690400
H	-1.92313300	3.91965200	-1.51048300
C	2.06007400	4.65409300	-0.10903200
C	0.58030300	4.92995400	-0.43980000
H	2.46123000	3.86484600	-0.74856000
H	2.66549300	5.55793700	-0.24999300
H	2.17649400	4.33475400	0.93444100
C	0.47446000	5.39139400	-1.90478000
C	0.08555000	6.05304500	0.49468400
H	-0.54779600	5.68693300	-2.16480900
H	1.12344100	6.25646400	-2.08791400

H	0.77680700	4.58637700	-2.58057600
H	0.75479100	6.92010900	0.43928300
H	-0.91853100	6.40189800	0.23458100
H	0.06472200	5.71966800	1.53995700
C	-0.23370000	3.60496200	-0.20208200
O	0.25661700	2.56170700	-1.00535900
H	-2.42032600	2.40660900	1.10805600
H	-2.13042300	4.65554400	0.07817500
C	1.75209200	-0.68230900	-0.04725300
C	2.05402100	-2.91078700	0.26703700
C	3.24032400	-2.29717100	0.52969900
N	3.04191200	-0.93373700	0.33281400
N	1.15101100	-1.91089100	-0.08303700
Cl	4.72995800	-2.98376900	1.01314900
Cl	1.66176000	-4.57429900	0.32649500
C	4.19154500	0.69089900	1.77110100
C	4.05657500	0.08573000	0.50550400
C	4.86357400	0.42667700	-0.59814000
C	5.82595800	1.42563800	-0.40364400
C	5.97778800	2.04956000	0.83170900
C	5.16952600	1.68443300	1.90512400
H	6.46328400	1.71954100	-1.23186000
H	6.72987100	2.82274200	0.95882600
H	5.29861900	2.17836300	2.86305400
C	-1.18716600	-2.14661900	0.62617600
C	-2.52775900	-2.34688200	0.27405000
C	-2.90531100	-2.52549700	-1.05444700
C	-1.94535900	-2.51194100	-2.06295500
C	-0.58938700	-2.31724600	-1.77124600
C	-0.24158300	-2.12878900	-0.41866000
H	-3.28468800	-2.36216200	1.05199500
H	-3.95106300	-2.67928500	-1.30407300
H	-2.25157200	-2.65552800	-3.09437700
C	3.31933200	0.32196800	2.96717500
H	2.68674400	-0.52394000	2.68327300
C	2.38073800	1.48398500	3.34767400
H	1.72697200	1.18884100	4.17550200
H	2.94860600	2.36472600	3.66616200
H	1.75151800	1.77535900	2.50057900
C	4.16408800	-0.12992300	4.17412600
H	3.50995100	-0.45267400	4.99075300
H	4.81895900	-0.96646900	3.91148700
H	4.79174400	0.68243000	4.55508900
C	4.72469100	-0.23185200	-1.96714700
H	3.94979700	-1.00073200	-1.90117000
C	4.26620700	0.78360300	-3.03201900
H	3.31914100	1.25301900	-2.74863200
H	5.00788600	1.57706000	-3.17227000
H	4.12634300	0.28305500	-3.99605700
C	6.02779000	-0.93572400	-2.39364200
H	5.88326700	-1.44548700	-3.35192600
H	6.84857600	-0.22168400	-2.51842100
H	6.33909800	-1.68082400	-1.65508700
C	-0.81280400	-1.95631200	2.09287100
C	0.43382500	-2.32073700	-2.90237400
C	-1.19568100	-3.18693800	2.93827100
H	-0.86820100	-3.04903300	3.97403800
H	-2.27952600	-3.34301600	2.95096200
H	-0.72864800	-4.09773900	2.55136500
C	0.46516600	-3.68033900	-3.62830700
H	0.67457200	-4.49915000	-2.93304000
H	-0.48885000	-3.89322600	-4.12203400
H	1.24445100	-3.67854400	-4.39760800
C	-1.43829900	-0.67139000	2.66945600
H	-2.53220800	-0.72381200	2.66644500
H	-1.11385000	-0.52540300	3.70537400
H	-1.14258400	0.20769500	2.08919500
H	0.27324700	-1.84357500	2.15907600
Cu	0.98333100	0.98421500	-0.46793300
H	-0.10150100	3.38145400	0.87678100
C	0.18265600	-1.16766000	-3.89369300
H	0.95337400	-1.16511700	-4.67173400
H	-0.78952000	-1.26978500	-4.38743200
H	0.20340600	-0.19752600	-3.38758000
H	1.42511900	-2.16317000	-2.46834000

49

C	8.42828700	-2.06578200	-0.83163300
C	7.49040900	-0.88379500	-0.55378700
H	7.90580700	-3.00541800	-0.60048800
H	8.65728200	-2.10310200	-1.90643400
C	6.17034600	-0.94359200	-1.33251400
H	7.27212900	-0.84132400	0.52311700

H	8.01043900	0.05488000	-0.79369300
H	6.38506400	-0.98508100	-2.41017500
H	5.64950700	-1.88166300	-1.09104900
C	5.23869900	0.24118300	-1.04553000
C	3.90568400	0.18598900	-1.80245700
H	5.75807600	1.17766100	-1.29590300
H	5.03655900	0.28762700	0.03429200
H	4.10402600	0.14011900	-2.88383500
H	3.38668500	-0.75064100	-1.55048800
C	9.73827700	-2.00728800	-0.03630700
C	10.67933500	-3.18771300	-0.30988900
H	9.50846200	-1.97049400	1.03847700
H	10.26142100	-1.06760400	-0.26583800
C	11.98084100	-3.12363800	0.49586400
H	10.15549500	-4.12689000	-0.08453000
H	10.91404800	-3.22156500	-1.38266100
H	12.62984700	-3.97853300	0.27832700
H	12.54403600	-2.21148700	0.26669600
H	11.77940500	-3.12425800	1.57341300
C	-1.02563800	1.61197000	-3.61759800
C	-0.30386900	2.85186500	-3.06024300
H	-1.57270800	1.07839200	-2.83227300
H	-1.75635600	1.90602000	-4.38014400
H	-0.33086100	0.90498000	-4.08196100
C	-1.35658000	3.85240500	-2.54773600
C	0.48198500	3.53260300	-4.20271900
H	-0.88082100	4.73809700	-2.11933100
H	-2.01226400	4.16588900	-3.36933600
H	-1.97406200	3.40568400	-1.76447900
H	-0.20033000	3.84244000	-5.00293100
H	1.00167500	4.42875300	-3.84420300
H	1.22879900	2.86954600	-4.65139600
C	0.69472000	2.49010900	-1.90267800
O	0.01355000	2.22261800	-0.67094400
C	-2.02066000	-0.86106300	0.22901900
C	-2.88580000	-2.54701800	1.48525100
C	-3.34214000	-2.71089800	0.21519900
N	-2.80326600	-1.67677900	-0.54517700
N	-2.08536200	-1.40845700	1.48375100
Cl	-4.38480700	-3.91549800	-0.40591400
Cl	-3.17419200	-3.51683400	2.86348700
C	-2.27073700	-2.19535400	-2.88789300
C	-3.06841100	-1.49729500	-1.95820600
C	-4.14339700	-0.66810900	-2.33904800
C	-4.39291800	-0.53307600	-3.71063100
C	-3.61427900	-1.19741800	-4.65431900
C	-2.56755600	-2.01930800	-4.24528200
H	-5.21160500	0.09765500	-4.04246400
H	-3.82756300	-1.07876000	-5.71262800
H	-1.97299600	-2.53784500	-4.99085500
C	-0.10586400	-1.27326700	2.93379200
C	0.48649500	-0.77530000	4.10110200
C	-0.21034500	0.07117100	4.95905500
C	-1.52177100	0.43802700	4.66847800
C	-2.16860800	-0.02982900	3.51766200
C	-1.43242400	-0.87913000	2.66543000
H	1.50604800	-1.05893900	4.34185800
H	0.26884400	0.44301600	5.86002600
H	-2.05617000	1.09494200	5.34728900
C	-1.13430600	-3.13000300	-2.48156400
H	-1.05100100	-3.11766600	-1.39090600
C	0.21961200	-2.65791700	-3.04414900
H	1.02191200	-3.31745700	-2.69701900
H	0.22673000	-2.67371300	-4.13910800
H	0.45046400	-1.63958500	-2.72022000
C	-1.42413500	-4.58397000	-2.90646700
H	-0.62542300	-5.24516500	-2.55421300
H	-2.37084600	-4.94323700	-2.49313300
H	-1.47567000	-4.67634200	-3.99652700
C	-5.04118100	0.05045800	-1.33566300
H	-4.65823600	-0.14400400	-0.33028200
C	-5.01962900	1.57749600	-1.53785900
H	-4.00196100	1.97345800	-1.47114600
H	-5.42901400	1.86030200	-2.51336900
H	-5.62731600	2.06609800	-0.76903000
C	-6.48310800	-0.49378100	-1.39012300
H	-7.10030300	-0.00373300	-0.62978100
H	-6.94374900	-0.30554200	-2.36572500
H	-6.51095800	-1.57251100	-1.20808200
C	0.67958900	-2.22328600	2.03497200
C	-3.61703800	0.37466500	3.25405800
C	0.91168400	-3.58023300	2.73024600

H	1.43882500	-4.26523800	2.05762500
H	1.52166200	-3.46157700	3.63227400
H	-0.03280500	-4.04898800	3.02286900
C	-4.56201200	-0.18530500	4.33691000
H	-4.49152300	-1.27426300	4.41046000
H	-4.32916100	0.23468800	5.32119700
H	-5.59949900	0.07457800	4.10152300
C	2.01323400	-1.60465100	1.57433400
H	2.70822700	-1.48437800	2.41230200
H	2.49555100	-2.25912800	0.84042400
H	1.85959000	-0.62198800	1.11935400
H	0.08667800	-2.41236000	1.13587900
Cu	-1.02500100	0.68157400	-0.26863300
H	1.28477400	3.39625100	-1.72578400
C	-3.77177800	1.90321000	3.13507700
H	-4.80630800	2.15541000	2.87849800
H	-3.53379200	2.40337800	4.07991500
H	-3.11257700	2.31059700	2.36375700
H	-3.92534600	-0.05554600	2.29683400
Si	0.17411400	3.21361100	1.08214900
H	-1.18932300	2.56745600	1.16537400
O	1.50989200	2.20630200	1.40129900
O	0.47991300	4.57767300	0.11201200
C	0.86536900	5.86062800	0.57909600
C	1.20134800	6.75241900	-0.61056500
H	1.74152600	5.79396800	1.24033400
H	0.05904700	6.31961900	1.16845300
H	1.50714700	7.74744300	-0.26846800
H	2.02001500	6.32329100	-1.19721200
H	0.33389800	6.86726800	-1.26838700
C	2.36964600	2.26065200	2.52992600
C	3.52478300	3.24116900	2.34228100
H	2.77404000	1.24966500	2.66812700
H	1.81634300	2.50741200	3.44390400
H	4.20667500	3.19814900	3.19989800
H	4.09369300	3.00069700	1.43862000
H	3.15986100	4.26933300	2.25067800
C	-0.06924600	4.08420300	2.80228400
H	-0.93124700	4.76186600	2.72628100
H	-0.33709900	3.32863700	3.55244300
H	0.76652400	4.66977700	3.20412000
C	1.65848900	1.34021800	-2.26252900
H	1.87531000	1.34966400	-3.33823000
H	1.14261900	0.39017300	-2.06413800
C	2.98520300	1.37445000	-1.49538300
H	2.77208100	1.41944800	-0.42296000
H	3.51236500	2.30782500	-1.74484200

TS18

C	-8.94791700	-0.27700900	0.64513600
C	-7.43561600	-0.48540500	0.49313000
H	-9.18278800	-0.08295800	1.70166000
H	-9.24528000	0.62904500	0.09774700
C	-6.59917000	0.69850600	0.99513700
H	-7.13841100	-1.39473000	1.03540000
H	-7.20044900	-0.67297600	-0.56449400
H	-6.90392100	1.60951400	0.46014100
H	-6.82786500	0.87964800	2.05537300
C	-5.08705500	0.49887600	0.82990500
C	-4.25144000	1.67863000	1.34301400
H	-4.85813900	0.32798800	-0.23188400
H	-4.78168200	-0.41735800	1.35598400
H	-4.57109400	2.59665500	0.82887600
H	-4.46891000	1.83900800	2.40933300
C	-9.78514200	-1.46342100	0.15093800
C	-11.29751500	-1.25208900	0.29828000
H	-9.49142900	-2.36941700	0.70076800
H	-9.54908300	-1.66036700	-0.90489800
C	-12.12605700	-2.44278500	-0.19498000
H	-11.53323900	-1.05342400	1.35281000
H	-11.59114700	-0.34839100	-0.25322600
H	-13.19966300	-2.26063900	-0.07847900
H	-11.93593000	-2.64463800	-1.25555100
H	-11.88056300	-3.35394200	0.36292600
H	-2.52604500	1.34781700	0.08593300
C	-2.74047700	1.49252400	1.15050900
C	1.94980000	3.36027000	1.92938900
C	0.45622200	3.62864400	2.20066900
H	2.16697300	3.42972600	0.86289200
H	2.56531700	4.09585700	2.46180600
H	2.24781000	2.36559300	2.27928500
C	0.09865300	5.03253900	1.67609800
C	0.23541700	3.60125600	3.73092600

H	-0.93366700	5.30600500	1.91735300
H	0.75381400	5.77915400	2.14162500
H	0.22372600	5.09196200	0.59450000
H	0.90412900	4.32031200	4.21750700
H	-0.78810200	3.86779700	4.01192800
H	0.45400000	2.61156900	4.14978900
O	0.01564900	2.12902800	0.21055800
C	1.82309600	-1.26907400	-0.10047500
C	3.44740800	-2.85312300	0.07820300
C	2.30773200	-3.48288300	-0.31216100
N	1.32097100	-2.50585400	-0.41774500
N	3.13840200	-1.50152800	0.21115100
Cl	2.04728500	-5.14476000	-0.62523700
Cl	4.99991300	-3.51262400	0.36514800
C	-0.44170800	-2.70065200	-2.12266900
C	-0.06046300	-2.76263100	-0.76690200
C	-0.96290100	-3.07976400	0.26953500
C	-2.29912300	-3.29951100	-0.08786700
C	-2.71192900	-3.22071100	-1.41535900
C	-1.79126100	-2.93204300	-2.41915200
H	-3.02339400	-3.54135200	0.68367200
H	-3.75335300	-3.39483200	-1.66976000
H	-2.12299200	-2.89085400	-3.45176100
C	4.78446100	0.26344600	-0.26593200
C	5.65839100	1.24169100	0.22635100
C	5.80753300	1.45442600	1.59394600
C	5.09171000	0.68221300	2.50506900
C	4.20547900	-0.31250100	2.07328700
C	4.06105900	-0.48913800	0.68108000
H	6.23227300	1.84176400	-0.47249100
H	6.48980600	2.22012300	1.95148200
H	5.22548700	0.85044200	3.56917700
C	0.54611800	-2.43785500	-3.25591800
H	1.51601000	-2.19233800	-2.81372900
C	0.12839200	-1.23765700	-4.12499200
H	0.88739100	-1.05152300	-4.89241600
H	-0.82083300	-1.42191900	-4.63932200
H	0.02191200	-0.33088600	-3.52429200
C	0.73668700	-3.70035900	-4.12210100
H	1.48196800	-3.51349300	-4.90256200
H	1.07496600	-4.55215600	-3.52475100
H	-0.19903900	-3.98560500	-4.61505000
C	-0.53915700	-3.22098500	1.72900900
H	0.53393600	-3.02100900	1.79605300
C	-1.24613500	-2.19737700	2.63672400
H	-1.04215900	-1.17317000	2.31180000
H	-2.33174800	-2.34196800	2.63633400
H	-0.89665100	-2.30443000	3.66919800
C	-0.76816000	-4.65900500	2.23680300
H	-0.39943900	-4.76008500	3.26300200
H	-1.83240500	-4.91703100	2.23865500
H	-0.24561200	-5.39022400	1.61286600
C	4.68163800	0.03007800	-1.77018500
C	3.46794300	-1.16241600	3.10549100
C	5.98140400	-0.59523500	-2.31773600
H	5.87968900	-0.80246100	-3.38835800
H	6.83137100	0.08347600	-2.18738700
H	6.22087600	-1.53455400	-1.81005100
C	4.45569700	-1.96751000	3.97401600
H	5.10694800	-2.59682400	3.36051600
H	5.09155500	-1.30585300	4.57135400
H	3.90745100	-2.61572000	4.66578800
C	4.32772500	1.31882900	-2.53593700
H	5.12891200	2.06240800	-2.46379900
H	4.18593100	1.09256000	-3.59823300
H	3.40845700	1.77277100	-2.15553800
H	3.87307400	-0.68379600	-1.95059100
Cu	0.96597700	0.41455600	-0.31211700
H	-2.42470100	0.57105200	1.66032300
C	2.53079800	-0.31530700	3.98717100
H	1.99733500	-0.95884500	4.69482400
H	3.08822700	0.42724400	4.56799100
H	1.78892000	0.21548000	3.38373200
H	2.84070600	-1.88324700	2.57371500
Si	-0.01137400	2.84495000	-1.47716300
H	0.61284100	1.36979600	-1.72110300
O	-1.39362700	3.76656900	-1.04038100
O	1.37819100	3.81459900	-1.36390000
C	1.55491600	5.00872400	-2.11328200
C	2.95957400	5.55222800	-1.88504000
H	0.81461400	5.76385900	-1.80703200
H	1.40156200	4.82430400	-3.18643800

H	3.11115700	6.47620000	-2.45392600
H	3.12406900	5.76932300	-0.82490600
H	3.71098600	4.82303700	-2.20461700
C	-2.18430700	4.56834300	-1.90068800
C	-3.23670700	5.31509400	-1.08798700
H	-2.68398800	3.95138200	-2.66132400
H	-1.56716300	5.29933300	-2.44485600
H	-3.85245500	5.94102900	-1.74369700
H	-3.89512400	4.61325600	-0.56640900
H	-2.76524100	5.96014400	-0.33981700
C	-0.37708800	2.73816700	-3.38335600
H	0.51813400	2.34611800	-3.88096600
H	-1.18178100	2.01156400	-3.56214700
H	-0.66674100	3.66821000	-3.88556600
C	-0.39886800	2.48613000	1.55414800
H	-0.15037200	1.58307800	2.13296400
C	-1.91949600	2.67805800	1.67007600
H	-2.21696600	3.57997500	1.13464800
H	-2.15751000	2.82827300	2.73091300
50			
C	-1.84370800	6.86233200	0.31946700
C	-2.06343700	5.52616400	-0.40117000
H	-2.63263800	7.56841500	0.02225700
H	-1.96236800	6.71365300	1.40245600
C	-3.43547700	4.89836400	-0.12350200
H	-1.94499900	5.67458400	-1.48416000
H	-1.27542500	4.81951700	-0.10386800
H	-3.55231600	4.74803800	0.95943800
H	-4.22403700	5.60596500	-0.41832000
C	-3.65812500	3.56368600	-0.84581000
C	-5.03180400	2.93967100	-0.56717900
H	-2.87107800	2.85533600	-0.55070800
H	-3.54113500	3.71346400	-1.92870000
H	-5.14949900	2.78945700	0.51583700
H	-5.81901000	3.64952800	-0.86052500
C	-0.47235900	7.49181400	0.04315000
C	-0.25338100	8.82875600	0.76268300
H	-0.35210000	7.64029900	-1.03978800
H	0.31729900	6.78716400	0.34162600
C	1.11904800	9.44957200	0.48172900
H	-1.04161800	9.53334500	0.46373000
H	-0.37361500	8.68062200	1.84466000
H	1.24489400	10.40143000	1.00860400
H	1.92795600	8.78246100	0.80170500
H	1.25466300	9.64140700	-0.58904100
H	-4.48779900	0.88918400	-0.98311500
C	-5.25845100	1.60638100	-1.28989900
C	-8.34874300	-2.22518500	-2.50809600
C	-8.31723800	-0.76967900	-2.00075600
H	-8.04427500	-2.92628500	-1.72864200
H	-9.36135200	-2.49104100	-2.83146700
H	-7.67724100	-2.36137800	-3.36416300
C	-9.24844900	-0.63123300	-0.78251300
C	-8.82368300	0.14066500	-3.14082100
H	-9.32246300	0.40908000	-0.44847300
H	-10.25917200	-0.96714300	-1.04118600
H	-8.89334400	-1.22630700	0.06240600
H	-9.82590700	-0.17364600	-3.45149300
H	-8.89127900	1.19089200	-2.84104700
H	-8.17067400	0.08158000	-4.01958300
O	-6.20677500	-1.40213700	-0.87809300
C	3.44708200	-0.68681400	-0.05619300
C	5.57205100	-1.31397600	-0.55414600
C	5.48608000	-1.20187600	0.80027500
N	4.18024600	-0.81738200	1.08979400
N	4.31668600	-0.99606200	-1.06424500
Cl	6.69045100	-1.46138500	1.98632800
Cl	6.91398300	-1.75053000	-1.52032900
C	3.07911100	-1.65782600	3.11871700
C	3.65765100	-0.57953800	2.42002300
C	3.74833100	0.72132400	2.95482900
C	3.21947500	0.92579000	4.23540700
C	2.63418100	-0.11714700	4.94846900
C	2.56721100	-1.39305600	4.39538000
H	3.26530100	1.91584900	4.67836100
H	2.22969100	0.06506900	5.93982700
H	2.10906700	-2.19772800	4.96195900
C	3.47945300	-2.17257700	-3.05182400
C	3.13760700	-2.12791100	-4.40930700
C	3.28067000	-0.95818400	-5.15074900
C	3.77247300	0.19691800	-4.54876000
C	4.13064300	0.21260700	-3.19482200

C	3.96735500	-0.98525700	-2.47054100
H	2.75300600	-3.02173600	-4.89037300
H	3.00801800	-0.94693400	-6.20199000
H	3.87892600	1.10279500	-5.13737500
C	2.98645900	-3.06901200	2.54650000
H	3.46472600	-3.07403600	1.56300400
C	1.51901300	-3.49251300	2.33962000
H	1.47310700	-4.48925500	1.88828900
H	0.97708800	-3.53047800	3.29044500
H	0.99486300	-2.79320300	1.68056300
C	3.74116800	-4.08626300	3.42472100
H	3.70655600	-5.07930400	2.96458300
H	4.79135900	-3.80444400	3.54882900
H	3.29396100	-4.16636200	4.42102000
C	4.37772400	1.88951400	2.20209400
H	4.76222000	1.51713200	1.24851900
C	3.32979400	2.97184900	1.87712800
H	2.49977500	2.55622200	1.29695000
H	2.91615700	3.41278700	2.79033600
H	3.78635200	3.77816200	1.29324700
C	5.57321400	2.48389400	2.97197000
H	6.04144000	3.27978400	2.38340800
H	5.26109600	2.91810200	3.92750900
H	6.33166500	1.72280900	3.17978500
C	3.30347600	-3.47123400	-2.27093300
C	4.66132000	1.49884400	-2.56952000
C	4.13630800	-4.61710100	-2.87776900
H	4.03745300	-5.51923700	-2.26502800
H	3.80132800	-4.86595800	-3.89012600
H	5.19743200	-4.35455900	-2.92928200
C	5.94936100	1.97979800	-3.26597500
H	6.72599300	1.20911200	-3.24330600
H	5.76660800	2.24319200	-4.31300600
H	6.33903900	2.87106100	-2.76308600
C	1.81557700	-3.85909500	-2.16455900
H	1.38362000	-4.05587400	-3.15150100
H	1.70308700	-4.76702600	-1.56258900
H	1.23225200	-3.06120400	-1.69411300
H	3.66865100	-3.31201400	-1.25246100
Cu	1.58428600	-0.16592700	-0.21704500
H	-5.12265900	1.75147600	-2.37085400
C	3.58424100	2.60128700	-2.56522300
H	3.96427400	3.50011600	-2.06811700
H	3.29425900	2.87928400	-3.58401800
H	2.68405500	2.27167200	-2.03675400
H	4.91668000	1.29424200	-1.52605000
Si	-5.75160400	-1.67300000	0.67855700
H	0.12482000	0.25113900	-0.34592800
O	-6.96032900	-1.08811000	1.66657800
O	-5.57893000	-3.31274700	0.86512600
C	-6.59345300	-4.28532900	0.59861200
C	-6.24354300	-5.58312500	1.31042100
H	-6.66050100	-4.45188900	-0.48408300
H	-7.57163500	-3.91903000	0.93883500
H	-6.99832600	-6.34810900	1.10028000
H	-5.27116100	-5.95650100	0.97445900
H	-6.19770800	-5.43058900	2.39326600
C	-6.90217500	-1.15428700	3.09646000
C	-8.16878200	-0.54698200	3.67823500
H	-6.02053700	-0.60950000	3.46114400
H	-6.79960800	-2.19936200	3.41842900
H	-8.14091400	-0.58678900	4.77207700
H	-8.27077600	0.49898000	3.37313800
H	-9.05255400	-1.09345900	3.33484700
C	-4.08406200	-0.97471300	1.14391000
H	-3.75867000	-1.37822100	2.10839300
H	-3.32818600	-1.24234000	0.39900500
H	-4.10616900	0.11558500	1.22737000
C	-6.84257700	-0.38018500	-1.66479900
H	-6.30455100	-0.39785000	-2.62376600
C	-6.65362400	1.01305200	-1.04160200
H	-6.85751600	0.94730700	0.03368000
H	-7.39942400	1.70284900	-1.45137500

51

C	6.68587600	-0.11400600	0.38499000
C	5.45406800	0.22584500	-0.46305800
H	6.86363000	0.69602100	1.10693400
H	6.47644800	-1.01210500	0.98370200
C	4.18410700	0.45633100	0.36530000
H	5.66314000	1.12270900	-1.06361300
H	5.27495500	-0.58548000	-1.18313400
H	3.98009400	-0.43789900	0.97157400

H	4.36073000	1.27267400	1.08030300
C	2.94845500	0.78398500	-0.48189400
C	1.68011100	1.01613200	0.34854000
H	2.77029200	-0.03439200	-1.19411900
H	3.15148300	1.67638600	-1.09094600
H	1.48703900	0.13013100	0.97066100
H	1.85176500	1.84476700	1.05059000
C	7.95751700	-0.34280800	-0.44091200
C	9.18757400	-0.68660000	0.40815700
H	8.16997000	0.55596200	-1.03770400
H	7.78048500	-1.15146000	-1.16471700
C	10.45413700	-0.91208900	-0.42310800
H	9.36380400	0.12103500	1.13179600
H	8.97553500	-1.58538700	1.00323400
H	11.31315600	-1.15295300	0.21185300
H	10.32160500	-1.73856800	-1.13080000
H	10.71023000	-0.01881600	-1.00444100
H	0.25510900	0.48163600	-1.18498700
C	0.43884200	1.31748900	-0.49947400
C	-4.48722200	2.50024500	-0.76357200
C	-3.23878200	2.57197100	0.13751800
H	-4.88511900	1.48507900	-0.81490900
H	-5.27251600	3.15700400	-0.37351900
H	-4.25711400	2.82396900	-1.78552200
C	-3.59843900	2.08484600	1.55315400
C	-2.78414100	4.04614600	0.20087900
H	-2.76219000	2.21399900	2.24842100
H	-4.44381900	2.66106100	1.94582100
H	-3.87173700	1.02708000	1.55426100
H	-3.59931200	4.67170700	0.57979800
H	-1.92681500	4.19254400	0.86471500
H	-2.51095100	4.42300900	-0.79162100
O	-2.58467300	0.44030200	-0.93543600
H	0.63639400	2.19148600	-1.13572500
Si	-2.54440900	-1.13466800	-0.46897000
O	-2.80060800	-1.18575800	1.17610700
O	-3.76196100	-1.91499500	-1.28038200
C	-5.14502900	-1.54660900	-1.23649400
C	-5.99402000	-2.73274400	-1.66471800
H	-5.31312800	-0.69534800	-1.90806600
H	-5.42185000	-1.22846500	-0.22253500
H	-7.05482700	-2.46176600	-1.66244200
H	-5.72294200	-3.05561200	-2.67452400
H	-5.85158500	-3.57747600	-0.98374400
C	-2.81155600	-2.40714000	1.92698700
C	-3.19233100	-2.10614600	3.36696900
H	-1.81888800	-2.87559700	1.88808500
H	-3.52689300	-3.11296100	1.48426000
H	-3.19571300	-3.02694100	3.95912400
H	-2.47929300	-1.40864300	3.81664000
H	-4.18982500	-1.65928900	3.41757700
C	-0.99408000	-2.05781300	-0.94759000
H	-1.12320100	-3.13215600	-0.78116400
H	-0.76367000	-1.91075100	-2.00708800
H	-0.13006500	-1.73015000	-0.36239900
C	-2.09674600	1.72401900	-0.50670200
H	-1.83230400	2.24103000	-1.44048000
C	-0.81909500	1.59009400	0.33855300
H	-0.96834200	0.79515100	1.07938600
H	-0.65958000	2.50984900	0.91158200

52

S	-0.11180600	1.13438100	0.13907800
O	-1.31737200	1.70590300	1.23184800
O	0.02054900	1.66351200	-1.48518400
C	-0.63752700	1.14915700	-2.62444000
C	-0.04893500	1.79108600	-3.87653200
H	-1.71720400	1.35661600	-2.57942200
H	-0.53430400	0.05715000	-2.68578200
H	-0.54363200	1.40912000	-4.77711400
H	-0.17235800	2.87901200	-3.85307900
H	1.02183700	1.57518400	-3.95582900
C	-1.08532600	2.48000100	2.39620400
C	-2.18315500	2.20237100	3.41904800
H	-1.07790800	3.55177500	2.15377700
H	-0.10420900	2.25686700	2.83133800
H	-2.02614200	2.79965300	4.32470900
H	-3.16960000	2.45352300	3.01447900
H	-2.19228200	1.14455200	3.70397800
C	0.90006900	-0.35558600	0.77023600
H	1.48856200	-0.77815100	-0.05515100
H	1.60674400	-0.07097800	1.55422500
H	0.25930900	-1.16045400	1.14530100

N	-4.45456400	-1.07551800	0.27753200	C	-7.80354600	-3.14960900	0.39616400
C	-3.42591200	-1.66257300	1.25943400	H	-9.38167900	-4.62349600	0.11336200
C	-3.50031900	-3.14781600	1.61084900	H	-8.36669200	-4.38004000	-1.31465900
H	-3.56367200	-1.08914700	2.17929500	H	-7.75012600	-5.30466500	0.06192200
H	-2.45922400	-1.37775800	0.83915100	C	-6.36060700	-2.85948500	-0.05160100
C	-2.36685500	-3.49639200	2.59204000	H	-8.44871400	-2.30468500	0.12288800
H	-4.45828000	-3.38548200	2.08622900	H	-7.83692000	-3.22219600	1.49076200
H	-3.40972900	-3.78353900	0.72725400	C	-5.87626900	-1.54956700	0.57006100
C	-2.38962500	-4.96782000	3.01475700	H	-5.72564100	-3.70191900	0.23219200
H	-1.40078800	-3.26067500	2.12837700	H	-6.33859600	-2.78849300	-1.14411800
H	-2.44504600	-2.85755300	3.48111700	H	-6.53226900	-0.74932700	0.22643400
H	-1.57658400	-5.18747100	3.71331700	H	-5.95232800	-1.58667000	1.65997000
H	-3.33323400	-5.22441700	3.50901700	F	-1.38751000	0.00495800	-0.39217800
H	-2.27493900	-5.63090100	2.15026100	C	9.33739900	-1.93261800	0.30823800
C	-4.41032800	0.44449600	0.56922100	C	7.93151900	-1.59731200	-0.20561700
C	-5.13006000	1.36220100	-0.41793200	H	10.02302300	-1.11213500	0.05198100
H	-3.34905500	0.70146400	0.61524200	H	9.32070400	-1.98154900	1.40652700
H	-4.84503800	0.55143400	1.56671100	C	7.36692700	-0.28198800	0.34441700
C	-5.08508900	2.81059600	0.10075900	H	7.94908700	-1.55136300	-1.30403900
H	-4.64612000	1.32775100	-1.39858400	H	7.24774800	-2.41917100	0.05126300
H	-6.17709800	1.07197100	-0.56571000	H	7.35082700	-0.32535100	1.44298300
C	-5.72920100	3.80125000	-0.87280600	H	8.04649300	0.54224100	0.08379400
H	-5.59425700	2.86523500	1.07175900	C	5.95834100	0.03883600	-0.17130100
H	-4.04110400	3.09202200	0.28070900	C	5.37898800	1.35237000	0.36817600
H	-5.68782200	4.82134600	-0.47897800	H	5.28179300	-0.78741200	0.09058100
H	-5.21483100	3.79626700	-1.83989900	H	5.97572400	0.07685400	-1.27016500
H	-6.78175700	3.55514500	-1.05309300	H	5.36804000	1.31859500	1.46740000
C	-4.02380200	-1.25656700	-1.18304200	H	6.04910900	2.18213700	0.09867000
C	-3.47441200	-2.61178200	-1.62834000	C	9.89328600	-3.24879700	-0.24808700
H	-3.23195000	-0.52014100	-1.32042600	C	11.29846200	-3.59094400	0.26306000
H	-4.89152000	-0.97745800	-1.78415200	H	9.91033000	-3.19969900	-1.34646100
C	-3.18877400	-2.57284600	-3.13984900	H	9.20702700	-4.06921200	0.00717300
H	-2.53783800	-2.82150000	-1.10267800	C	11.84260600	-4.90777700	-0.29892800
H	-4.16349100	-3.43369000	-1.41978700	H	11.98525700	-2.77248900	0.00731900
C	-2.57994000	-3.88032900	-3.65394900	H	11.28164100	-3.64065400	1.36042800
H	-4.12043600	-2.36317200	-3.68170800	H	12.84640200	-5.12248900	0.08240200
H	-2.50893200	-1.73992500	-3.35874700	H	11.19642600	-5.75072300	-0.02811400
H	-2.38769200	-3.82761400	-4.72991000	H	11.90172300	-4.87639800	-1.39297100
H	-1.62909400	-4.09693900	-3.15515700	H	3.29820500	0.82437100	0.13680700
H	-3.25094400	-4.72800900	-3.47567300	C	3.96340300	1.64708200	-0.14456000
C	-8.35660300	-4.43732300	-0.22076100	C	0.01143700	4.83802300	-0.41808000

C	1.47628900	4.71123100	0.04179000
H	-0.63689100	4.17497700	0.15556200
H	-0.34238900	5.86970300	-0.29855700
H	-0.09049600	4.56415400	-1.47328800
C	1.59999700	5.20646000	1.49490600
C	2.33232700	5.60732700	-0.87793800
H	2.64398400	5.23037200	1.82642600
H	1.20122800	6.22343400	1.59567000
H	1.04584700	4.55359800	2.17417200
H	1.93606700	6.62988000	-0.89024100
H	3.37601100	5.66960800	-0.55451300
H	2.32241500	5.23826500	-1.91081900
O	1.06687400	2.35210200	0.63750800
H	3.97697900	1.66835900	-1.24455300
C	1.92120000	3.20938000	-0.08743900
H	1.86333200	2.97370200	-1.15974200
C	3.37594700	2.96472000	0.37322600
H	3.39544000	2.96649100	1.47077700
H	4.02648000	3.78606300	0.04750700

TS19

Si	-0.31586800	-0.55994300	0.40867500
O	-1.17057000	0.36338100	1.49400800
O	-0.60362000	-0.15837000	-1.17712400
C	0.42546900	0.11281900	-2.13919400
C	-0.16546800	0.87966900	-3.31054400
H	0.84237000	-0.84099200	-2.49484500
H	1.21438300	0.68147200	-1.64436500
H	0.61014400	1.08648800	-4.05584600
H	-0.96289800	0.30921600	-3.79926100
H	-0.58160300	1.83432200	-2.97521400
C	-0.59834400	1.07493600	2.60494400
C	-0.59546000	0.22000200	3.86614300
H	-1.22109000	1.96448900	2.76114800
H	0.40127300	1.40761600	2.31174900
H	-0.21546600	0.80130400	4.71413800
H	-1.60418800	-0.12720400	4.11520600
H	0.04666800	-0.65872600	3.74597000
C	1.30709400	-1.30763000	0.92974500
H	1.76417400	-1.82514600	0.07894900
H	1.97306300	-0.50646400	1.24693700
H	1.15202600	-2.04462000	1.72461400
N	-4.88272000	-0.29947300	0.18973800
C	-4.35678500	-1.19020900	1.32836700
C	-4.99737400	-2.55878200	1.55572300
H	-4.49145500	-0.59429000	2.23388000
H	-3.28591300	-1.28631300	1.14817100
C	-4.23475000	-3.28668900	2.67732400
H	-6.04768900	-2.45302000	1.84858100
H	-4.96962100	-3.17657100	0.65606500
C	-4.83087200	-4.66046300	2.99536100
H	-3.18479500	-3.39551200	2.37953600
H	-4.23686100	-2.66674500	3.58334300
H	-4.26735500	-5.15772100	3.79062100
H	-5.87177800	-4.57507700	3.32666000
H	-4.81349800	-5.31340900	2.11582200
C	-4.42076600	1.12339900	0.58145500
C	-4.56476300	2.21859500	-0.47464900
H	-3.37328300	1.01700000	0.87645200
H	-5.00769700	1.37568100	1.46840700
C	-4.23927500	3.58810100	0.14759800
H	-3.88232800	2.04015800	-1.31081500
H	-5.57905900	2.25424300	-0.88842700
C	-4.33192800	4.72693900	-0.87155100
H	-4.92707300	3.78192300	0.98068500
H	-3.22947600	3.56151200	0.57393300
H	-4.10054800	5.68913800	-0.40479700
H	-3.62607700	4.57778300	-1.69555900
H	-5.33783600	4.79680100	-1.30059000
C	-4.22457600	-0.63012000	-1.15608500
C	-4.04489000	-2.09707500	-1.54735900
H	-3.23325300	-0.17455700	-1.11380800
H	-4.81011500	-0.09767800	-1.90824600
C	-3.42250600	-2.17326900	-2.95258800
H	-3.36600900	-2.58240500	-0.84140900
H	-4.99007200	-2.64477500	-1.54636400
C	-3.18533100	-3.61649200	-3.40638900
H	-4.07712500	-1.66450400	-3.67265900
H	-2.47198900	-1.62699000	-2.94904000
H	-2.73872800	-3.64494100	-4.40504100
H	-2.50760600	-4.13915600	-2.72285800
H	-4.12327600	-4.18179100	-3.44391600
C	-9.46421700	-2.16691200	-1.33993400

C	-8.66562200	-1.13232000	-0.54206800
H	-10.53951400	-1.98749900	-1.24730100
H	-9.20953800	-2.12937700	-2.40464600
H	-9.26315400	-3.18330500	-0.98437100
C	-7.14686000	-1.35461000	-0.64865300
H	-8.91287600	-0.12368600	-0.89732100
H	-8.96586600	-1.17054900	0.51290900
C	-6.41194500	-0.27255000	0.14179000
H	-6.90771000	-2.35559300	-0.28326400
H	-6.85840200	-1.31427100	-1.70416500
H	-6.67928800	0.69634500	-0.28025900
H	-6.73110200	-0.27140300	1.18717500
F	-1.32618500	-1.89145800	0.45194700
C	10.21550600	-1.13405500	0.04737700
C	8.74377100	-1.10588500	-0.38327900
H	10.72956800	-0.25085000	-0.35837400
H	10.27396600	-1.04181100	1.14151600
C	7.99154200	0.15032700	0.07308600
H	8.68505900	-1.18731200	-1.47826600
H	8.23381300	-1.99553300	0.01353100
H	8.05280900	0.22975700	1.16816500
H	8.49935000	1.04160300	-0.32304200
C	6.51807400	0.17460200	-0.35206900
C	5.75253000	1.41315000	0.13126000
H	6.01768800	-0.72762000	0.02847500
H	6.45644500	0.11314800	-1.44842200
H	5.82229500	1.47205300	1.22761300
H	6.25033900	2.31754600	-0.24932600
C	10.96113800	-2.39967400	-0.39269700
C	12.43237100	-2.42919800	0.03940000
H	10.90418200	-2.49401700	-1.48681400
H	10.44754700	-3.28286200	0.01393000
C	13.16752200	-3.69968800	-0.39836300
H	12.94698200	-1.54923800	-0.37026400
H	12.48965300	-2.33182500	1.13223600
H	14.21303200	-3.69065600	-0.07277600
H	12.69551000	-4.59477900	0.02287800
H	13.15991700	-3.80584500	-1.48929300
H	3.78527800	0.51422800	0.08181900
C	4.27489400	1.42493600	-0.28063100
C	-0.23479000	3.79646100	-0.20185000
C	1.24892400	3.95939900	0.17093800
H	-0.66301600	2.94244900	0.32568000
H	-0.80774100	4.70170800	0.03999200
H	-0.34666900	3.61476200	-1.27886600
C	1.35162800	4.33576900	1.66010900
C	1.83347400	5.10522700	-0.67876700
H	2.38357300	4.56176400	1.95084100
H	0.74774600	5.22491100	1.88522800
H	0.99679800	3.51716600	2.29160800
H	1.22872000	6.01620900	-0.57871500
H	2.85628300	5.36312200	-0.38472200
H	1.85097900	4.83747100	-1.74286400
O	1.37507200	1.48803000	0.43211600
H	4.20793300	1.39323900	-1.37949700
C	1.97608000	2.57803600	-0.13447100
H	1.96340900	2.53810800	-1.26214800
C	3.48895600	2.63265000	0.23850300
H	3.56875200	2.65953700	1.33461200
H	3.96400600	3.55031700	-0.13833500

53

N	2.80905900	-1.29050300	-0.29718900
C	1.84421900	-0.91589400	-1.43484800
C	0.79736700	-1.93865800	-1.87414000
H	2.49468900	-0.71623500	-2.29120500
H	1.42050600	0.04565500	-1.11109400
C	-0.06942900	-1.33814400	-2.99515600
H	1.27762500	-2.84740300	-2.25566400
H	0.14664700	-2.24050900	-1.05069700
C	-1.12106100	-2.32269300	-3.51403300
H	-0.56313800	-0.43166100	-2.62385800
H	0.57520100	-1.01862400	-3.82432600
H	-1.72468400	-1.87216900	-4.30794800
H	-0.65285300	-3.22553900	-3.92198000
H	-1.80128800	-2.63387600	-2.71346400
C	3.96463000	-0.27307900	-0.46249100
C	4.99591900	-0.20945500	0.66417400
H	3.45315300	0.69522300	-0.54880300
H	4.44757600	-0.54573900	-1.40526500
C	6.20631800	0.62906900	0.21847700
H	4.55084500	0.25391400	1.55019400
H	5.35345900	-1.20165300	0.96557000

C	7.24400300	0.79969400	1.33126000
H	6.67526200	0.15488300	-0.65358600
H	5.86057300	1.61517900	-0.11463600
H	8.09803300	1.39060200	0.98592800
H	6.81306600	1.31129900	2.19866500
H	7.62462100	-0.16996000	1.67161300
C	2.19202200	-1.01159600	1.08104800
C	0.78784000	-1.53390700	1.38703400
H	2.14940000	0.08786700	1.11397900
H	2.90920200	-1.40129300	1.80704800
C	0.43591600	-1.19974700	2.84697600
H	0.06078200	-1.03919900	0.73629400
H	0.68655400	-2.61145900	1.23596400
C	-0.98424900	-1.63233200	3.22235600
H	1.15737800	-1.68592200	3.51710700
H	0.54532500	-0.11977200	3.00460400
H	-1.20827700	-1.38837000	4.26555600
H	-1.72863500	-1.12939300	2.59534600
H	-1.11730700	-2.71281500	3.09629000
C	2.75982000	-6.43100300	0.33391900
C	3.42761000	-5.18134000	-0.24673600
H	3.32210600	-7.33332500	0.07504200
H	2.69976000	-6.37659100	1.42640900
H	1.74077000	-6.55084000	-0.04993800
C	2.66198300	-3.89183700	0.09520600
H	4.45608300	-5.10643600	0.12996900
H	3.50565300	-5.27942500	-1.33728100
C	3.40505300	-2.68267500	-0.47273800
H	1.64611500	-3.96545200	-0.29966100
H	2.58327800	-3.80620700	1.18403000
H	4.39096700	-2.64860200	-0.00859800
H	3.55999800	-2.79776400	-1.54910700
C	-7.32449000	0.41583500	-0.19059500
C	-5.92414400	0.38557600	0.43424100
H	-7.70920100	1.44557800	-0.16689000
H	-7.25302500	0.14422900	-1.25365000
C	-4.92354800	1.32349900	-0.25219600
H	-5.99703300	0.65090500	1.49874900
H	-5.53661500	-0.64312500	0.40508500
H	-4.85268700	1.06154800	-1.31779100
H	-5.31126800	2.35193500	-0.21943100
C	-3.52219500	1.29299200	0.37059500
C	-2.52409400	2.24543600	-0.30043800
H	-3.12916100	0.26641800	0.32684800
H	-3.59635000	1.54198100	1.43916100
H	-2.45668200	2.00299900	-1.37151100
H	-2.91877400	3.27123300	-0.25060800
C	-8.32775900	-0.51388900	0.50261000
C	-9.72803300	-0.48319300	-0.12228900
H	-8.40071600	-0.24170700	1.56547800
H	-7.94453000	-1.54440200	0.48002900
C	-10.72427600	-1.41270500	0.57747700
H	-10.11054600	0.54642200	-0.10013800
H	-9.65581100	-0.75657200	-1.18387800
H	-11.71305600	-1.36690700	0.10913600
H	-10.38660600	-2.45487700	0.54042800
H	-10.84334300	-1.14245500	1.63305800
H	-0.70562400	1.19446500	0.23963100
C	-1.12112100	2.20593000	0.31714300
C	3.61641900	3.99388700	0.53316600
C	2.29269000	4.16133300	-0.23450700
H	3.99250500	2.97596100	0.40901100
H	4.37912900	4.70250800	0.18515800
H	3.46870500	4.16545800	1.60752300
C	2.56486400	4.01338000	-1.74040600
C	1.74182800	5.56824400	0.06409100
H	1.67233600	4.23639300	-2.33684100
H	3.36162500	4.68971000	-2.07611600
H	2.86378000	2.98331100	-1.95495900
H	2.50526000	6.33589900	-0.11852100
H	0.87662900	5.81881300	-0.55827700
H	1.43420500	5.65565500	1.11433700
O	1.80856900	1.75971100	0.03683500
H	-1.19685700	2.42465200	1.39382900
C	1.31260500	3.01381700	0.26211000
H	1.19588900	3.24189800	1.36089900
C	-0.12252300	3.17569600	-0.32029100
H	-0.08072100	2.98522300	-1.40257400
H	-0.49697200	4.20083400	-0.19013600

4a

C	4.96845900	0.45690300	0.18627600
C	3.69976800	-0.31926600	-0.18812800

H	4.96836000	1.42492500	-0.33494300
H	4.94646000	0.69124100	1.26031100
C	2.40134100	0.42585300	0.14528800
H	3.71978000	-0.54913800	-1.26310500
H	3.70291700	-1.28951200	0.32885300
H	2.37941500	0.65145800	1.22118100
H	2.39860400	1.39799200	-0.36815000
C	1.13469000	-0.35081600	-0.23483300
C	-0.16613600	0.38513900	0.10979400
H	1.14203100	-1.32664100	0.27136500
H	1.15309600	-0.56885300	-1.31225400
H	-0.18622800	0.59778300	1.18847700
H	-0.17381200	1.36363900	-0.39151900
C	6.26542300	-0.29334000	-0.14040900
C	7.53550300	0.48195500	0.23112600
H	6.28767200	-0.52993600	-1.21403100
H	6.26683400	-1.26055700	0.38252600
C	8.82516200	-0.27739200	-0.09529900
H	7.53613400	1.44710600	-0.29354900
H	7.51272400	0.71990100	1.30342200
H	9.71263100	0.30065200	0.18283200
H	8.86829800	-1.23222300	0.44115100
H	8.89412000	-0.49811600	-1.16672600
H	-1.41804500	-1.37796800	0.21110900
C	-1.42741000	-0.39633500	-0.27682300
C	-6.47781300	-0.65595500	-0.57232200
C	-5.35231200	0.25816500	-0.04694800
H	-6.45496400	-1.62872700	-0.07517200
H	-7.45882800	-0.20014000	-0.39945900
H	-6.37342100	-0.82666400	-1.65035600
C	-5.58683300	0.53293300	1.45147300
C	-5.39420900	1.58776300	-0.82589400
H	-4.83193600	1.20602500	1.87060100
H	-6.56476100	1.00229900	1.60222900
H	-5.58141700	-0.39419800	2.03529200
H	-6.40035400	2.01896800	-0.78265900
H	-4.70241300	2.33044400	-0.41715400
H	-5.14430000	1.43814900	-1.88303200
H	-1.41483400	-0.59437100	-1.35821700
C	-2.72964400	0.33119400	0.08503800
H	-2.73780000	0.54431200	1.16385500
H	-2.74972500	1.30420500	-0.41855500
C	-3.98933600	-0.46530700	-0.28916400
H	-3.93994200	-0.69114700	-1.36351800
O	-3.96690900	-1.75794300	0.33809800
H	-3.86095100	-1.61632800	1.28935400

55

C	8.45121000	-1.04153500	0.63272200
C	7.25404300	-0.42934600	-0.10573300
H	9.20793000	-0.26266600	0.80508100
H	8.12958800	-1.37707200	1.62914800
C	6.60102500	0.74064100	0.64118500
H	7.57651100	-0.09008700	-1.10064400
H	6.50040800	-1.21072500	-0.28249400
H	6.27588000	0.40024600	1.63471700
H	7.35362800	1.52217600	0.81947700
C	5.40465200	1.34813100	-0.10245700
C	4.73879300	2.51036700	0.64514500
H	4.65545200	0.56490900	-0.28573500
H	5.73204500	1.69464900	-1.09334000
H	4.40061000	2.16016000	1.63081700
H	5.48595100	3.29339700	0.83989600
C	9.09558900	-2.21679700	-0.11319300
C	10.29200800	-2.83204000	0.62408300
H	9.41827700	-1.88187500	-1.10964200
H	8.33859500	-2.99554000	-0.28633600
C	10.92645200	-4.00704400	-0.12721000
H	11.04963300	-2.05498200	0.79514000
H	9.96973900	-3.16548100	1.62006200
H	11.77644200	-4.42345500	0.42363700
H	10.20196500	-4.81505300	-0.28194600
H	11.28917300	-3.69635400	-1.11389800
H	2.81079600	2.33028300	-0.32396000
C	3.55071500	3.11080200	-0.11664000
C	2.87016000	4.25288400	0.64126800
H	2.50276200	3.89272700	1.61313300
C	-0.27591300	6.44225300	-0.20082800
C	1.12781300	6.21902500	0.38508000
H	-0.97999500	5.68826600	0.16458800
H	-0.64971500	7.42928800	0.09095100
H	-0.26139700	6.38337900	-1.29150200
C	1.06995300	6.29485800	1.92539700

C	2.08656100	7.31139200	-0.15337100
H	2.05922200	6.20477500	2.38309500
H	0.65311500	7.26112500	2.22908300
H	0.42880400	5.50950800	2.33964600
H	1.71560400	8.30006700	0.13738900
H	3.09934000	7.20515200	0.24760200
H	2.14582300	7.28083700	-1.24627700
C	1.67492600	4.85421500	-0.08978000
O	1.17517100	4.27889600	-1.04529600
H	3.88728300	3.47668900	-1.09545000
H	3.58911000	5.04593900	0.88271000
C	-2.08077000	-0.70324100	0.11097600
C	-3.53206200	-2.11308400	-0.92060700
C	-2.27898400	-2.61470800	-1.09899200
N	-1.40119900	-1.74045900	-0.46429900
N	-3.39496600	-0.94389400	-0.17861700
Cl	-1.78994500	-4.03357600	-1.91934200
Cl	-5.03150600	-2.72756700	-1.46772600
C	0.59250300	-2.60362400	0.68200000
C	0.03742800	-1.90495600	-0.40933100
C	0.81751200	-1.36719000	-1.45247300
C	2.20509200	-1.54143300	-1.36974700
C	2.78457500	-2.21909600	-0.30035900
C	1.98571500	-2.74238500	0.71283600
H	2.83868900	-1.14025200	-2.15444200
H	3.86288900	-2.34246900	-0.25807900
H	2.44925000	-3.26898200	1.54112700
C	-5.10387100	-0.37486900	1.49095400
C	-6.15053600	0.46619700	1.88910400
C	-6.56759900	1.52627400	1.08858100
C	-5.94633200	1.76735700	-0.13381200
C	-4.89461400	0.95967800	-0.58501100
C	-4.49079200	-0.09943100	0.25213800
H	-6.64330000	0.28883500	2.83994100
H	-7.38057700	2.16653000	1.41834000
H	-6.28143800	2.59701200	-0.74849000
C	-0.24897200	-3.19796000	1.80736600
H	-1.30389000	-3.02416200	1.57717700
C	0.04400100	-2.50088700	3.15043700
H	-0.60246800	-2.90597400	3.93624400
H	1.08333900	-2.65343500	3.46029600
H	-0.13319600	-1.42274300	3.08223600
C	-0.05367500	-4.72287400	1.91686100
H	-0.71045700	-5.13148900	2.69196500
H	-0.28810400	-5.22412700	0.97266500
H	0.97637600	-4.97781700	2.18702100
C	0.22116200	-0.62389200	-2.64392600
H	-0.86446800	-0.58836600	-2.51710800
C	0.72068500	0.83215500	-2.71122400
H	0.49902000	1.38161300	-1.79184800
H	1.80285900	0.87522700	-2.87400700
H	0.23988900	1.35591900	-3.54428900
C	0.50368200	-1.36472100	-3.96641300
H	0.01884800	-0.84565900	-4.79985800
H	1.57718000	-1.40492800	-4.17935500
H	0.12700400	-2.39167900	-3.93910300
C	-4.67473300	-1.52522400	2.39651100
C	-4.23666600	1.25756100	-1.92835500
C	-5.82514500	-2.52497400	2.62572200
H	-5.47500000	-3.36972800	3.22807900
H	-6.66082600	-2.06056100	3.15968600
H	-6.20716700	-2.91725300	1.67817100
C	-5.25119900	1.18628800	-3.08615100
H	-5.74879100	0.21212400	-3.12161800
H	-6.02407500	1.95621200	-2.99177000
H	-4.74181100	1.34372400	-4.04259000
C	-4.11418100	-1.00441200	3.73439500
H	-4.87710900	-0.46217900	4.30309000
H	-3.76913800	-1.84102800	4.35133900
H	-3.26934300	-0.32755700	3.57207300
H	-3.86721100	-2.07090600	1.90025600
Cu	-1.36141600	0.76569100	1.15638700
H	-0.80954500	1.90169700	2.00916100
C	-3.51308800	2.61813900	-1.90288700
H	-3.00722200	2.79606800	-2.85763400
H	-4.21723800	3.44066900	-1.73798000
H	-2.76275400	2.65133300	-1.10671900
H	-3.47801900	0.49276400	-2.11676800

TS20

C	8.62350000	0.80060600	0.16376500
C	7.14861100	0.53074100	-0.16053100
H	8.94790600	1.71335000	-0.35639000

H	8.72626900	1.01128200	1.23803900	H	2.22159400	2.05391300	-1.12982800
C	6.21105500	1.68379300	0.22038100	H	1.73061600	4.33592800	-0.25878600
H	7.04680400	0.32163500	-1.23524000	C	-1.63116500	-0.60161100	0.04808800
H	6.82570800	-0.38380500	0.35783200	C	-3.11936800	-2.28867700	-0.29349300
H	6.30909900	1.89015100	1.29598800	C	-1.88167400	-2.84618700	-0.22711100
H	6.53529800	2.59956600	-0.29467200	N	-0.97945800	-1.80484600	-0.01929700
C	4.73856800	1.40940400	-0.11101000	N	-2.95418300	-0.91568000	-0.12320200
C	3.79568800	2.55694000	0.27147800	Cl	-1.42788000	-4.49065800	-0.36020300
H	4.41548300	0.49157100	0.39925800	Cl	-4.63453900	-3.04597700	-0.53492800
H	4.64145000	1.20651000	-1.18733000	C	1.01063200	-2.17684300	1.37182100
H	3.89417700	2.76302900	1.34718900	C	0.45351700	-1.97233400	0.09301500
H	4.11700100	3.47439200	-0.24294000	C	1.22706600	-1.94497000	-1.08531400
C	9.55636500	-0.35631100	-0.21610700	C	2.60989800	-2.11966700	-0.94827900
C	11.03251000	-0.08851000	0.10415700	C	3.19114700	-2.31767500	0.30158500
H	9.45263300	-0.56858800	-1.29012300	C	2.39912600	-2.34538600	1.44654100
H	9.23346100	-1.26911200	0.30530200	H	3.23888100	-2.10198500	-1.83268200
C	11.95513900	-1.25046900	-0.27845700	H	4.26549600	-2.45503900	0.38298800
H	11.35588400	0.82256200	-0.41773900	H	2.86446300	-2.50506500	2.41429000
H	11.13687000	0.12349400	1.17709800	C	-4.67750000	0.35663200	1.07913900
H	13.00031500	-1.02919100	-0.03760600	C	-5.71370400	1.29804400	1.03561100
H	11.67788900	-2.16767400	0.25405300	C	-6.09379600	1.89735900	-0.16250200
H	11.89897600	-1.46325800	-1.35238100	C	-5.44439700	1.56495300	-1.34843900
H	1.98989600	1.37748900	0.47404800	C	-4.39916400	0.63241500	-1.36699500
C	2.32377100	2.27720800	-0.06240400	C	-4.03213700	0.05019800	-0.13645700
C	1.40673500	3.44469600	0.30077200	H	-6.23203400	1.56043100	1.95259000
H	1.51386600	3.68883600	1.36132700	H	-6.90186300	2.62310100	-0.17250500
C	-2.50047000	3.94571100	0.26845000	H	-5.75297000	2.03459800	-2.27723700
C	-1.03846900	4.41091400	0.34615300	C	0.17391000	-2.23804600	2.64610600
H	-2.70641200	3.18111500	1.02516100	H	-0.87243700	-2.07015500	2.37684900
H	-3.17554300	4.79011100	0.44798100	C	0.56854800	-1.12639400	3.63763800
H	-2.72838700	3.52464500	-0.71288000	H	-0.07713900	-1.16443400	4.52154800
C	-0.75897100	4.98308600	1.74619800	H	1.60372600	-1.23946200	3.97713700
C	-0.82542300	5.52404700	-0.71240100	H	0.46478700	-0.13792700	3.18015700
H	0.22162000	5.46417100	1.81049100	C	0.26108700	-3.62818900	3.30716300
H	-1.51106200	5.74048900	1.99417100	H	-0.38780500	-3.66804400	4.18845900
H	-0.80639100	4.19784400	2.50795200	H	-0.05099200	-4.41909900	2.61819800
H	-1.51188800	6.35565400	-0.51891300	H	1.28191400	-3.85138400	3.63517400
H	0.19303200	5.92483500	-0.68855300	C	0.62553600	-1.74401100	-2.47346200
H	-1.02210800	5.14412200	-1.71893200	H	-0.46108700	-1.67748200	-2.37033100
C	-0.07678300	3.24008300	-0.04446000	C	1.10177400	-0.42302500	-3.10947000
O	-0.35428200	2.59090200	-1.11952100	H	0.82732700	0.43833200	-2.49359100

H	2.18910100	-0.41694200	-3.24342600
H	0.64491500	-0.29687800	-4.09721900
C	0.92196500	-2.94348700	-3.39526800
H	0.42162900	-2.80850100	-4.35989800
H	1.99477600	-3.04519700	-3.59027200
H	0.56894000	-3.88183600	-2.95652300
C	-4.30641300	-0.29514900	2.40835200
C	-3.72509200	0.28190000	-2.69043200
C	-5.48878800	-1.09645500	2.98934000
H	-5.18439500	-1.60089800	3.91243300
H	-6.33460700	-0.44387000	3.23055300
H	-5.84099500	-1.85682100	2.28561700
C	-4.72582100	-0.35792200	-3.67384200
H	-5.19784500	-1.24730700	-3.24483600
H	-5.51979800	0.34455800	-3.94917600
H	-4.21155600	-0.65518000	-4.59386500
C	-3.78831800	0.74149100	3.42373900
H	-4.55641800	1.48379900	3.66551500
H	-3.50033700	0.24405300	4.35610400
H	-2.91269300	1.26900700	3.03394400
H	-3.49192600	-1.00214700	2.22827400
Cu	-0.88262800	1.12338200	0.38095100
H	-0.39841500	2.25464400	1.39109400
C	-3.03404200	1.50767600	-3.32011600
H	-2.53617400	1.21630200	-4.25163500
H	-3.76065000	2.28988200	-3.56643700
H	-2.28300400	1.93266500	-2.64774400
H	-2.94574400	-0.45906600	-2.49148000

56

C	8.63796900	-0.26056600	-0.33117300
C	7.14697200	-0.20274500	0.02515500
H	8.75049200	-0.22939400	-1.42448000
H	9.13756700	0.64152600	0.05041900
C	6.42920700	1.03673500	-0.52478500
H	6.64895800	-1.10670300	-0.35434000
H	7.03437200	-0.23167400	1.11859700
H	6.92416800	1.94143400	-0.14321000
H	6.54435600	1.06670000	-1.61786600
C	4.93696800	1.08809300	-0.17245200
C	4.21091700	2.32130600	-0.72590300
H	4.82231400	1.06033900	0.92093200
H	4.44501200	0.18061800	-0.55142800
H	4.69882400	3.23011300	-0.34387800
H	4.33122000	2.35054400	-1.81867100
C	9.35240100	-1.50327200	0.21513300
C	10.84290700	-1.56340000	-0.14301100
H	8.85273900	-2.40590400	-0.16557400
H	9.24194300	-1.53487300	1.30880400
C	11.54755300	-2.80893600	0.40464600
H	10.95306000	-1.53105200	-1.23559800
H	11.34291300	-0.66269800	0.23879700
H	12.60839200	-2.82218700	0.13292900
H	11.48363200	-2.85101800	1.49823500
H	11.09211900	-3.72578300	0.01263300
H	2.59698500	2.33511000	0.71196700
C	2.71590800	2.35817100	-0.38209600
C	1.98524300	3.58386600	-0.94177800
H	2.46935300	4.48709200	-0.54874900
C	-1.70565100	4.87388700	-0.56733700
C	-0.22824400	4.95880500	-0.99688600
H	-1.78999700	4.70873900	0.51434600
H	-2.23542300	5.80492800	-0.80357100
H	-2.21060600	4.04882100	-1.07472500
C	0.41763000	6.14350400	-0.24983100
C	-0.16476400	5.20799300	-2.51512200
H	1.43595400	6.34919600	-0.59391700
H	-0.16813800	7.05785100	-0.40325800
H	0.45949700	5.95675300	0.83063200
H	-0.74362500	6.09920900	-2.78674300
H	0.86312600	5.36788900	-2.85847600
H	-0.57476300	4.35344500	-3.06092700
C	0.47451900	3.60400800	-0.61359400
O	-0.16363600	2.52117700	-1.23942100
H	2.23227600	1.45119500	-0.76382900
H	2.10788600	3.60742700	-2.03299900
C	-1.76049600	-0.51889300	0.11396500
C	-2.83597400	-2.51967200	0.11062900
C	-2.66134800	-2.15254600	1.40919200
N	-2.00097900	-0.92661000	1.39801700
N	-2.28069600	-1.51152700	-0.67229200
Cl	-3.12792300	-2.97172700	2.83609200
Cl	-3.57653400	-3.92365900	-0.52590100

C	-2.52808200	0.77357700	3.09026400	H	-6.68400300	-0.61138600	-1.90464500
C	-1.62197600	-0.17656100	2.57746000	H	-6.07161300	-0.95103800	-3.52837300
C	-0.36791100	-0.43664700	3.16615100	H	-5.77789600	-2.10285800	-2.21679100
C	-0.02070100	0.31830600	4.29375200	C	0.13820500	-4.22695000	-2.37833200
C	-0.88619600	1.27704100	4.81391800	H	-0.78928900	-4.76447500	-2.15838200
C	-2.12642500	1.49687600	4.22053700	H	0.37202400	-4.37816400	-3.43749500
H	0.93966700	0.15103800	4.77141000	H	0.94346900	-4.68196800	-1.79211600
H	-0.59552300	1.85072300	5.68915200	C	-4.65566000	1.20898700	-2.40397800
H	-2.79623200	2.23985300	4.64220900	H	-4.83212400	1.39193800	-3.46921500
C	-3.33614600	-0.91600300	-2.80937600	H	-5.49515200	1.64008000	-1.84824900
C	-3.27970700	-0.91472700	-4.20880200	H	-3.74393100	1.74157400	-2.11639700
C	-2.20019300	-1.47372700	-4.88744200	H	-4.39346300	-0.39971100	-1.02384100
C	-1.15028800	-2.05099400	-4.17837400	Cu	-0.92241500	1.05307300	-0.48782500
C	-1.15146200	-2.08229600	-2.77822500	H	0.38934500	3.53849600	0.49069800
C	-2.25493100	-1.50204700	-2.12074700	C	1.33742000	-1.98686300	-2.31377000
H	-4.09283000	-0.46883300	-4.77305100	H	2.15059200	-2.43769700	-1.73491900
H	-2.17758000	-1.46040700	-5.97320000	H	1.61215700	-2.04026400	-3.37253500
H	-0.31476000	-2.48462200	-4.71883900	H	1.26448900	-0.93049500	-2.03739300
C	-3.90561200	1.02571000	2.48448800	H	-0.17718300	-2.65505300	-0.96331300
H	-4.01970000	0.38094300	1.60868800	57			
C	-4.05602400	2.47954800	1.99796700	C	8.42828700	-2.06578200	-0.83163300
H	-5.03606600	2.62017900	1.52981000	C	7.49040900	-0.88379500	-0.55378700
H	-3.97892300	3.19079500	2.82723200	H	7.90580700	-3.00541800	-0.60048800
H	-3.28656400	2.73259600	1.26269700	H	8.65728200	-2.10310200	-1.90643400
C	-5.02660400	0.65283300	3.47523500	C	6.17034600	-0.94359200	-1.33251400
H	-6.00623400	0.79030700	3.00549600	H	7.27212900	-0.84132400	0.52311700
H	-4.94546600	-0.39035600	3.79571800	H	8.01043900	0.05488000	-0.79369300
H	-4.99472100	1.28340400	4.37006000	H	6.38506400	-0.98508100	-2.41017500
C	0.59706000	-1.49398600	2.63850900	H	5.64950700	-1.88166300	-1.09104900
H	0.13955000	-1.97300400	1.76824800	C	5.23869900	0.24118300	-1.04553000
C	1.92264300	-0.86709800	2.16664700	C	3.90568400	0.18598900	-1.80245700
H	1.75246700	-0.11184100	1.39415200	H	5.75807600	1.17766100	-1.29590300
H	2.45593700	-0.38917600	2.99538000	H	5.03655900	0.28762700	0.03429200
H	2.57801300	-1.64009900	1.75136200	H	4.10402600	0.14011900	-2.88383500
C	0.84903200	-2.59662900	3.68620700	H	3.38668500	-0.75064100	-1.55048800
H	1.49524700	-3.37437100	3.26589800	C	9.73827700	-2.00728800	-0.03630700
H	1.34629000	-2.19665400	4.57611800	C	10.67933500	-3.18771300	-0.30988900
H	-0.08629400	-3.06641900	4.00529500	H	9.50846200	-1.97049400	1.03847700
C	-4.53883900	-0.29807800	-2.10302100	H	10.26142100	-1.06760400	-0.26583800
C	0.01495200	-2.72861700	-2.03743500	C	11.98084100	-3.12363800	0.49586400
C	-5.84288600	-1.03810400	-2.46104600	H	10.15549500	-4.12689000	-0.08453000

H	10.91404800	-3.22156500	-1.38266100
H	12.62984700	-3.97853300	0.27832700
H	12.54403600	-2.21148700	0.26669600
H	11.77940500	-3.12425800	1.57341300
C	-1.02563800	1.61197000	-3.61759800
C	-0.30386900	2.85186500	-3.06024300
H	-1.57270800	1.07839200	-2.83227300
H	-1.75635600	1.90602000	-4.38014400
H	-0.33086100	0.90498000	-4.08196100
C	-1.35658000	3.85240500	-2.54773600
C	0.48198500	3.53260300	-4.20271900
H	-0.88082100	4.73809700	-2.11933100
H	-2.01226400	4.16588900	-3.36933600
H	-1.97406200	3.40568400	-1.76447900
H	-0.20033000	3.84244000	-5.00293100
H	1.00167500	4.42875300	-3.84420300
H	1.22879900	2.86954600	-4.65139600
C	0.69472000	2.49010900	-1.90267800
O	0.01355000	2.22261800	-0.67094400
C	-2.02066000	-0.86106300	0.22901900
C	-2.88580000	-2.54701800	1.48525100
C	-3.34214000	-2.71089800	0.21519900
N	-2.80326600	-1.67677900	-0.54517700
N	-2.08536200	-1.40845700	1.48375100
Cl	-4.38480700	-3.91549800	-0.40591400
Cl	-3.17419200	-3.51683400	2.86348700
C	-2.27073700	-2.19535400	-2.88789300
C	-3.06841100	-1.49729500	-1.95820600
C	-4.14339700	-0.66810900	-2.33904800
C	-4.39291800	-0.53307600	-3.71063100
C	-3.61427900	-1.19741800	-4.65431900
C	-2.56755600	-2.01930800	-4.24528200
H	-5.21160500	0.09765500	-4.04246400
H	-3.82756300	-1.07876000	-5.71262800
H	-1.97299600	-2.53784500	-4.99085500
C	-0.10586400	-1.27326700	2.93379200
C	0.48649500	-0.77530000	4.10110200
C	-0.21034500	0.07117100	4.95905500
C	-1.52177100	0.43802700	4.66847800
C	-2.16860800	-0.02982900	3.51766200
C	-1.43242400	-0.87913000	2.66543000
H	1.50604800	-1.05893900	4.34185800
H	0.26884400	0.44301600	5.86002600
H	-2.05617000	1.09494200	5.34728900
C	-1.13430600	-3.13000300	-2.48156400
H	-1.05100100	-3.11766600	-1.39090600
C	0.21961200	-2.65791700	-3.04414900
H	1.02191200	-3.31745700	-2.69701900
H	0.22673000	-2.67371300	-4.13910800
H	0.45046400	-1.63958500	-2.72022000
C	-1.42413500	-4.58397000	-2.90646700
H	-0.62542300	-5.24516500	-2.55421300
H	-2.37084600	-4.94323700	-2.49313300
H	-1.47567000	-4.67634200	-3.99652700
C	-5.04118100	0.05045800	-1.33566300
H	-4.65823600	-0.14400400	-0.33028200
C	-5.01962900	1.57749600	-1.53785900
H	-4.00196100	1.97345800	-1.47114600
H	-5.42901400	1.86030200	-2.51336900
H	-5.62731600	2.06609800	-0.76903000
C	-6.48310800	-0.49378100	-1.39012300
H	-7.10030300	-0.00373300	-0.62978100
H	-6.94374900	-0.30554200	-2.36572500
H	-6.51095800	-1.57251100	-1.20808200
C	0.67958900	-2.22328600	2.03497200
C	-3.61703800	0.37466500	3.25405800
C	0.91168400	-3.58023300	2.73024600
H	1.43882500	-4.26523800	2.05762500
H	1.52166200	-3.46157700	3.63227400
H	-0.03280500	-4.04898800	3.02286900
C	-4.56201200	-0.18530500	4.33691000
H	-4.49152300	-1.27426300	4.41046000
H	-4.32916100	0.23468800	5.32119700
H	-5.59949900	0.07457800	4.10152300
C	2.01323400	-1.60465100	1.57433400
H	2.70822700	-1.48437800	2.41230200
H	2.49555100	-2.25912800	0.84042400
H	1.85959000	-0.62198800	1.11935400
H	0.08667800	-2.41236000	1.13587900
Cu	-1.02500100	0.68157400	-0.26863300
H	1.28477400	3.39625100	-1.72578400
C	-3.77177800	1.90321000	3.13507700

H	-4.80630800	2.15541000	2.87849800
H	-3.53379200	2.40337800	4.07991500
H	-3.11257700	2.31059700	2.36375700
H	-3.92534600	-0.05554600	2.29683400
Si	0.17411400	3.21361100	1.08214900
H	-1.18932300	2.56745600	1.16537400
O	1.50989200	2.20630200	1.40129900
O	0.47991300	4.57767300	0.11201200
C	0.86536900	5.86062800	0.57909600
C	1.20134800	6.75241900	-0.61056500
H	1.74152600	5.79396800	1.24033400
H	0.05904700	6.31961900	1.16845300
H	1.50714700	7.74744300	-0.26846800
H	2.02001500	6.32329100	-1.19721200
H	0.33389800	6.86726800	-1.26838700
C	2.36964600	2.26065200	2.52992600
C	3.52478300	3.24116900	2.34228100
H	2.77404000	1.24966500	2.66812700
H	1.81634300	2.50741200	3.44390400
H	4.20667500	3.19814900	3.19989800
H	4.09369300	3.00069700	1.43862000
H	3.15986100	4.26933300	2.25067800
C	-0.06924600	4.08420300	2.80228400
H	-0.93124700	4.76186600	2.72628100
H	-0.33709900	3.32863700	3.55244300
H	0.76652400	4.66977700	3.20412000
C	1.65848900	1.34021800	-2.26252900
H	1.87531000	1.34966400	-3.33823000
H	1.14261900	0.39017300	-2.06413800
C	2.98520300	1.37445000	-1.49538300
H	2.77208100	1.41944800	-0.42296000
H	3.51236500	2.30782500	-1.74484200

TS21

C	8.66237900	-1.33721500	-0.83913500
C	7.60482500	-0.32403400	-0.38211200
H	8.23049600	-2.34818500	-0.81499500
H	8.91915100	-1.14280200	-1.89047800
C	6.32480400	-0.34786200	-1.22719800
H	7.34877800	-0.51679800	0.66968700
H	8.03701100	0.68662700	-0.40792200
H	6.58254500	-0.16204200	-2.27992100
H	5.88871300	-1.35694300	-1.19614900
C	5.27144100	0.67319200	-0.77803400
C	3.99105600	0.65013700	-1.62277000
H	5.70849400	1.68163200	-0.81162100
H	5.01414600	0.49010200	0.27511900
H	4.25319400	0.81583400	-2.67834900
H	3.54593100	-0.35437500	-1.57664500
C	9.94196200	-1.31361100	0.00630700
C	11.00163800	-2.32344300	-0.45312600
H	9.68692000	-1.51093900	1.05762200
H	10.37329400	-0.30235200	-0.01561300
C	12.27590500	-2.29284200	0.39711500
H	10.57102200	-3.33399700	-0.43124100
H	11.25746600	-2.12566500	-1.50312400
H	13.01121000	-3.02394300	0.04464100
H	12.74840400	-1.30420100	0.36623300
H	12.05694700	-2.52063900	1.44680500
C	-0.97189200	1.78792300	-3.48640700
C	-0.36150400	3.05165500	-2.85499800
H	-1.49851800	1.18328200	-2.74097600
H	-1.69883600	2.06107200	-4.25995900
H	-0.21318900	1.15568200	-3.95761300
C	-1.50131000	3.95255700	-2.34622800
C	0.41056400	3.83748000	-3.93848000
H	-1.11377900	4.84906500	-1.85398500
H	-2.13620600	4.26390500	-3.18485600
H	-2.12369100	3.42909000	-1.61814500
H	-0.26772100	4.13220200	-4.74746000
H	0.85083100	4.75215800	-3.52453500
H	1.21766200	3.25103300	-4.38843400
C	0.62070100	2.71752300	-1.68022700
O	-0.07050200	2.30391000	-0.48460700
C	-1.73580900	-1.11422900	0.17536000
C	-2.38020400	-3.05103200	1.18236300
C	-2.90506900	-3.05092400	-0.07135000
N	-2.49973300	-1.86564400	-0.68019500
N	-1.67395900	-1.86071200	1.32478200
Cl	-3.89431200	-4.22689700	-0.82204800
Cl	-2.49827200	-4.24735400	2.39863000
C	-2.09471000	-1.97883700	-3.10275600
C	-2.87046000	-1.49306200	-2.03014400

C	-4.02385600	-0.70329300	-2.21561100	H	0.78884700	-4.51378700	2.54983400
C	-4.37455200	-0.37905500	-3.53232200	C	-4.08066200	-1.28854800	4.44046000
C	-3.62167300	-0.83250500	-4.61179800	H	-3.90824000	-2.36585100	4.36333600
C	-2.49753100	-1.62516400	-4.39671500	H	-3.83048800	-0.97949800	5.46090000
H	-5.25446400	0.23048300	-3.71285800	H	-5.14905500	-1.10199100	4.28872900
H	-3.91520500	-0.57215400	-5.62454200	C	2.35220600	-1.71513600	1.14382600
H	-1.92315400	-1.97906300	-5.24712700	H	3.06564300	-1.49227000	1.94427800
C	0.35696500	-1.77797000	2.70646800	H	2.88806800	-2.26871600	0.36549800
C	0.97277300	-1.38334200	3.90124400	H	2.01617800	-0.76485700	0.71859500
C	0.25856000	-0.71985600	4.89500000	H	0.51315900	-2.74710100	0.80623000
C	-1.09404500	-0.44101200	4.71710900	Cu	-0.95893400	0.61375600	-0.06593200
C	-1.76233500	-0.80526900	3.54193600	H	1.13223900	3.65090400	-1.42465700
C	-1.00661400	-1.46063300	2.54756700	C	-3.54521700	1.00500200	3.49997500
H	2.02333600	-1.60783000	4.05666300	H	-4.60993500	1.19236700	3.32373600
H	0.75559700	-0.42599700	5.81486100	H	-3.30128500	1.39545200	4.49374500
H	-1.64197400	0.06794100	5.50381400	H	-2.96589400	1.56875100	2.76424300
C	-0.87028400	-2.87132500	-2.91546200	H	-3.57861800	-0.83116800	2.41028600
H	-0.71200400	-3.01823900	-1.84319700	Si	-0.10137500	3.16679600	1.23474000
C	0.40517000	-2.21445400	-3.47643000	H	-0.97277000	1.88148800	1.43061100
H	1.27272400	-2.85531000	-3.28674900	O	1.47349600	3.68209500	0.83610300
H	0.33484200	-2.06289700	-4.55873400	O	-1.13607800	4.46160300	0.86776200
H	0.59073600	-1.24228400	-3.01213100	C	-2.51659200	4.44702200	1.18053900
C	-1.08631400	-4.26250100	-3.54499600	C	-3.11318700	5.82665500	0.92976100
H	-0.21854400	-4.90152200	-3.35067900	H	-2.67789500	4.16426100	2.23267400
H	-1.97190300	-4.75626800	-3.13521300	H	-3.04213200	3.69929600	0.56524600
H	-1.21122900	-4.19210300	-4.63071800	H	-4.18429100	5.83225300	1.16025300
C	-4.90344300	-0.22332200	-1.06459900	H	-2.62149300	6.57824000	1.55590100
H	-4.45969600	-0.56439700	-0.12533500	H	-2.98335800	6.11794600	-0.11730400
C	-4.97039700	1.31415000	-1.00061700	C	2.38773300	4.43527600	1.60751600
H	-3.97237300	1.74956400	-0.89368000	C	2.14148900	5.94018300	1.51153800
H	-5.42746300	1.73458300	-1.90254100	H	3.39217400	4.20850600	1.22247600
H	-5.57415400	1.62987000	-0.14325600	H	2.37688500	4.12516800	2.66012800
C	-6.31639500	-0.83492300	-1.15108700	H	2.91650400	6.49248300	2.05609600
H	-6.91393200	-0.52694000	-0.28663800	H	2.15812200	6.26501400	0.46586100
H	-6.84068300	-0.50329600	-2.05354400	H	1.16690400	6.20622900	1.93213300
H	-6.27804100	-1.92846700	-1.16703900	C	0.04157300	3.26794500	3.16909600
C	1.16287000	-2.54428900	1.66217900	H	-0.95084300	3.07434100	3.59505800
C	-3.25256300	-0.50442400	3.40206700	H	0.70132000	2.47967900	3.55831400
C	1.63369100	-3.90633600	2.21092800	H	0.39490500	4.22454200	3.57264100
H	2.16412700	-4.46404900	1.43188900	C	1.68324700	1.66631700	-2.05123000
H	2.31850700	-3.78101600	3.05637400	H	1.97995400	1.79109100	-3.09988400

H	1.21541700	0.67397100	-1.98262900
C	2.95077900	1.69109000	-1.18860100
H	2.68290000	1.54156500	-0.13738700
H	3.40024500	2.69212400	-1.24061200
58			
C	8.93553200	4.95053900	-0.38838100
C	8.14833000	3.69801800	-0.79389000
H	8.44966600	5.41887300	0.47975500
H	9.93859200	4.65338800	-0.04982400
C	8.02101200	2.66285800	0.33126900
H	7.14430400	3.99382300	-1.13059600
H	8.63355000	3.23062000	-1.66286100
H	9.02566200	2.37201700	0.67064200
H	7.53185900	3.12887900	1.19877100
C	7.24204200	1.40509500	-0.07376700
C	7.12233800	0.36967000	1.05201700
H	7.73038500	0.94046600	-0.94246800
H	6.23586900	1.69339600	-0.41033400
H	8.12930500	0.09020000	1.39441000
H	6.62604400	0.83163700	1.91765100
C	9.06797300	5.98567100	-1.51269000
C	9.85781700	7.23628300	-1.10640800
H	8.06561700	6.28564900	-1.85114700
H	9.55329500	5.51814500	-2.38168700
C	9.98777500	8.26448500	-2.23499600
H	9.37202100	7.70449200	-0.23925700
H	10.85904000	6.93665600	-0.76745500
H	10.55523700	9.14402300	-1.91278400
H	10.50212800	7.83645900	-3.10324300
H	9.00326000	8.60906100	-2.57214900
C	4.64906000	-3.88929200	3.66954200
C	5.51643400	-4.33127400	2.47539500
H	3.63497800	-3.63968300	3.34505000
H	4.58157100	-4.69587600	4.40817200
H	5.06867300	-3.01431300	4.17659300
C	4.92598900	-5.61976000	1.86797300
C	6.94758600	-4.64392500	2.96115500
H	5.54580600	-5.98296200	1.03920100
H	4.88180000	-6.41280000	2.62278600
H	3.91720100	-5.45753300	1.48293100
H	6.93534000	-5.51955500	3.61935500
H	7.61465200	-4.87126300	2.12092500
H	7.38565100	-3.81607400	3.52648100
C	5.56431000	-3.23296300	1.36826600
O	4.22843500	-2.92223700	0.92693400
C	-3.86377500	0.52692100	0.11186800
C	-5.70893500	1.46355700	-0.82307800
C	-5.30705200	2.27802500	0.19152400
N	-4.17685400	1.69214600	0.75398100
N	-4.81623100	0.39662700	-0.85996400
Cl	-5.99386500	3.74692300	0.73535200
Cl	-7.03421200	1.63922800	-1.88991900
C	-2.34983700	3.10616500	1.58831700
C	-3.42283900	2.23557300	1.86557600
C	-3.79283000	1.86653600	3.17422300
C	-3.03364600	2.39234100	4.22715400
C	-1.96058300	3.24614400	3.98584700
C	-1.62545800	3.59868000	2.68115900
H	-3.28589300	2.12663100	5.24896200
H	-1.38415600	3.63970500	4.81794600
H	-0.78726600	4.26595400	2.50629300
C	-4.17842400	-0.57816100	-3.02195800
C	-4.23559400	-1.66360500	-3.90527700
C	-4.95259100	-2.81412700	-3.58796400
C	-5.63528000	-2.90284100	-2.37765000
C	-5.61600300	-1.84890200	-1.45546400
C	-4.87195100	-0.70323500	-1.80150500
H	-3.70975000	-1.60630900	-4.85331700
H	-4.98114500	-3.64430400	-4.28767000
H	-6.19155500	-3.80490700	-2.14340000
C	-1.95439200	3.51519800	0.17296400
H	-2.66746900	3.06803800	-0.52542900
C	-0.55811900	2.97541200	-0.19407900
H	-0.31079600	3.23697400	-1.22849600
H	0.21620000	3.40124600	0.45292800
H	-0.51725900	1.88593100	-0.09664100
C	-2.02875200	5.04258500	-0.01855700
H	-1.79850200	5.30330900	-1.05683300
H	-3.02672600	5.42596300	0.21548200
H	-1.30906500	5.56352200	0.62142500
C	-4.95923700	0.93136700	3.47676600
H	-5.43868700	0.66424400	2.53087500

C	-4.47103100	-0.37885800	4.12542400
H	-3.74021100	-0.88724800	3.48842300
H	-4.00001600	-0.19183900	5.09631900
H	-5.31495000	-1.05753800	4.28855100
C	-6.02717300	1.61986000	4.34894400
H	-6.87575800	0.94591300	4.50613600
H	-5.62982500	1.88837600	5.33330400
H	-6.40035100	2.53326900	3.87569900
C	-3.38321600	0.66576600	-3.40534700
C	-6.37344800	-1.98274200	-0.13791300
C	-3.93421300	1.31505000	-4.68987600
H	-3.38361800	2.23480900	-4.91359200
H	-3.83138200	0.64843100	-5.55252500
H	-4.99356000	1.56906600	-4.58501300
C	-7.87470800	-2.24473800	-0.36715200
H	-8.32688100	-1.46259800	-0.98471200
H	-8.04496900	-3.20599500	-0.86305400
H	-8.40235800	-2.26915900	0.59199100
C	-1.88109100	0.34873200	-3.54006800
H	-1.69480000	-0.36487000	-4.34966800
H	-1.31991600	1.26217200	-3.76385400
H	-1.48376000	-0.07973600	-2.61455000
H	-3.48614500	1.40090900	-2.60219200
Cu	-2.39944200	-0.68519300	0.50193900
H	6.12337500	-3.65310600	0.52053800
C	-5.74851700	-3.07318700	0.75452300
H	-6.27742200	-3.12863400	1.71196800
H	-5.81016900	-4.05836500	0.28001100
H	-4.69366700	-2.86205100	0.95752300
H	-6.29066000	-1.03554100	0.40247500
Si	3.52503500	-3.16400200	-0.54651000
H	-1.25584800	-1.64304100	0.81285700
O	4.75023100	-3.42426300	-1.63273300
O	2.59259100	-4.53991100	-0.59581900
C	1.34456400	-4.71141700	0.08643700
C	0.69735900	-6.00691800	-0.37640900
H	0.67890000	-3.86248200	-0.11751600
H	1.51896800	-4.74031300	1.17046300
H	-0.25535600	-6.16028500	0.14095900
H	0.50513500	-5.97863700	-1.45352600
H	1.34753400	-6.86155400	-0.16503400
C	4.55845200	-3.91680800	-2.96364700
C	5.91285300	-4.07531700	-3.63555700
H	3.93348000	-3.21559300	-3.53425200
H	4.03089500	-4.87768000	-2.92913500
H	5.78862600	-4.45144800	-4.65632500
H	6.43638100	-3.11542100	-3.68229900
H	6.53777400	-4.78187100	-3.08069600
C	2.48929400	-1.65992800	-0.93587600
H	1.97321500	-1.77329600	-1.89514900
H	1.72697100	-1.49274300	-0.16764100
H	3.11397200	-0.76294000	-0.98885900
C	6.24014200	-1.91831800	1.78124300
H	7.24473300	-2.14414200	2.15614300
H	5.68422400	-1.47118100	2.61478500
C	6.35668300	-0.89527400	0.64364100
H	5.35245900	-0.61742200	0.30254900
H	6.85660500	-1.36162900	-0.21705400

59

C	6.86957800	0.37086600	-0.25276900
C	5.45751900	-0.17107200	0.00167100
H	6.91327200	0.80886000	-1.26030000
H	7.07197000	1.19616700	0.44496500
C	4.35907800	0.89057200	-0.13294700
H	5.25390200	-0.99420500	-0.69822100
H	5.41421300	-0.61172800	1.00800600
H	4.56117100	1.71178300	0.56965800
H	4.40500500	1.33406000	-1.13794800
C	2.94590700	0.34891000	0.11577500
C	1.84969500	1.41350100	-0.01367300
H	2.90000500	-0.09853400	1.11896100
H	2.74182900	-0.46895000	-0.59010200
H	2.05074600	2.22812100	0.69690400
H	1.90072000	1.86575000	-1.01453600
C	7.96935400	-0.68867200	-0.11433200
C	9.38106100	-0.14688900	-0.37094700
H	7.76762100	-1.51512800	-0.81106700
H	7.92786500	-1.12591500	0.89371600
C	10.47346700	-1.21121000	-0.22966600
H	9.42291000	0.28881300	-1.37857600
H	9.58290800	0.67901100	0.32479700
H	11.46750500	-0.79371700	-0.42120200

H	10.48107900	-1.63907900	0.77943100
H	10.31697900	-2.03502200	-0.93557800
C	-3.34276400	3.16123400	-1.03891700
C	-3.18708100	2.51947800	0.35233900
H	-3.57116000	2.40548500	-1.79571100
H	-4.16088600	3.88997200	-1.02911200
H	-2.43612800	3.69032000	-1.34964400
C	-4.52168800	1.86413900	0.76067300
C	-2.85418700	3.60996400	1.39218000
H	-4.45498100	1.43122000	1.76593100
H	-5.32472500	2.60932200	0.77217800
H	-4.80777600	1.06630800	0.07199300
H	-3.70809700	4.28574400	1.50979600
H	-2.64061700	3.17381800	2.37524100
H	-1.99430300	4.21884500	1.09828300
C	-2.07145500	1.42888700	0.35808900
O	-2.36537500	0.41787100	-0.62785000
H	-2.08475100	0.95937300	1.35141200
Si	-2.76670000	-1.16951300	-0.43057100
O	-2.42617100	-1.57515100	1.13762700
O	-4.39754700	-1.43756800	-0.62046000
C	-5.10364800	-1.30627900	-1.85913400
C	-6.53931800	-1.76617000	-1.66728600
H	-4.61475800	-1.90746300	-2.63759900
H	-5.08082000	-0.25863200	-2.18785800
H	-7.09817500	-1.66735800	-2.60342100
H	-6.56996700	-2.81451600	-1.35507700
H	-7.03803400	-1.16438800	-0.90158700
C	-2.87035300	-2.77581100	1.78268500
C	-2.42912500	-2.75194500	3.23626900
H	-2.44466400	-3.65051100	1.27199200
H	-3.96210200	-2.84859200	1.71236800
H	-2.76031800	-3.66149200	3.74766800
H	-1.33898400	-2.69217300	3.30934700
H	-2.85737300	-1.88864900	3.75451300
C	-1.79993000	-2.16349900	-1.68242200
H	-2.05975900	-3.22606400	-1.63370400
H	-1.99756900	-1.81790200	-2.70245800
H	-0.72469900	-2.06876200	-1.50330000
C	-0.65128000	1.94301000	0.08660800
H	-0.42972800	2.75642400	0.78634200
H	-0.61115800	2.37324800	-0.92180100
C	0.43528800	0.86907800	0.22295800
H	0.23689700	0.05939700	-0.48902800
H	0.38078100	0.42016400	1.22485200

60

C	8.73636700	-2.41213400	0.30685200
C	7.75371100	-1.47154200	-0.40157100
H	9.34104300	-1.83321600	1.01980400
H	8.17219100	-3.13851100	0.90942100
C	6.82024200	-0.72378800	0.55832600
H	8.31784700	-0.74240200	-1.00075600
H	7.15091100	-2.04905000	-1.11719000
H	6.25324900	-1.45420000	1.15337200
H	7.42387800	-0.15206000	1.27804500
C	5.84096400	0.22489600	-0.14418900
C	4.90369600	0.96351300	0.81911000
H	5.24025700	-0.34430200	-0.86825200
H	6.40854700	0.95913400	-0.73410100
H	4.33552100	0.22710100	1.40586900
H	5.50615000	1.52706500	1.54708200
C	9.66803400	-3.16562600	-0.65003700
C	10.65220200	-4.10227400	0.06134700
H	10.23186200	-2.44065200	-1.25467000
H	9.06481600	-3.74817000	-1.36137900
C	11.57904500	-4.85253700	-0.90000700
H	11.25575800	-3.51996900	0.77111100
H	10.08881300	-4.82606600	0.66605900
H	12.26979300	-5.50912600	-0.36059800
H	11.00667000	-5.47397000	-1.59835500
H	12.17959800	-4.15540900	-1.49562000
C	2.49805300	4.36382800	-1.72058200
C	1.99292900	4.66753600	-0.29735900
H	1.83784000	3.64829100	-2.21496000
H	2.52247200	5.28268500	-2.31986400
H	3.50927500	3.94853400	-1.72062200
C	0.64105300	5.40349500	-0.41299400
C	2.99022700	5.60398400	0.41149200
H	0.28404300	5.72760700	0.57114000
H	0.73364100	6.29316400	-1.04792800
H	-0.11935800	4.74549300	-0.83899400
H	3.04066400	6.57065900	-0.10411000

H	2.68775300	5.79962100	1.44771000	C	-5.12425000	0.88320500	-1.23184400
H	4.00358000	5.18999000	0.43008000	H	-3.98669100	0.73437100	0.59297500
C	1.75109300	3.37013500	0.55478500	H	-5.71521900	0.31427300	0.77387100
O	0.93359800	2.47231800	-0.16165800	C	-5.65870200	2.31157500	-1.02464700
H	1.21288200	3.72642000	1.44551900	H	-4.20724400	0.93228900	-1.82562500
Si	-0.42431100	1.51229000	0.43380600	H	-5.86028500	0.31556900	-1.81285200
O	-0.91487900	2.81790700	1.42923200	C	-5.92407200	3.03412500	-2.34809700
O	-1.05813000	1.29906300	-1.15027700	H	-6.58378700	2.27271100	-0.43496000
C	-0.52798300	1.83883800	-2.34900500	H	-4.93632800	2.88607300	-0.43169600
C	-1.38651100	1.39549900	-3.52897200	H	-6.30523300	4.04488100	-2.17355000
H	0.50865300	1.51177100	-2.50118800	H	-5.00780700	3.12131300	-2.94190400
H	-0.50155700	2.93471700	-2.30515500	H	-6.66410600	2.49733300	-2.95226700
H	-0.98907900	1.80175700	-4.46619600	C	-3.31864200	-1.42423800	-0.88608700
H	-1.40755800	0.30366500	-3.61307600	C	-2.38680800	-2.62820000	-0.75126900
H	-2.41783500	1.74802700	-3.41731300	H	-2.71409000	-0.52230900	-0.77410500
C	-1.99732200	2.85188500	2.33686600	H	-3.79538200	-1.41713300	-1.86848800
C	-1.86991400	4.08767900	3.22094000	C	-1.35168700	-2.59580500	-1.88969000
H	-2.02650000	1.94864400	2.96012100	H	-1.85205300	-2.57891600	0.20237900
H	-2.95732700	2.88711000	1.79866400	H	-2.92093800	-3.58130900	-0.78078800
H	-2.70843400	4.15202400	3.92401100	C	-0.32772800	-3.72903200	-1.78152200
H	-0.93959000	4.05694400	3.79818700	H	-1.87103400	-2.66097300	-2.85512800
H	-1.85986300	4.99898400	2.61395300	H	-0.83878300	-1.62700800	-1.87646400
C	0.62504200	0.08623000	1.15371900	H	0.39177400	-3.68809000	-2.60505200
H	0.10601500	-0.87610200	1.10197000	H	0.23535800	-3.66444400	-0.84410600
H	1.59383700	-0.00530000	0.65602400	H	-0.81455200	-4.71040600	-1.81166100
H	0.82642600	0.27796400	2.21661100	C	-6.90006300	-5.48239400	-1.60723300
N	-4.46154100	-1.26066900	0.12705100	C	-6.97489600	-4.06949300	-1.02185700
C	-3.99972400	-1.51937100	1.57111400	H	-7.90103100	-5.88826900	-1.78169900
C	-3.97514300	-2.95497000	2.09403700	H	-6.36585200	-5.48692800	-2.56360200
H	-4.69508900	-0.94683400	2.19031900	H	-6.37592300	-6.16501100	-0.92946200
H	-3.02482400	-1.03348400	1.63968000	C	-5.58254900	-3.46777200	-0.76434300
C	-3.44459100	-2.96374700	3.53906200	H	-7.53394400	-3.41755400	-1.70542300
H	-4.98295800	-3.38452800	2.09054800	H	-7.54206800	-4.09064000	-0.08240700
H	-3.34376200	-3.60303000	1.48269500	C	-5.72449500	-2.04669200	-0.21968600
C	-3.43095700	-4.36874300	4.14744100	H	-5.03847600	-4.11467700	-0.07252600
H	-2.43090400	-2.54477700	3.55514400	H	-5.02431200	-3.45622600	-1.70655400
H	-4.06200100	-2.30063500	4.15868300	H	-6.25178200	-1.45059100	-0.96465900
H	-3.04987500	-4.34844400	5.17291300	H	-6.33035100	-2.03897200	0.69027300
H	-4.43787000	-4.80002000	4.17350100	F	-1.88507000	0.62131600	0.94844700
H	-2.79351800	-5.04538700	3.56781200	C	3.01042800	2.65445100	1.11180300
C	-4.83914500	0.23954400	0.12410600	H	3.60373300	3.36598200	1.70125500

H	2.63788600	1.91677900	1.83352600	H	1.76168000	4.88155300	1.81273700
C	3.92414600	1.91815800	0.12270400	H	3.19426200	4.92816800	0.77274900
H	4.50159600	2.63443300	-0.47508500	C	1.93450300	2.27662600	0.91927300
H	3.30060600	1.35687900	-0.58325500	O	1.48063500	1.11173100	0.36655100
TS22				H	1.41640500	2.52222900	1.88755700
C	10.18988100	-1.33692100	0.16514100	Si	-0.42860300	-0.77649400	0.33558700
C	8.94517100	-0.71219700	-0.47727500	O	-1.08545400	0.05683400	1.61315000
H	10.70263200	-0.57889100	0.77456700	O	-0.79360500	-0.11899000	-1.14486100
H	9.87778200	-2.12615300	0.86420400	C	0.20056300	0.15137600	-2.15133100
C	7.95289000	-0.13929900	0.54252800	C	-0.40787100	1.02037000	-3.23851600
H	9.25460300	0.08272700	-1.17100500	H	0.53596100	-0.80148700	-2.58673200
H	8.43631600	-1.46884900	-1.09159800	H	1.04225100	0.64387700	-1.65538900
H	7.65249500	-0.93542500	1.23903000	H	0.33036500	1.20876800	-4.02586000
H	8.46063500	0.62043700	1.15425900	H	-1.27630200	0.53520800	-3.69784800
C	6.69739200	0.47551700	-0.08859800	H	-0.72577600	1.98567100	-2.83284800
C	5.70085800	1.02492300	0.94054200	C	-0.34009800	0.52257100	2.74603800
H	6.19520200	-0.28173600	-0.70785000	C	-0.58111500	-0.37201500	3.95478200
H	6.99371900	1.28019600	-0.77715300	H	-0.67624900	1.54353700	2.96115400
H	5.42586800	0.21932200	1.63749000	H	0.71653900	0.57526900	2.47502200
H	6.20147300	1.79063500	1.55241800	H	-0.04992600	0.02088700	4.82904800
C	11.17942100	-1.92408300	-0.84883400	H	-1.64734300	-0.42733100	4.19883500
C	12.41966100	-2.55341500	-0.20238900	H	-0.22237500	-1.38986800	3.76824900
H	11.49609400	-1.13597000	-1.54716300	C	1.15211100	-1.74011300	0.52638900
H	10.66688500	-2.68137000	-1.45949200	H	1.19487900	-2.54227500	-0.21867000
C	13.39980600	-3.14427700	-1.22061500	H	1.99197200	-1.05580500	0.41365700
H	12.93450200	-1.79604800	0.40435700	H	1.19002700	-2.20616400	1.51710200
H	12.10232600	-3.33810300	0.49801100	N	-4.91206900	-0.10789600	0.15943500
H	14.27156900	-3.58783500	-0.72818300	C	-4.51435700	-1.05890300	1.30076600
H	12.92212600	-3.92743200	-1.82057400	C	-5.33767000	-2.32688200	1.52412000
H	13.76363400	-2.37555800	-1.91204600	H	-4.57070400	-0.44879000	2.20508200
C	2.20543200	3.52611100	-1.35648300	H	-3.46550500	-1.29899000	1.12398900
C	1.61010900	3.57523600	0.06164900	C	-4.71130500	-3.14277000	2.66934600
H	1.95716600	2.58169300	-1.84655400	H	-6.37043000	-2.07771700	1.79160600
H	1.81248400	4.34449800	-1.97489900	H	-5.37438100	-2.95021400	0.62836000
H	3.29526400	3.62437800	-1.34564500	C	-5.50012100	-4.41841200	2.97645300
C	0.07509700	3.65095700	-0.05575000	H	-3.67879200	-3.39989100	2.40311000
C	2.10158900	4.85222600	0.76931300	H	-4.65217000	-2.52075100	3.57188800
H	-0.38113600	3.78422000	0.93415300	H	-5.03244800	-4.98182800	3.78947200
H	-0.23892500	4.49690400	-0.68156500	H	-6.52780800	-4.18745500	3.27795300
H	-0.31566000	2.72390900	-0.48047300	H	-5.54884700	-5.07446100	2.10049200
H	1.71474100	5.75203100	0.27274200	C	-4.28454900	1.24814600	0.55768300

C	-4.26415300	2.34009000	-0.51220100	H	3.40960400	1.40811700	2.19426400
H	-3.26681800	1.01847000	0.88410000	C	4.42286100	1.61032200	0.32473600
H	-4.85872700	1.57956700	1.42690800	H	4.70443200	2.40316700	-0.38034700
C	-3.87119800	3.68725700	0.11883400	H	3.90544100	0.84013700	-0.25905800
H	-3.54273100	2.09139200	-1.29593000	61			
H	-5.24038000	2.45343800	-0.99784900	C	7.38077300	0.41554300	-0.37400400
C	-3.79273500	4.81296700	-0.91586400	C	5.99110000	0.33439400	0.26984000
H	-4.60105200	3.95054800	0.89527200	H	7.29682000	0.19401000	-1.44768500
H	-2.90242000	3.58375500	0.62130300	H	7.75075200	1.44871800	-0.30638300
H	-3.52360600	5.76178400	-0.44207800	C	4.96475400	1.28562700	-0.35786700
H	-3.03823100	4.59608400	-1.67946800	H	5.61924200	-0.69814200	0.20067200
H	-4.75328800	4.95324100	-1.42429200	H	6.07725100	0.55317800	1.34391500
C	-4.28668900	-0.51754200	-1.18145700	H	5.34201300	2.31656100	-0.29536400
C	-4.28717200	-1.99445100	-1.57629000	H	4.87134500	1.06281700	-1.43058400
H	-3.24651400	-0.18996800	-1.12860500	C	3.57972700	1.21603700	0.29738200
H	-4.79502100	0.08431000	-1.93747000	C	2.55271200	2.17612400	-0.31671600
C	-3.65650700	-2.14196400	-2.97247600	H	3.67825600	1.43214700	1.37114600
H	-3.68479900	-2.56506500	-0.86508500	H	3.19883300	0.18623600	0.23110000
H	-5.29263500	-2.42137200	-1.59365400	H	2.94522900	3.20251100	-0.26402300
C	-3.58113300	-3.60289000	-3.42508600	H	2.44300100	1.95242900	-1.38823500
H	-4.23724300	-1.56110700	-3.70121000	C	8.40778200	-0.53092800	0.25924600
H	-2.64990200	-1.70799700	-2.95565900	C	9.79950500	-0.44511500	-0.37955200
H	-3.13084200	-3.68331600	-4.41920800	H	8.04115000	-1.56530300	0.18896900
H	-2.97498900	-4.19931300	-2.73474100	H	8.48976900	-0.31152200	1.33360600
H	-4.57750700	-4.05668400	-3.47182200	C	10.81898400	-1.39255600	0.26011400
C	-9.66004500	-1.35964600	-1.48118200	H	9.71842200	-0.66500700	-1.45285100
C	-8.75580000	-0.44688600	-0.64814200	H	10.16576400	0.58820300	-0.30888600
H	-10.70626000	-1.04855700	-1.40580200	H	11.80108100	-1.30646600	-0.21654000
H	-9.37980600	-1.33629800	-2.53989800	H	10.94674000	-1.17472200	1.32674600
H	-9.59508800	-2.39908800	-1.14170600	H	10.49765600	-2.43694700	0.17350200
C	-7.27505400	-0.85697800	-0.72954900	C	-2.58178100	4.04938700	-1.43910100
H	-8.86720100	0.59056000	-0.98884200	C	-2.21595900	4.16588300	0.04965800
H	-9.08120400	-0.46450100	0.39982800	H	-2.93718500	3.03669500	-1.65056700
C	-6.42599300	0.10880400	0.09578900	H	-3.36955600	4.76131900	-1.71774400
H	-7.17164300	-1.88662000	-0.38015400	H	-1.71829700	4.24601600	-2.08515100
H	-6.96054100	-0.83458500	-1.77811700	C	-3.49844300	4.02592900	0.88892800
H	-6.56575700	1.11198400	-0.30687800	C	-1.60869700	5.55312100	0.33129100
H	-6.75889600	0.12794100	1.13653900	H	-3.28023500	4.14140200	1.95874300
F	-1.56904400	-1.99755200	0.30847400	H	-4.24299600	4.78498000	0.61632800
C	3.43148800	2.13730400	1.37038000	H	-3.93212400	3.03423000	0.74252000
H	3.80864500	3.07086300	1.81231300	H	-2.35836000	6.34455500	0.20122700

H	-1.23845900	5.61846900	1.36269800
H	-0.77407300	5.78694900	-0.33760600
C	-1.23781500	2.98967200	0.47941000
O	-1.79350600	1.75096700	0.32897100
H	-1.01653500	3.23269500	1.55936700
N	-2.78531300	-1.32340400	0.42444200
C	-1.60554100	-1.12016400	1.38946800
C	-0.52092800	-2.19458200	1.45523400
H	-2.06895400	-1.05209300	2.37781500
H	-1.23229100	-0.11836800	1.13043000
C	0.56032000	-1.77415600	2.46679000
H	-0.94271600	-3.15370900	1.77796000
H	-0.04838800	-2.36202100	0.48485400
C	1.66384300	-2.82517600	2.61511700
H	0.99889900	-0.81979900	2.15103900
H	0.09416300	-1.59031200	3.44353100
H	2.41937000	-2.50371100	3.33862400
H	1.25723700	-3.78254800	2.95999100
H	2.17110100	-3.00414700	1.66052800
C	-3.85661600	-0.34151600	0.95998800
C	-5.09061300	-0.12620000	0.08379800
H	-3.30788000	0.60500000	1.07307200
H	-4.14789100	-0.74466600	1.93414800
C	-6.16465400	0.64431400	0.87097400
H	-4.82187200	0.45029700	-0.80681000
H	-5.52775900	-1.06948000	-0.26618900
C	-7.40272000	0.95561600	0.02569000
H	-6.45799300	0.05919000	1.75240100
H	-5.73475000	1.57937500	1.25028400
H	-8.15259700	1.49723300	0.61062500
H	-7.14522000	1.57416600	-0.84094700
H	-7.87014900	0.03741500	-0.34763800
C	-2.44493600	-0.84244500	-0.99329100
C	-1.13792400	-1.29834100	-1.64340300
H	-2.38954300	0.24896000	-0.88234700
H	-3.29736500	-1.12935000	-1.61328500
C	-1.07533900	-0.74945800	-3.07940700
H	-0.28769400	-0.89498900	-1.08549400
H	-1.02756500	-2.38512600	-1.67342800
C	0.23323600	-1.10807200	-3.78909300
H	-1.92482100	-1.13788200	-3.65683600
H	-1.19155100	0.34097300	-3.05083700
H	0.25188300	-0.70810500	-4.80772300
H	1.09747100	-0.69874700	-3.25455500
H	0.36595100	-2.19394100	-3.85444100
C	-2.99825500	-6.30450900	-0.97098000
C	-3.50339700	-5.16353500	-0.08332100
H	-3.52233700	-7.23851900	-0.74666600
H	-3.15460000	-6.08004200	-2.03178600
H	-1.92697500	-6.47850000	-0.82182300
C	-2.78691500	-3.83312500	-0.37032200
H	-4.58390000	-5.03561300	-0.22967200
H	-3.36520100	-5.43060600	0.97244500
C	-3.37099500	-2.72816200	0.50959200
H	-1.71522500	-3.96209500	-0.20145500
H	-2.92191200	-3.57995800	-1.42710400
H	-4.42856000	-2.62948900	0.26392500
H	-3.31082900	-3.00431200	1.56592900
C	0.14602200	3.08996000	-0.22849400
H	0.01191100	2.86403300	-1.29652800
H	0.55307300	4.10930500	-0.16731200
C	1.17702700	2.12172800	0.35894100
H	0.77152300	1.10469700	0.29557100
H	1.29814000	2.33579000	1.43246000

4a’

C	-4.96846000	0.45689600	0.18631500
C	-3.69974700	-0.31927700	-0.18799900
H	-4.94649700	0.69131000	1.26033400
H	-4.96836100	1.42488200	-0.33497200
C	-2.40133900	0.42592900	0.14530300
H	-3.70285800	-1.28945900	0.32910600
H	-3.71976000	-0.54928600	-1.26294600
H	-2.39863000	1.39798800	-0.36828800
H	-2.37941600	0.65170400	1.22116000
C	-1.13467600	-0.35077000	-0.23470400
C	0.16614700	0.38530200	0.10969400
H	-1.15311900	-0.56904600	-1.31207600
H	-1.14195900	-1.32648400	0.27170900
H	0.17379600	1.36367000	-0.39187500
H	0.18627100	0.59822800	1.18832100
C	-6.26540200	-0.29338800	-0.14036300
C	-7.53550500	0.48191500	0.23107600

H	-6.26681700	-1.26057300	0.38263200
H	-6.28761400	-0.53005100	-1.21397100
C	-8.82514500	-0.27744700	-0.09539200
H	-7.51278200	0.71990100	1.30336400
H	-7.53611300	1.44704700	-0.29363500
H	-9.71263100	0.30060800	0.18266300
H	-8.89404100	-0.49821800	-1.16681400
H	-8.86831200	-1.23225500	0.44109700
H	1.41478500	-0.59460800	-1.35810900
C	1.42740500	-0.39626800	-0.27677100
C	6.47779100	-0.65623900	-0.57196900
C	5.35233100	0.25810500	-0.04693200
H	6.37347800	-0.82727900	-1.64995700
H	7.45883800	-0.20046300	-0.39916800
H	6.45486600	-1.62887200	-0.07453600
C	5.39451900	1.58755900	-0.82607700
C	5.58661600	0.53307700	1.45150200
H	4.70262100	2.33032400	-0.41768000
H	6.40066900	2.01873200	-0.78258900
H	5.14495200	1.43775800	-1.88326700
H	6.56462800	1.00222600	1.60236600
H	4.83179500	1.20644700	1.87033000
H	5.58082500	-0.39394700	2.03547000
H	1.41802400	-1.37777300	0.21142100
C	2.72965000	0.33134900	0.08481100
H	2.74969400	1.30423900	-0.41902600
H	2.73794800	0.54474400	1.16357400
C	3.98931100	-0.46526100	-0.28926300
H	3.93999500	-0.69112900	-1.36360600
O	3.96672000	-1.75787900	0.33803700
H	3.86099200	-1.61622600	1.28930300

63

C	7.08885100	0.87703100	-0.95516600
C	5.88125600	0.81962500	-0.01078800
H	6.73619200	0.86009900	-1.99642700
H	7.60544900	1.83896600	-0.82568300
C	4.87741500	1.96002200	-0.22284800
H	5.36517400	-0.14256000	-0.13862400
H	6.23490600	0.83753900	1.03024000
H	5.39015500	2.92395900	-0.09103600
H	4.52317500	1.94345700	-1.26338000
C	3.67300300	1.88926400	0.72439600
C	2.67423200	3.04146500	0.50993400
H	4.03050300	1.89159700	1.76190400
H	3.14783800	0.93616000	0.58074000
H	3.19970900	3.99716100	0.64471300
H	2.33238400	3.00552600	-0.52516800
C	8.08856500	-0.26633300	-0.74066400
C	9.29898100	-0.21104700	-1.68164200
H	7.57270000	-1.22866600	-0.87171400
H	8.44013100	-0.25098000	0.30121300
C	10.29054400	-1.35788700	-1.45988100
H	8.94828100	-0.22629700	-2.72268000
H	9.81535800	0.74968100	-1.54978000
H	11.14187600	-1.29047100	-2.14546100
H	10.68519100	-1.34759400	-0.43721300
H	9.81171800	-2.33116700	-1.61841400
C	1.47218000	2.97681600	1.44328000
C	1.62640400	2.92022500	2.77608300
H	0.77056300	2.87298400	3.44065000
H	2.60995800	2.92953400	3.23768800
O	-0.81745900	2.27671300	1.55309700
C	-0.49008800	4.25925200	0.18821300
C	-1.85066500	3.96022200	-0.46455800
C	-0.69505100	5.32188400	1.30185300
C	0.45781400	4.83739500	-0.87569200
H	-1.74786700	3.21699900	-1.26260900
H	-2.56865600	3.58008500	0.26408900
H	-2.25786000	4.87600200	-0.90705800
H	0.24816100	5.56543600	1.80035700
H	-1.09755800	6.24268100	0.86589400
H	-1.40060800	4.96305100	2.05747800
H	-0.01609400	5.70954000	-1.34009700
H	1.40722400	5.17253000	-0.45090700
H	0.66550600	4.10577400	-1.66138300
C	0.04536700	2.99477000	0.92668100
C	-1.31033900	-0.59241000	-0.03532100
C	-2.83338600	-2.23550900	-0.43471600
C	-1.72402400	-2.82687500	0.08181500
N	-0.80003100	-1.81133900	0.32026300
N	-2.56806300	-0.86856800	-0.49965800
Cl	-1.43840300	-4.48149800	0.41517200

Cl	-4.30465900	-2.95349100	-0.93548000
C	0.63853600	-1.95952900	2.30342000
C	0.51167700	-2.01175500	0.90013300
C	1.60090600	-2.26815500	0.04206900
C	2.85574800	-2.45285100	0.63723600
C	3.01656900	-2.38802500	2.01895500
C	1.91886000	-2.14624000	2.84017900
H	3.71740600	-2.65501900	0.00867200
H	3.99977600	-2.53304300	2.45716800
H	2.05450300	-2.10693200	3.91651900
C	-4.39555000	0.70845800	-0.04270500
C	-5.29420800	1.66736200	-0.52798800
C	-5.31084200	2.02601700	-1.87323700
C	-4.42986400	1.42534600	-2.76826700
C	-3.51005700	0.45807300	-2.34263600
C	-3.50748600	0.12761300	-0.97184200
H	-5.99305100	2.13596600	0.15795700
H	-6.01724800	2.77178500	-2.22632700
H	-4.45897800	1.70620600	-3.81642900
C	-0.54468500	-1.73925300	3.24211300
H	-1.44791500	-1.62623300	2.63618100
C	-0.38835300	-0.44655700	4.06561000
H	-1.25918200	-0.31115400	4.71655200
H	0.50014100	-0.48677100	4.70535700
H	-0.30703500	0.42855300	3.41559600
C	-0.76151700	-2.95976800	4.15944500
H	-1.65008300	-2.80943800	4.78165700
H	-0.90305400	-3.87704800	3.57966500
H	0.09118900	-3.11356100	4.82934400
C	1.46274600	-2.38246800	-1.47359200
H	0.43548900	-2.12292000	-1.74396400
C	2.38667900	-1.39640200	-2.21286000
H	2.18475100	-0.36649200	-1.90604800
H	3.44312300	-1.61511100	-2.02369700
H	2.22334900	-1.47095400	-3.29346900
C	1.71537300	-3.82972900	-1.94386100
H	1.56361600	-3.90727300	-3.02575300
H	2.74284100	-4.14200900	-1.72776000
H	1.03936300	-4.53664900	-1.45375100
C	-4.43512500	0.32111200	1.43302500
C	-2.58923200	-0.20358400	-3.36408500
C	-5.76591300	-0.37393300	1.78590700
H	-5.75744000	-0.69525500	2.83282300
H	-6.61573900	0.30406300	1.65213100
H	-5.93693300	-1.25491700	1.15995000
C	-3.39675800	-1.03195500	-4.38418400
H	-4.01306600	-1.78776200	-3.88807900
H	-4.05977300	-0.39493900	-4.97943600
H	-2.71833800	-1.54412400	-5.07473500
C	-4.18261700	1.53093400	2.35324800
H	-4.96788700	2.28719600	2.24481900
H	-4.18119900	1.20740000	3.39999500
H	-3.21777400	1.99711300	2.13669600
H	-3.63187300	-0.39686200	1.62059000
Cu	-0.33938400	1.15262600	-0.06759600
H	0.59016600	1.48136200	-1.24495400
C	-1.69026000	0.82508400	-4.07600400
H	-1.01940700	0.31489000	-4.77556700
H	-2.28125100	1.54669100	-4.65014100
H	-1.07754800	1.37417800	-3.35563700
H	-1.92803500	-0.89388700	-2.83311000

TS23

C	7.89240100	0.11895200	0.99382900
C	6.98551300	0.60971200	-0.14192400
H	7.86076500	0.84177000	1.82177500
H	7.49123500	-0.82186500	1.39753900
C	5.52821800	0.82835400	0.28421900
H	7.38859100	1.54881700	-0.54749900
H	7.01610600	-0.11482200	-0.96841400
H	5.12432100	-0.10962000	0.69139600
H	5.49622000	1.55581000	1.10792300
C	4.62790500	1.31424400	-0.85958100
C	3.17431900	1.52259700	-0.41877000
H	4.66848600	0.58369800	-1.67807000
H	5.02906200	2.25324800	-1.26493800
H	2.77172100	0.57326500	-0.03862700
H	3.15253100	2.19385700	0.44566100
C	9.34938400	-0.09518200	0.56463800
C	10.25801600	-0.59206000	1.69641900
H	9.75215800	0.84660900	0.16460700
H	9.38121200	-0.81477800	-0.26633200
C	11.71124900	-0.80040700	1.25788100

H	10.22559000	0.12574500	2.52751600	C	-4.06428000	2.49402600	2.63125900
H	9.85696700	-1.53446100	2.09411100	C	-4.74968200	3.25713800	1.68944000
H	12.33311700	-1.15774300	2.08551300	C	-4.86058400	2.81235400	0.37470800
H	11.77843200	-1.53708700	0.44884200	C	-4.28709900	1.60084500	-0.03245400
H	12.15144500	0.13371500	0.89007600	C	-3.59047300	0.85723200	0.94155000
C	2.21658400	2.02767900	-1.47942300	H	-3.98963100	2.84785000	3.65483400
C	2.53135600	2.07183000	-2.78215100	H	-5.20265800	4.19990900	1.98232400
H	1.80441700	2.39517700	-3.51939500	H	-5.40203500	3.41324200	-0.34925500
H	3.51098000	1.78785900	-3.15185400	C	0.48083600	-2.79155900	1.75130400
O	-0.15399800	2.07928800	-1.86493800	H	-0.48791000	-2.32482700	1.95077700
C	0.64992100	3.97198100	-0.58016800	C	1.55083500	-1.91995900	2.43662700
C	-0.75311200	4.16449300	0.01861000	H	1.35635200	-1.86312000	3.51301100
C	1.70737600	4.38234900	0.45586000	H	2.55505100	-2.33610100	2.30238600
C	0.78636800	4.89247600	-1.81969900	H	1.54586000	-0.90264400	2.03418000
H	-1.52769400	3.89957700	-0.70400500	C	0.44296200	-4.20637200	2.36265100
H	-0.88580600	3.54024100	0.90879200	H	0.24107500	-4.14774700	3.43739200
H	-0.89572500	5.21062300	0.31207600	H	-0.33756100	-4.81946400	1.90196500
H	2.71936000	4.35674200	0.04042900	H	1.39907200	-4.72409900	2.23123700
H	1.51609100	5.40975200	0.78591500	C	-1.16372300	-2.02398100	-3.08197800
H	1.67517300	3.73578500	1.33848300	H	-2.02338300	-1.64215500	-2.52435000
H	0.64291600	5.93709700	-1.52260900	C	-0.65069000	-0.87164700	-3.96732300
H	1.77542000	4.80321900	-2.27865200	H	-0.35025200	-0.00936000	-3.36489100
H	0.03311500	4.64177600	-2.57166300	H	0.20646600	-1.18680600	-4.57275100
C	0.80444600	2.50483000	-1.11430500	H	-1.44084600	-0.55168200	-4.65558600
C	-1.68270100	-0.49205500	0.09017100	C	-1.66206800	-3.20581500	-3.93767600
C	-3.58701500	-1.63766700	0.56741600	H	-2.46161100	-2.87433200	-4.60865500
C	-2.67331100	-2.53763600	0.11535100	H	-0.85822900	-3.61768300	-4.55718400
N	-1.51198500	-1.82426700	-0.17375600	H	-2.05458400	-4.01515300	-3.31409700
N	-2.96915600	-0.38880400	0.54629300	C	-2.74765700	0.45618900	3.34884800
Cl	-2.83002200	-4.22913900	-0.09102400	C	-4.44579600	1.13978200	-1.47843800
Cl	-5.19824100	-1.89662900	1.08249500	C	-3.72666100	-0.02490200	4.43880700
C	0.68219400	-2.84750000	0.23983900	H	-3.20402900	-0.65773300	5.16385300
C	-0.28402800	-2.39698500	-0.68299900	H	-4.16199900	0.81863700	4.98513200
C	-0.10693200	-2.47736000	-2.07919100	H	-4.54773700	-0.60659300	4.00860100
C	1.10104900	-3.01511700	-2.54196500	C	-5.93014300	0.92731700	-1.83773000
C	2.07929500	-3.45863300	-1.65619700	H	-6.40854200	0.21404100	-1.15946700
C	1.86870800	-3.37806800	-0.28196600	H	-6.49172500	1.86625500	-1.78994500
H	1.27515000	-3.08717600	-3.61102000	H	-6.01836700	0.53948600	-2.85802100
H	3.00790500	-3.87290200	-2.03816900	C	-1.56916800	1.23493500	3.96408500
H	2.63651500	-3.73444400	0.39764100	H	-1.91040800	2.13604700	4.48455700
C	-3.47019600	1.27443900	2.28289800	H	-1.04430300	0.60865100	4.69338700

H	-0.85290300	1.53516200	3.19340800
H	-2.32862100	-0.43419400	2.87203900
Cu	-0.39121800	0.90063600	-0.10080900
H	0.76549900	1.74944400	0.55544200
C	-3.76935800	2.11389100	-2.46299400
H	-3.87969700	1.74397800	-3.48835200
H	-4.23073400	3.10680900	-2.41927500
H	-2.70170600	2.21961500	-2.24976600
H	-3.94546700	0.17344200	-1.58665800
64			
C	7.23164100	0.23747400	-0.48109200
C	5.72500400	0.32615000	-0.20578000
H	7.51069600	1.00004700	-1.22240500
H	7.78289700	0.49051500	0.43600200
C	5.26987700	1.70512600	0.28817500
H	5.17375400	0.07069100	-1.12230600
H	5.44591600	-0.43455400	0.53695200
H	5.83138000	1.96771200	1.19654100
H	5.53631000	2.46381300	-0.46188500
C	3.76601500	1.79004600	0.58218700
C	3.33236500	3.18718100	1.07241100
H	3.49415400	1.04291100	1.33898800
H	3.20302000	1.52769100	-0.32336700
H	3.88194600	3.42217500	1.99331800
H	3.65017700	3.92212300	0.32447700
C	7.68437800	-1.14088000	-0.97907700
C	9.19153300	-1.23382000	-1.24997700
H	7.13626200	-1.39295500	-1.89857800
H	7.40293500	-1.90474400	-0.23955300
C	9.63249300	-2.61334000	-1.75016700
H	9.47374200	-0.46982100	-1.98727200
H	9.73962500	-0.98524300	-0.33088000
H	10.71171500	-2.64797100	-1.93290100
H	9.39353000	-3.39435500	-1.01894500
H	9.12777100	-2.87412800	-2.68770200
C	1.84055800	3.30082400	1.33190300
C	1.35756900	3.17682900	2.57476800
H	0.28949300	3.18950100	2.76292700
H	2.01525400	3.03785900	3.43025500
O	-0.32222200	2.85219700	0.26408700
C	0.64203200	5.01796700	-0.22123000
C	-0.10855000	5.06756700	-1.56718200
C	-0.22634800	5.67515500	0.86530600
C	1.94675800	5.82193700	-0.37134200
H	0.50080800	4.63652100	-2.37181200
H	-1.04255500	4.50454500	-1.51173500
H	-0.34070900	6.10287200	-1.84535700
H	0.28787400	5.68595300	1.83156100
H	-0.45660800	6.71268700	0.59409800
H	-1.16746700	5.13349100	0.98744300
H	1.72120100	6.84392200	-0.69907500
H	2.49631300	5.89571500	0.57240200
H	2.61295300	5.37918200	-1.12153700
C	0.91108900	3.49325300	0.12076600
C	-1.50853900	-0.63220900	0.03931700
C	-3.02692400	-2.29037600	-0.28789000
C	-1.87676400	-2.87035100	0.15062200
N	-0.95526500	-1.84450400	0.34654900
N	-2.78840300	-0.92082700	-0.35283600
Cl	-1.53750200	-4.52258300	0.43314100
Cl	-4.51738700	-3.01967900	-0.70171500
C	0.65106000	-1.99683300	2.19898400
C	0.40189800	-2.03880700	0.81262200
C	1.41056900	-2.27954900	-0.14156100
C	2.71173300	-2.47597000	0.33719700
C	2.99122200	-2.43796400	1.70098800
C	1.97177700	-2.19940300	2.61879500
H	3.51639900	-2.65938300	-0.36753000
H	4.00750100	-2.59659100	2.04984200
H	2.20243000	-2.17133500	3.67909500
C	-4.58422000	0.66776300	0.18586500
C	-5.50208000	1.62678600	-0.26101900
C	-5.59048200	1.96811000	-1.60785000
C	-4.76062200	1.35394100	-2.54203500
C	-3.82370100	0.38791800	-2.15469800
C	-3.75385400	0.06993200	-0.78325800
H	-6.15587500	2.11264200	0.45652400
H	-6.30972400	2.71508200	-1.93082300
H	-4.83939200	1.62872300	-3.58918800
C	-0.43906400	-1.74075800	3.23450000
H	-1.39108500	-1.62303600	2.70949400
C	-0.18015700	-0.43080900	4.00414400

H	-1.00382300	-0.23172400	4.69810700	C	2.57446300	-0.68708700	-0.10675100
H	0.74299100	-0.48943900	4.59072600	C	4.57658200	-1.25803700	-1.01373100
H	-0.09164200	0.41934200	3.32084600	C	3.84702700	-2.39955600	-0.88443000
C	-0.59552900	-2.93141000	4.20101500	N	2.62188500	-2.03609000	-0.33107100
H	-1.41749800	-2.74310600	4.89963700	N	3.78677500	-0.21727700	-0.53316500
H	-0.81255800	-3.85881400	3.66203500	Cl	4.27382600	-4.00633500	-1.28559700
H	0.31262100	-3.08991800	4.79218500	Cl	6.15669300	-1.04902400	-1.63385300
C	1.14301700	-2.31454200	-1.64323800	C	0.61293300	-3.24307600	-1.06379300
H	0.06556100	-2.21764300	-1.80261400	C	1.53746500	-2.95118600	-0.04050900
C	1.81398600	-1.12157400	-2.35224400	C	1.45774400	-3.51428500	1.24920600
H	1.46515100	-0.17044900	-1.93764200	C	0.39344700	-4.38927000	1.50194700
H	2.90346900	-1.15730900	-2.24523200	C	-0.53924800	-4.69410900	0.51386400
H	1.58097700	-1.13607200	-3.42239100	C	-0.42769600	-4.12780200	-0.75354700
C	1.57568700	-3.65202200	-2.27396200	H	0.29674600	-4.83875700	2.48531900
H	1.30931000	-3.66937200	-3.33590500	H	-1.35420800	-5.37842600	0.73123000
H	2.65809600	-3.80096100	-2.20265600	H	-1.16006800	-4.37567500	-1.51551500
H	1.08572600	-4.50008900	-1.78591600	C	3.88381700	2.00839000	-1.56948100
C	-4.51658300	0.32088700	1.66984700	C	4.27344200	3.35066300	-1.47794700
C	-2.92699800	-0.25806700	-3.20634500	C	4.93551200	3.83441500	-0.35273300
C	-5.85533300	-0.24598200	2.18147200	C	5.22634300	2.98240400	0.70947900
H	-5.76157200	-0.54307200	3.23130100	C	4.86195900	1.63068700	0.67472800
H	-6.65657900	0.49774000	2.11789600	C	4.18644800	1.17379000	-0.47496700
H	-6.16398400	-1.12384700	1.60546700	H	4.05344800	4.02534800	-2.29938400
C	-3.74888100	-0.97918600	-4.29219700	H	5.22700000	4.87952500	-0.30383800
H	-4.41383100	-1.73124300	-3.85655200	H	5.74369700	3.37146100	1.58096200
H	-4.36339500	-0.27623900	-4.86424700	C	0.70142300	-2.64420300	-2.46425900
H	-3.07955200	-1.48315400	-4.99733500	H	1.56877300	-1.97884100	-2.49950800
C	-4.07048700	1.53505900	2.50814700	C	-0.53860500	-1.78934200	-2.79017200
H	-4.79489600	2.35374600	2.44123100	H	-0.42075400	-1.31309600	-3.76941000
H	-3.98116900	1.25336500	3.56275300	H	-1.44619500	-2.40155100	-2.82643300
H	-3.10085700	1.91429500	2.17067600	H	-0.69089900	-1.00538700	-2.04253700
H	-3.76222200	-0.45930900	1.80516000	C	0.91653300	-3.73626200	-3.53102100
Cu	-0.76753000	1.09440700	0.15146800	H	1.02660100	-3.28019800	-4.52045900
H	1.46817800	3.10509300	-0.75578300	H	1.81515900	-4.32569500	-3.32536200
C	-1.96886700	0.77629200	-3.82989100	H	0.06514800	-4.42369500	-3.57432600
H	-1.29924900	0.28822800	-4.54606900	C	2.46352100	-3.21181100	2.35573400
H	-2.51997800	1.55716900	-4.36459300	H	3.21497400	-2.52327200	1.95933500
H	-1.35755600	1.26065600	-3.06208000	C	1.78875400	-2.50862800	3.54973700
H	-2.30910800	-1.01381300	-2.71355800	H	1.29796500	-1.58204100	3.23562200
65				H	1.03472500	-3.15054900	4.01753700
O	-0.09013600	1.36340100	1.43583900	H	2.53474800	-2.25970400	4.31190300

C	3.20581500	-4.48521300	2.80700200	H	-6.11780500	2.35761700	-1.99376200
H	3.95961400	-4.23420100	3.56055300	H	-5.38250700	2.00900400	-0.41675800
H	2.51978400	-5.21304600	3.25294100	C	-4.58131600	6.89397800	-2.65205700
H	3.71215100	-4.97080400	1.96701500	H	-4.05760100	7.84863700	-2.77512200
C	3.16524100	1.51458800	-2.82139200	H	-4.71987800	6.45970900	-3.64802600
C	5.19756900	0.72720200	1.85716400	H	-5.57028000	7.11122800	-2.23499700
C	4.06133200	1.63948400	-4.06958000	C	-6.26949600	-4.73608700	0.26338800
H	3.54612100	1.23210600	-4.94583500	C	-5.61598400	-3.42797900	-0.20078200
H	4.30546200	2.68537100	-4.28378500	H	-5.48857400	-5.48903200	0.44372900
H	5.00148200	1.09382500	-3.94265300	H	-6.76095000	-4.57142900	1.23308000
C	6.71814400	0.65042100	2.09680500	C	-4.59177300	-2.86133300	0.79060300
H	7.24550200	0.30309400	1.20307100	H	-5.12721600	-3.59197100	-1.17204100
H	7.13044300	1.62653800	2.37310300	H	-6.39886300	-2.67701300	-0.37982500
H	6.93635700	-0.04549400	2.91361200	H	-5.07779200	-2.70441100	1.76433400
C	1.82315000	2.24364100	-3.02613100	H	-3.80104900	-3.60593600	0.96222400
H	1.97152300	3.31514300	-3.19662000	C	-3.95679800	-1.54567500	0.32065800
H	1.30302000	1.83618200	-3.89948500	C	-2.93359600	-0.98403400	1.31215300
H	1.17165300	2.12734500	-2.15469200	H	-4.74871000	-0.80368100	0.14987100
H	2.93715300	0.45298900	-2.69048100	H	-3.47436100	-1.70763900	-0.65239000
Cu	1.17558200	0.30748600	0.66280000	H	-3.41021700	-0.88047600	2.29645500
C	4.45517000	1.17399900	3.13173500	H	-2.13853200	-1.73082700	1.46613200
H	4.67136800	0.48547900	3.95559100	C	-7.29205400	-5.29594800	-0.73338100
H	4.76586000	2.17665100	3.44423000	C	-7.95533200	-6.59950400	-0.27025800
H	3.37244000	1.19038800	2.97329900	H	-6.80009900	-5.46517100	-1.70223100
H	4.85551400	-0.28505800	1.62338900	H	-8.06999300	-4.54083300	-0.91731300
Si	-3.60134100	5.73369400	-1.55220500	C	-8.97648800	-7.14792500	-1.27229300
H	-2.29030400	5.39230700	-2.16497600	H	-7.17908200	-7.35533600	-0.08767300
O	-4.35955700	4.27344000	-1.34756200	H	-8.44697800	-6.43016500	0.69754800
O	-3.37554700	6.39424400	-0.03979600	H	-9.43263500	-8.07635000	-0.91268100
C	-2.54070700	7.52806000	0.21070000	H	-9.78335800	-6.42725100	-1.44892100
C	-2.42752000	7.74375700	1.71148200	H	-8.50709000	-7.36071400	-2.23980100
H	-2.96596500	8.42154800	-0.26835800	C	-2.26190900	0.32731100	0.94649100
H	-1.54364300	7.36470500	-0.22327900	C	-2.44758100	0.93810200	-0.23135200
H	-1.79329600	8.61043100	1.92472000	H	-1.91064000	1.84875200	-0.47323700
H	-3.41434300	7.92087100	2.15028900	H	-3.11671900	0.54956900	-0.99245600
H	-1.98841300	6.86478600	2.19290000	C	-1.90799200	2.01157000	2.91241600
C	-5.67624400	4.11193200	-0.80616200	C	-0.91012100	2.28890800	4.05464900
C	-6.09186300	2.65622200	-0.94106700	C	-2.13232800	3.31135600	2.12104300
H	-6.38604700	4.76078500	-1.33796700	C	-3.24227500	1.55573600	3.53140900
H	-5.67785500	4.41211400	0.24936000	H	-0.74188700	1.38688000	4.65664800
H	-7.08813100	2.50378000	-0.51297400	H	0.05266700	2.61348800	3.65349500

H	-1.29001700	3.06980100	4.72477400
H	-2.87308400	3.18039400	1.32684800
H	-2.49107800	4.10633700	2.78626100
H	-1.19770800	3.64183500	1.66071600
H	-3.61826800	2.31736900	4.22522300
H	-4.01215200	1.39637800	2.76948400
H	-3.12642100	0.62488600	4.10005200
C	-1.28253400	0.88518400	1.99715800
H	-1.08232400	0.04556700	2.69387100
TS24			
O	0.12609300	2.25760400	-0.17581600
C	1.43289300	-1.36689300	0.02606000
C	1.90415000	-3.56974000	-0.29138000
C	2.14744200	-3.28676700	1.01595900
N	1.84746900	-1.93939000	1.20108200
N	1.47336600	-2.38814500	-0.88899700
Cl	2.73138200	-4.31734200	2.25042600
Cl	2.06009100	-5.05889600	-1.11896600
C	0.92608700	-1.29959600	3.38867700
C	1.98129800	-1.22877600	2.45581500
C	3.16917000	-0.50745400	2.69622800
C	3.26444000	0.18378000	3.91084900
C	2.23162300	0.14981000	4.84356700
C	1.07916000	-0.58784400	4.58530300
H	4.16310800	0.75151100	4.12987800
H	2.32799400	0.69419900	5.77841500
H	0.28560600	-0.61524600	5.32547000
C	-0.13614600	-2.37622300	-2.75059900
C	-0.37120600	-2.22244800	-4.12309700
C	0.66913400	-1.95123600	-5.00720300
C	1.97446300	-1.83632100	-4.53680700
C	2.27138100	-1.98237000	-3.17595200
C	1.19303300	-2.23978000	-2.30310500
H	-1.38320600	-2.31961600	-4.50296200
H	0.46292400	-1.83457300	-6.06715400
H	2.77862100	-1.63112800	-5.23648800
C	-0.33921400	-2.12271700	3.16068300
H	-0.27738600	-2.58075500	2.16916400
C	-1.60410000	-1.24476300	3.17770700
H	-2.48917400	-1.85439600	2.96709600
H	-1.75135500	-0.77215700	4.15460000
H	-1.54872400	-0.45373300	2.42524200
C	-0.45748500	-3.26435900	4.19117100
H	-1.33863800	-3.87729000	3.97404200
H	0.42196800	-3.91391500	4.17439600
H	-0.56736900	-2.87163000	5.20758900
C	4.34551100	-0.48820000	1.72455300
H	4.04103400	-0.99875700	0.80705700
C	4.75285500	0.94387000	1.33072900
H	3.91340200	1.50074900	0.90506100
H	5.12984400	1.50578600	2.19192700
H	5.55431300	0.90946500	0.58493100
C	5.54658800	-1.26356000	2.30462100
H	6.36864000	-1.28334100	1.58124100
H	5.91814200	-0.79091800	3.22030300
H	5.27927000	-2.29727800	2.54492200
C	-1.29906400	-2.70567200	-1.82073100
C	3.72071700	-1.87566700	-2.70921600
C	-1.84417000	-4.12226000	-2.09521900
H	-2.64575800	-4.36287000	-1.38879000
H	-2.25625200	-4.19850000	-3.10722500
H	-1.06154900	-4.88015100	-1.99325900
C	4.59221400	-2.98752000	-3.32793000
H	4.19468900	-3.98173200	-3.10381700
H	4.65278800	-2.88615500	-4.41671300
H	5.61154800	-2.93061600	-2.93173800
C	-2.42267000	-1.65716800	-1.91821100
H	-2.87874000	-1.64685900	-2.91366900
H	-3.21348000	-1.88663000	-1.19623500
H	-2.04869700	-0.65044100	-1.70917400
H	-0.92944200	-2.69000500	-0.79166600
Cu	1.06186000	0.46346000	-0.32072200
C	4.31326800	-0.48504300	-3.00661400
H	5.33666900	-0.42262300	-2.62125700
H	4.35117100	-0.28883400	-4.08342400
H	3.72039700	0.30562400	-2.53904700
H	3.74453300	-2.00950800	-1.62393700
Si	1.36397000	3.14489900	-1.26386300
H	1.84837900	1.62227800	-1.32942800
O	0.18068600	4.32887300	-1.64499300
O	2.39391800	3.76182500	-0.06504400
C	2.98341000	5.05255100	-0.15490100

C	4.02671700	5.21620300	0.94253000	H	11.62879400	-2.29056500	-1.21561000
H	2.21166900	5.82989400	-0.05100900	C	-2.36552400	2.31549800	-0.09256300
H	3.45722500	5.19661900	-1.13725400	C	-2.60868600	3.01247800	-1.20831400
H	4.48187100	6.21153200	0.89385600	H	-1.85442700	3.67431700	-1.61293700
H	3.57148100	5.09336600	1.93034200	H	-3.54578000	2.91446000	-1.74814000
H	4.81955100	4.46884700	0.83629500	C	-0.95474200	3.56510000	1.74567800
C	0.29928700	5.35165200	-2.62386200	C	0.35393600	3.39191700	2.54301200
C	-0.87036900	6.32375300	-2.50910800	C	-1.01637500	4.98256000	1.15433200
H	0.31600500	4.91822100	-3.63392700	C	-2.13346500	3.41932600	2.73447600
H	1.23935900	5.90855100	-2.50401000	H	0.39652300	2.40422700	3.01899400
H	-0.77548500	7.11520600	-3.26103900	H	1.22486000	3.50295100	1.89554600
H	-1.82556000	5.81451700	-2.66940200	H	0.40953900	4.14403500	3.33972100
H	-0.89594100	6.78982900	-1.51959800	H	-1.94283200	5.13434000	0.59232600
C	2.37929900	3.27495800	-2.91839200	H	-0.98991100	5.71801600	1.96789600
H	3.32303300	2.73526600	-2.77596200	H	-0.18528500	5.17273700	0.47781000
H	1.83506100	2.75198800	-3.71767700	H	-2.02233700	4.15202000	3.54163500
H	2.61396400	4.27817700	-3.29134800	H	-3.09889200	3.60538600	2.25396000
C	-7.99036500	-0.87280600	0.48706200	H	-2.16258000	2.42557200	3.19623200
C	-7.05926900	0.15566400	-0.16762900	C	-1.04065900	2.41022800	0.67921600
H	-7.52201500	-1.86664400	0.44061900	H	-1.00083900	1.50092800	1.29511700
H	-8.09642300	-0.63768900	1.55595000	66			
C	-5.67016800	0.22556800	0.47939300	O	-5.59851500	1.42382300	0.21261200
H	-6.95012600	-0.08219600	-1.23549600	C	2.90088900	0.66143600	-0.15650600
H	-7.52863600	1.14894900	-0.12496200	C	5.08288000	0.05426100	0.00967000
H	-5.77934900	0.47065200	1.54565300	C	4.81117500	0.88954900	1.05007600
H	-5.20408700	-0.76989800	0.44381000	N	3.47257500	1.25303200	0.93509200
C	-4.73799800	1.24738200	-0.18532600	N	3.90476900	-0.07549800	-0.71998100
C	-3.35694100	1.30894700	0.47437400	Cl	5.84664700	1.43888900	2.29540500
H	-5.20473900	2.24108600	-0.15030500	Cl	6.54991200	-0.72570200	-0.39619500
H	-4.63065100	0.99706300	-1.24893400	C	2.12074300	1.56988100	2.96129800
H	-3.49046500	1.49068400	1.54803900	C	2.77024200	2.13484700	1.84548300
H	-2.89030100	0.31352400	0.41725400	C	2.76637000	3.51784000	1.57476400
C	-9.38128200	-0.93912800	-0.15612900	C	2.06722900	4.34297500	2.46473100
C	10.31015500	-1.97271200	0.49372200	C	1.40899800	3.81465900	3.57202800
H	-9.27625600	-1.16977800	-1.22618000	C	1.43804900	2.44425200	3.81615400
H	-9.85270500	0.05301700	-0.10532600	H	2.03637600	5.41305500	2.28545400
C	11.69800200	-2.03054600	-0.15293500	H	0.87201700	4.47372100	4.24793200
H	-9.84002900	-2.96433600	0.44069500	H	0.92116500	2.04480800	4.68319300
H	10.41382400	-1.74325200	1.56316200	C	3.35960700	-2.22516700	-1.77634600
H	12.33563900	-2.77763300	0.33147700	C	3.20959200	-2.97384600	-2.95053300
H	12.20761500	-1.06251300	-0.08316500	C	3.44330500	-2.40803100	-4.20102600

C	3.83719900	-1.07671400	-4.30514900	Cu	1.07021100	0.83117600	-0.77748300
C	4.00506100	-0.27917000	-3.16609400	C	3.36993000	1.99851800	-4.06854800
C	3.75218900	-0.87905400	-1.91624300	H	3.67566900	3.04840700	-4.12921400
H	2.90389800	-4.01329900	-2.88354700	H	3.22803300	1.63199800	-5.09086600
H	3.31891900	-3.00751300	-5.09810300	H	2.40367900	1.95199700	-3.55636600
H	4.01654900	-0.64740900	-5.28586100	H	4.53854500	1.61098200	-2.32218500
C	2.12691300	0.07403300	3.26021700	Si	-5.42832800	1.69283900	-1.41324300
H	2.73299200	-0.42656100	2.49984900	H	-0.36492900	0.96624600	-1.27107500
C	0.70664800	-0.51815800	3.17084700	O	-6.98335000	1.50623300	-1.97415200
H	0.73642000	-1.59989800	3.33919100	O	-4.90079300	3.24055300	-1.70754400
H	0.04449100	-0.08033400	3.92548300	C	-5.56327100	4.42321000	-1.24527500
H	0.26386500	-0.33578400	2.18654600	C	-4.77748600	5.64370600	-1.69677100
C	2.77118700	-0.22885900	4.62711900	H	-5.63956100	4.40272000	-0.15053300
H	2.81809100	-1.31067400	4.78997200	H	-6.58554800	4.45848200	-1.64534200
H	3.78914300	0.16871600	4.68489600	H	-5.26916500	6.56045600	-1.35490200
H	2.19262500	0.20553600	5.44904800	H	-3.76274900	5.62178100	-1.28772400
C	3.47059900	4.13308400	0.36938500	H	-4.70732400	5.67564300	-2.78853500
H	3.98707600	3.33487200	-0.17102300	C	-7.35524000	1.75418500	-3.33405300
C	2.45639000	4.75997300	-0.60739800	C	-8.85661300	1.56538300	-3.48137100
H	1.72321600	4.02013500	-0.94406000	H	-6.82046000	1.06226900	-3.99954100
H	1.91128400	5.58659400	-0.13944500	H	-7.06968000	2.77451200	-3.62370300
H	2.97389700	5.15596000	-1.48760500	H	-9.16321100	1.74518500	-4.51699600
C	4.53978500	5.15771700	0.79613100	H	-9.14545500	0.54618100	-3.20692600
H	5.06721400	5.53950700	-0.08426500	H	-9.39807000	2.26223100	-2.83419200
H	4.09380100	6.01430200	1.31225800	C	-4.19690500	0.57537100	-2.25339200
H	5.27862100	4.70810500	1.46668400	H	-4.16071800	0.78369000	-3.32753400
C	3.09266600	-2.87907300	-0.42454300	H	-3.18766300	0.72443400	-1.85573200
C	4.43699700	1.17574700	-3.32021300	H	-4.46842400	-0.47555600	-2.11857600
C	4.04699900	-4.06220800	-0.16987800	C	-1.78199600	-6.45957000	0.67040000
H	3.87352600	-4.47877600	0.82791100	C	-3.06785800	-5.62319100	0.65756300
H	3.89171100	-4.86607100	-0.89698600	H	-1.12068100	-6.11936700	-0.13956000
H	5.09412400	-3.75013900	-0.23139100	H	-1.23636700	-6.27145300	1.60636200
C	5.81133100	1.29001000	-4.00852200	C	-2.81987500	-4.11576000	0.79640900
H	6.57813700	0.73059700	-3.46384800	H	-3.61562400	-5.81507500	-0.27614200
H	5.77980500	0.90811300	-5.03426700	H	-3.72733200	-5.95910800	1.47066500
H	6.12289500	2.33877600	-4.05460000	H	-2.27101700	-3.92274300	1.72924400
C	1.61942500	-3.31308200	-0.29549200	H	-2.16187000	-3.78084900	-0.01807900
H	1.36449000	-4.08418700	-1.03034700	C	-4.10773400	-3.28162000	0.78283900
H	1.43244700	-3.72689700	0.70099100	C	-3.83825300	-1.77791300	0.89850900
H	0.94361600	-2.46551000	-0.44732900	H	-4.75869800	-3.60441900	1.60660900
H	3.27992600	-2.13886700	0.35839700	H	-4.65981000	-3.48669300	-0.14397000

H	-3.24485100	-1.59112800	1.80249400
H	-3.18388600	-1.46704300	0.06956200
C	-2.02746900	-7.96652500	0.52278700
C	-0.74156700	-8.80291100	0.53529400
H	-2.57263400	-8.15557900	-0.41324400
H	-2.68861200	-8.30797200	1.33241200
C	-0.99515400	-10.30677900	0.38776200
H	-0.08129100	-8.46236400	-0.27417200
H	-0.19685600	-8.61389100	1.47058400
H	-0.05874100	-10.87452100	0.40197400
H	-1.62526300	-10.68371400	1.20170900
H	-1.50616700	-10.53142400	-0.55561800
C	-5.04877900	-0.86219000	0.89134900
C	-6.30092200	-1.29395100	0.70037100
H	-7.12877900	-0.59609400	0.63900300
H	-6.53530300	-2.34564500	0.57466200
C	-4.85382900	1.19708900	2.50362500
C	-4.33208500	2.64827400	2.49389700
C	-6.31263300	1.18559300	2.99544700
C	-3.98705300	0.37261400	3.47410700
H	-3.29092800	2.69244700	2.15301500
H	-4.93277300	3.27808900	1.83346800
H	-4.37284800	3.07496700	3.50227900
H	-6.70643500	0.16705600	3.05965800
H	-6.37274700	1.63314700	3.99374800
H	-6.95742100	1.75962700	2.32500200
H	-4.01012900	0.83108800	4.46882800
H	-4.35236000	-0.65368700	3.57676600
H	-2.93958500	0.33627000	3.15311000
C	-4.74124500	0.63089200	1.04570400
H	-3.69603700	0.78392700	0.73750500

67

C	6.07341200	0.30574900	0.42281700
C	4.88709800	-0.10677200	-0.45713800
H	5.85328800	1.27223300	0.89856800
H	6.18470800	-0.41739300	1.24342000
C	3.55988800	-0.19892000	0.30581300
H	4.78062900	0.61166700	-1.28240200
H	5.10386800	-1.07713900	-0.92623500
H	3.66707000	-0.91140200	1.13600000
H	3.33934500	0.77411100	0.76747900
C	2.37881100	-0.62175000	-0.57705600
C	1.05610400	-0.68641800	0.19196800
H	2.59257600	-1.60201200	-1.02367800
H	2.28374500	0.08277500	-1.41389400
H	1.17670500	-1.35469100	1.05472200
H	0.84656800	0.30053600	0.63336300
C	7.39813300	0.40980100	-0.34274300
C	8.58643200	0.81661600	0.53727000
H	7.28855900	1.13652400	-1.16059100
H	7.61737500	-0.55493600	-0.82265600
C	9.90411100	0.92415400	-0.23632500
H	8.36591500	1.77871000	1.01963400
H	8.69875700	0.08803100	1.35177200
H	10.73168400	1.21406600	0.41953100
H	10.16850500	-0.03185200	-0.70279300
H	9.83445700	1.67211900	-1.03446500
C	-0.17302800	-1.10401500	-0.59426600
C	-0.16543400	-1.32566400	-1.91344700
H	-1.07875000	-1.56836300	-2.44526200
H	0.73996100	-1.25220900	-2.50615700
C	-1.87073700	-2.62568100	0.70410200
C	-3.07175000	-2.48420400	1.66137500
C	-2.26897300	-3.52692200	-0.47768400
C	-0.70640300	-3.28013800	1.47139800
H	-2.81914300	-1.85549800	2.52340900
H	-3.92912900	-2.03558200	1.15417200
H	-3.37448000	-3.46583800	2.04197800
H	-1.42833900	-3.69090300	-1.15777800
H	-2.59644900	-4.50443500	-0.10700100
H	-3.09127300	-3.08603500	-1.04716600
H	-1.02681000	-4.24623800	1.87604300
H	0.15689100	-3.46396400	0.82450700
H	-0.37857600	-2.66329600	2.31608400
C	-1.46604600	-1.19130300	0.22136800
H	-1.32325100	-0.58631900	1.12683800
O	-2.57987100	-0.65239000	-0.50983500
Si	-2.94429300	0.94952900	-0.71650200
O	-4.58459500	1.07071600	-0.90878600
O	-2.42292400	1.69360000	0.67682200
C	-2.51838800	3.10448800	0.90940700
C	-2.03472300	3.41200700	2.31653400

H	-3.55824300	3.43405300	0.78376000	H	3.68080100	-0.58401800	-2.10791300
H	-1.90919000	3.64492400	0.17241400	H	2.60478300	-1.08778200	-0.81010800
H	-2.09613700	4.48715800	2.51315100	C	2.61960500	-3.00681000	-2.77728000
H	-2.64658600	2.88918100	3.05777400	H	4.70908600	-2.81441300	-2.28373800
H	-0.99473500	3.09649100	2.44400800	H	3.71146200	-3.42829500	-0.96765700
C	-5.55090500	0.55569200	0.01727600	C	2.73410700	-4.41602000	-3.36509700
C	-6.89707300	1.20856900	-0.25002000	H	1.64968000	-2.89217100	-2.27761900
H	-5.23045200	0.75306000	1.04851800	H	2.63672700	-2.26769700	-3.58847800
H	-5.62232300	-0.53230400	-0.10497900	H	1.91986900	-4.61484600	-4.06848300
H	-7.65415900	0.81151300	0.43397100	H	3.67962300	-4.54621200	-3.90329700
H	-6.83737000	2.29198000	-0.10801900	H	2.69005200	-5.17839200	-2.57948900
H	-7.22341400	1.01345900	-1.27609400	C	4.44647000	0.80463500	-0.32995100
C	-2.20815400	1.70979200	-2.24990300	C	5.11630600	1.63853400	0.76185600
H	-1.11701500	1.64296700	-2.22900300	H	3.37117600	0.99937500	-0.35122600
H	-2.56005500	1.18270800	-3.14204800	H	4.87050400	1.05337100	-1.30649600
H	-2.48976300	2.76284000	-2.34993800	C	4.99364600	3.13432400	0.42167800
68				H	4.63874500	1.46074700	1.73012200
Si	0.05628600	1.02178500	-0.02811000	H	6.17775000	1.38997900	0.87869200
O	1.22179500	1.78104000	-1.04176700	C	5.61120800	4.03154500	1.49782500
O	-0.26305700	1.57326500	1.55925300	H	5.47943500	3.32948100	-0.54307000
C	0.33623500	1.16256800	2.77083100	H	3.93444800	3.38696600	0.29301800
C	1.48471100	2.08381600	3.17410500	H	5.51480300	5.08805700	1.22989100
H	0.69941900	0.13082500	2.70810500	H	5.11768700	3.88661300	2.46493200
H	-0.44005900	1.19196300	3.55076000	H	6.67733400	3.81620300	1.63127300
H	1.90399100	1.79081000	4.14437300	C	4.17542200	-1.10923600	1.21280200
H	2.27787200	2.04043800	2.42227200	C	3.71101400	-2.53682200	1.50066200
H	1.14069300	3.12082700	3.24751700	H	3.34278500	-0.44252800	1.43625700
C	0.98814900	2.80988200	-1.98786000	H	5.02959300	-0.84886000	1.84118800
C	2.24444700	3.01560600	-2.82842900	C	3.43499400	-2.68689100	3.00714100
H	0.72233300	3.74977300	-1.48437700	H	2.78529900	-2.74288300	0.95464400
H	0.14244100	2.56061400	-2.63903100	H	4.44697000	-3.28602400	1.20035000
H	2.08458900	3.80391100	-3.57307300	C	2.91449300	-4.08018000	3.37070500
H	3.09534100	3.30641900	-2.20334000	H	4.35563400	-2.48079800	3.56890700
H	2.51232800	2.09505000	-3.35889400	H	2.70550800	-1.92910200	3.31974500
C	-0.69904600	-0.64037500	-0.58661900	H	2.73067000	-4.16210700	4.44630400
H	-0.55925100	-1.41641500	0.17389800	H	1.97389400	-4.29887900	2.85374300
H	-1.75662600	-0.57630700	-0.84946900	H	3.63556500	-4.85768200	3.09480400
H	-0.16122200	-0.98356300	-1.48121000	C	8.70245400	-3.86798100	-0.11226700
N	4.58242800	-0.73392400	-0.21718500	C	8.05606000	-2.55849900	-0.57280600
C	3.58356000	-1.26563200	-1.25952700	H	9.73590500	-3.94017000	-0.46425400
C	3.74581100	-2.69442100	-1.77565100	H	8.71573100	-3.94060200	0.98070100

H	8.15674100	-4.73613400	-0.49756500	C	-2.74648500	4.42617100	-1.45059200
C	6.59932600	-2.42316600	-0.09724200	C	-4.27014300	4.00888700	0.49465700
H	8.64176400	-1.70842400	-0.19981100	H	-1.89727700	4.04410800	1.89239300
H	8.08832100	-2.49828900	-1.66827400	H	-0.82310400	4.31998000	0.51985900
C	6.02817500	-1.08488300	-0.56464200	H	-2.04849800	5.53774300	0.94570200
H	6.01973000	-3.26665800	-0.47901900	H	-3.48681800	4.01557400	-2.14349000
H	6.57944500	-2.48134300	0.99598100	H	-2.91765400	5.50722300	-1.37833100
H	6.63791200	-0.28925000	-0.13565300	H	-1.75251000	4.26243500	-1.87381500
H	6.09546600	-0.99423100	-1.65189000	H	-4.46508600	5.08333800	0.59436800
F	1.46413500	0.10084600	0.56688400	H	-5.03994400	3.59573200	-0.16501200
C	-8.85262800	-2.04908200	0.63612100	H	-4.39455300	3.56147500	1.48800200
C	-7.88114500	-1.39058500	-0.35116000	C	-2.50333100	2.23661200	-0.11808700
H	-8.30686200	-2.78116200	1.24855600	H	-2.51457900	1.89809700	0.92970700
H	-9.22828200	-1.28890700	1.33615200	O	-1.21787400	2.07715700	-0.66192400
C	-6.70133900	-0.68281200	0.32630800	TS25			
H	-7.49789500	-2.15252500	-1.04503800	Si	0.39958300	-0.63386100	-0.18730900
H	-8.42956900	-0.66609000	-0.97017500	O	1.07646100	0.12364100	-1.49180700
H	-7.08660000	0.07944000	1.01873600	O	0.80038700	0.03999700	1.27142300
H	-6.15239800	-1.40556800	0.94684400	C	-0.06733300	0.76286600	2.16485000
C	-5.73292400	-0.02463000	-0.66489600	C	0.77537900	1.49331400	3.19680900
C	-4.57048200	0.69560900	0.02501200	H	-0.73089800	0.04422000	2.66682600
H	-6.28444300	0.68957100	-1.29156600	H	-0.66818800	1.44553100	1.55747800
H	-5.34217000	-0.79085600	-1.34749700	H	0.12615100	2.02306400	3.90247300
H	-4.97788900	1.41121500	0.75107400	H	1.40490200	0.80158100	3.76736200
H	-4.01088400	-0.02894300	0.63801000	H	1.42496700	2.23217900	2.71529700
C	-10.04065000	-2.74215600	-0.04188300	C	0.48575500	0.98338200	-2.48643000
C	-11.01141300	-3.40467600	0.94339700	C	0.07799000	0.17774400	-3.71218500
H	-9.66662700	-3.50042000	-0.74506000	H	1.26099900	1.71093200	-2.76047500
H	-10.58865300	-2.00896800	-0.65117900	H	-0.36189000	1.50717400	-2.03120100
C	-12.19839400	-4.08707100	0.25672600	H	-0.29770200	0.84587100	-4.49572900
H	-10.46537500	-4.14148400	1.54835900	H	0.92443600	-0.38573600	-4.12024300
H	-11.38222200	-2.64859900	1.64892600	H	-0.71838600	-0.53172300	-3.46444300
H	-12.87009700	-4.55306200	0.98529700	C	-1.25615500	-1.45972500	-0.36466000
H	-12.78592600	-3.36742600	-0.32488700	H	-1.57486200	-1.85327300	0.60744000
H	-11.86048400	-4.86969500	-0.43243400	H	-2.00494100	-0.75297700	-0.72023400
C	-3.56521600	1.40629000	-0.86347700	H	-1.17633400	-2.30570800	-1.05625900
C	-3.55999900	1.28009300	-2.19548000	N	4.88566600	-0.13425900	-0.27155300
H	-2.78497200	1.74673700	-2.79335300	C	4.44609500	-1.17241600	-1.31854700
H	-4.29840000	0.68915200	-2.72833800	C	5.24809800	-2.46545600	-1.46469700
C	-2.85201600	3.77674000	-0.05983300	H	4.48215600	-0.63933000	-2.27141900
C	-1.84300300	4.46189800	0.88154400	H	3.39942200	-1.38123200	-1.09441700

C	4.59149500	-3.34787200	-2.54189800	H	8.87782700	0.61566700	0.69433000
H	6.27863600	-2.25045100	-1.76737700	H	9.04143400	-0.54121200	-0.61799300
H	5.29256700	-3.02734200	-0.52917000	C	6.40085600	0.07698400	-0.26860900
C	5.36162000	-4.64953600	-2.77967900	H	7.15060000	-1.88672200	0.32392100
H	3.56137100	-3.57619000	-2.24185000	H	6.99160400	-0.73656900	1.64891600
H	4.52194400	-2.78562400	-3.48201100	H	6.55553300	1.10439100	0.06168900
H	4.87370700	-5.25818000	-3.54691300	H	6.70259600	0.02375100	-1.31761000
H	6.38589100	-4.44949200	-3.11312700	F	1.45702600	-1.90750300	-0.12818800
H	5.41968300	-5.24951200	-1.86494100	C	-9.40903400	-1.56466100	0.72444000
C	4.24761900	1.18616600	-0.76551700	C	-8.32398900	-1.08619700	-0.24833800
C	4.27573300	2.37616700	0.19212800	H	-8.95871500	-2.24036900	1.46580700
H	3.21478600	0.93081900	-1.01654400	H	-9.79198500	-0.70460200	1.29235600
H	4.78103600	1.42966500	-1.68805600	C	-7.15096100	-0.37696200	0.43952600
C	3.70530300	3.62197700	-0.50894500	H	-7.94315500	-1.94623600	-0.81767600
H	3.67377700	2.16856200	1.08136300	H	-8.77366500	-0.40878600	-0.98846600
H	5.29282400	2.59957400	0.53419500	H	-7.53176300	0.48318900	1.00884700
C	3.68223200	4.84663300	0.40984800	H	-6.70330400	-1.05501300	1.18049700
H	4.30225900	3.84375100	-1.40298900	C	-6.06451800	0.09815300	-0.53415500
H	2.68795200	3.40712900	-0.85752900	C	-4.89346600	0.79173000	0.16983400
H	3.27508700	5.71825900	-0.11122200	H	-6.50984700	0.78251600	-1.26932800
H	3.06030200	4.66614300	1.29311400	H	-5.69385200	-0.76292500	-1.10634200
H	4.68962800	5.10369300	0.75594800	H	-5.28387100	1.61896100	0.77723800
C	4.30097600	-0.42559000	1.11713200	H	-4.45908800	0.09633100	0.90619200
C	4.29394000	-1.86766200	1.62301000	C	-10.57971700	-2.27770600	0.03683500
H	3.26515800	-0.08397000	1.07505700	C	-11.66409400	-2.75813200	1.00935800
H	4.84379700	0.22361900	1.80701400	H	-10.19742800	-3.13783800	-0.53160700
C	3.69379600	-1.90435400	3.03977500	H	-11.03181600	-1.60246700	-0.70393700
H	3.67012500	-2.48221600	0.96910100	C	-12.82840100	-3.47030900	0.31389600
H	5.29529200	-2.30406800	1.64829900	H	-11.21209300	-3.43235600	1.74972000
C	3.61300400	-3.32722800	3.59989700	H	-12.04720400	-1.89877500	1.57638200
H	4.29801500	-1.27903700	3.71025700	H	-13.58351100	-3.80276600	1.03392700
H	2.69211700	-1.45971000	3.01292800	H	-13.32347200	-2.80833400	-0.40584700
H	3.18430000	-3.32878200	4.60672800	H	-12.48075100	-4.35285500	-0.23540600
H	2.98464300	-3.96479300	2.96866800	C	-3.75376600	1.30377600	-0.69207100
H	4.60488600	-3.78925600	3.65844900	C	-3.68774800	1.06683800	-2.00870900
C	9.67686500	-1.29818700	1.30504200	H	-2.82071300	1.38838400	-2.57614400
C	8.75042100	-0.44339800	0.43574100	H	-4.46231100	0.53371800	-2.55288900
H	10.72197400	-1.00402500	1.17000500	C	-2.81502500	3.63495500	0.01887900
H	9.43392600	-1.19081600	2.36778400	C	-1.78238800	4.23384700	0.99007600
H	9.59256200	-2.35991500	1.04907500	C	-2.53535000	4.17875300	-1.39016300
C	7.27110500	-0.83550400	0.59486600	C	-4.22119400	4.07043500	0.46406300

H	-1.97984100	3.91132300	2.02085300
H	-0.78336400	3.88874900	0.71453400
H	-1.80257600	5.33130500	0.97452200
H	-3.28492900	3.83263500	-2.10925300
H	-2.54319700	5.27673200	-1.39847400
H	-1.55497300	3.83328700	-1.72895000
H	-4.29185500	5.16511600	0.51529500
H	-4.99425700	3.72640000	-0.23150400
H	-4.46412800	3.68263000	1.46126300
C	-2.61019500	2.04571200	0.05799900
H	-2.80003100	1.80506800	1.14387100
O	-1.35643600	1.69628900	-0.34048600

69

N	-3.30999400	-0.70535100	0.38590800
C	-2.12244200	-0.95192400	1.33340800
C	-1.52581000	-2.35521100	1.42524400
H	-2.50598200	-0.68792400	2.32325600
H	-1.39841600	-0.17794500	1.03590500
C	-0.36694800	-2.34438000	2.43867400
H	-2.27458100	-3.08224800	1.76171600
H	-1.14709000	-2.70454600	0.46206100
C	0.29454400	-3.71696300	2.59035400
H	0.37815600	-1.60217400	2.12697000
H	-0.74216600	-2.00918600	3.41465700
H	1.10889300	-3.68328900	3.32083900
H	-0.42578900	-4.47058100	2.92849600
H	0.71437900	-4.06238500	1.63902100
C	-3.90560300	0.62453700	0.90718700
C	-4.97822100	1.29021100	0.04583800
H	-3.03835900	1.28751400	0.99640900
H	-4.30891200	0.38822000	1.89597700
C	-5.54511100	2.51789400	0.77964600
H	-4.55126100	1.61686700	-0.90699100
H	-5.80582800	0.60957300	-0.18801200
C	-6.59613500	3.26202300	-0.04883900
H	-5.98550600	2.20179600	1.73419800
H	-4.72315700	3.20027500	1.02930900
H	-6.98281800	4.13013500	0.49385600
H	-6.17371800	3.62019200	-0.99401800
H	-7.44554900	2.61251800	-0.28878300
C	-2.84708400	-0.42710000	-1.05138900
C	-1.78689600	-1.33457200	-1.67345000
H	-2.40208700	0.57552300	-0.97841100
H	-3.75599400	-0.42065900	-1.65700100
C	-1.57515800	-0.93158000	-3.14295900
H	-0.84182200	-1.20035300	-1.13833600
H	-2.04649300	-2.39539700	-1.63220600
C	-0.45915400	-1.73446600	-3.81729400
H	-2.51299800	-1.06814600	-3.69764800
H	-1.33938700	0.13879000	-3.19326000
H	-0.33214800	-1.43371800	-4.86200300
H	0.49888300	-1.58320900	-3.30787200
H	-0.67746900	-2.80833100	-3.80339900
C	-5.40803400	-5.25761400	-0.88907200
C	-5.44690300	-3.98638800	-0.03634100
H	-6.24906900	-5.91607000	-0.65153700
H	-5.46064700	-5.01987700	-1.95715500
H	-4.48404600	-5.82086600	-0.71837000
C	-4.27549400	-3.03774600	-0.34271200
H	-6.39612800	-3.46089100	-0.20342800
H	-5.42802500	-4.25714100	1.02728800
C	-4.38865700	-1.77421300	0.51045100
H	-3.33525700	-3.56393100	-0.16171000
H	-4.30180800	-2.77663400	-1.40589700
H	-5.33062800	-1.28388000	0.26235800
H	-4.42680700	-2.02934800	1.57324400
C	7.28390800	-0.38848200	-0.53065600
C	6.08429800	-0.08701500	0.37594800
H	6.96548000	-1.06021500	-1.34087000
H	7.61246500	0.54009000	-1.01913900
C	4.88707800	0.52039100	-0.36577900
H	5.76641800	-1.01371000	0.87520200
H	6.39905500	0.59563800	1.17829300
H	5.20223200	1.44691100	-0.86691400
H	4.57383900	-0.16477300	-1.16687100
C	3.68890100	0.81531800	0.54564600
C	2.48268300	1.38289300	-0.20985300
H	3.99657000	1.51832100	1.33169900
H	3.39522900	-0.10825500	1.06262300
H	2.79477900	2.28483200	-0.75302100
H	2.19677200	0.67454500	-1.00434400
C	8.47026100	-1.01804900	0.20962300

C	9.67101800	-1.32022400	-0.69525400
H	8.14158600	-1.94775200	0.69626000
H	8.78948600	-0.34856700	1.02143900
C	10.84753500	-1.95619200	0.05151600
H	9.35160700	-1.98581900	-1.50880900
H	10.00303700	-0.39050900	-1.17718100
H	11.68834600	-2.15681300	-0.62070600
H	11.21025000	-1.30003100	0.85116800
H	10.55600200	-2.90685900	0.51271700
C	1.23173100	1.68684500	0.59498800
C	1.13839600	1.41864800	1.90414500
H	0.19936800	1.58373300	2.42190700
H	1.96238300	1.01915900	2.48830100
C	-0.05675500	3.82911900	-0.18579400
C	-1.15745100	4.22709700	-1.18554100
C	-0.44907300	4.33382300	1.21073900
C	1.26353300	4.48942100	-0.61574500
H	-0.87818800	3.94378800	-2.20904400
H	-2.08388600	3.70544600	-0.93370100
H	-1.33914300	5.30952200	-1.17766800
H	0.34206100	4.13909500	1.94213800
H	-0.64330900	5.41408800	1.20198400
H	-1.35216400	3.81550300	1.54347900
H	1.14597500	5.57785600	-0.70052800
H	2.06517400	4.30414700	0.10726500
H	1.59739400	4.12243500	-1.59460800
C	0.00905500	2.23062300	-0.19816900
H	0.26076900	2.00555500	-1.27237500
O	-1.17400700	1.67713500	0.19038300

70

C	4.22088700	0.39499100	-0.32906200
C	2.99533400	-0.39222000	0.15081700
H	4.25473200	0.37996000	-1.42787200
H	4.10760600	1.45073000	-0.04380400
C	1.66873200	0.13137900	-0.41306100
H	3.11300300	-1.44996000	-0.12480000
H	2.95686900	-0.36788500	1.24921900
H	1.55618100	1.19292400	-0.15062700
H	1.70106000	0.09182000	-1.51117200
C	0.44636300	-0.64786100	0.08893700
C	-0.86993500	-0.13422300	-0.50188400
H	0.40537200	-0.58876700	1.18466700
H	0.56993900	-1.71081500	-0.15707500
H	-0.95877600	0.94006100	-0.29501600
H	-0.82111600	-0.20044300	-1.60005300
C	5.54738100	-0.13926700	0.22466400
C	6.77400000	0.65280900	-0.24449800
H	5.66457600	-1.19292800	-0.06717700
H	5.51154600	-0.13200900	1.32360600
C	8.09412200	0.10777200	0.30913500
H	6.80848000	0.64867200	-1.34252600
H	6.65949500	1.70461900	0.05117900
H	8.94924900	0.69482700	-0.04182200
H	8.10279100	0.12948100	1.40496900
H	8.25414100	-0.93129100	-0.00099800
C	-2.13891800	-0.83614200	-0.05579200
C	-2.14537200	-1.90907600	0.74504000
H	-3.07374700	-2.41019600	0.99772500
H	-1.23542000	-2.32673900	1.16144100
C	-4.22609200	0.75098600	0.18551700
C	-5.42485100	1.23376900	-0.65822000
C	-4.74320600	0.13998900	1.49974900
C	-3.33199100	1.96214300	0.50634800
H	-5.08754000	1.69717900	-1.59289100
H	-6.08825000	0.40388300	-0.91211900
H	-6.00324500	1.98186600	-0.10500600
H	-3.91858900	-0.18898300	2.13876700
H	-5.32389900	0.88465500	2.05522200
H	-5.38828000	-0.72047400	1.30532900
H	-3.92418200	2.73752000	1.00442800
H	-2.50944000	1.69651800	1.17727100
H	-2.90704100	2.40580400	-0.40138000
C	-3.44169100	-0.30708900	-0.66066200
H	-3.17892100	0.19255200	-1.60985500
O	-4.36158100	-1.37131700	-0.92806600
H	-3.85252100	-2.08981600	-1.32727700

71

C	-1.17415700	4.05736200	1.62789900
C	-2.59150500	4.25575500	1.06084700
H	-0.64440000	5.02110700	1.63203700
H	-1.24810700	3.72500400	2.66967900
C	-3.42365700	5.24805000	1.88197200

H	-2.51751600	4.60648900	0.02287300	C	2.36825200	-0.77624000	2.31452000
H	-3.09496900	3.28204100	1.03092900	C	2.22766100	-1.03661400	0.93633600
C	-4.83547100	5.44916100	1.32184700	H	5.33514300	-0.24728400	-0.16572100
H	-3.48849700	4.89188700	2.91915100	H	5.61804100	0.26729000	2.23180200
H	-2.90445600	6.21534200	1.92265300	H	3.75472900	-0.08990100	3.81037600
H	-5.40882800	6.15793900	1.92851200	C	-1.20674800	-0.46732000	-3.12459000
H	-4.80305900	5.83737500	0.29730300	H	-0.31204300	-0.76172100	-2.57039700
H	-5.38944400	4.50375800	1.29994700	C	-1.01497400	1.00376600	-3.53741700
C	-0.35645000	3.08185000	0.86103200	H	-0.10799500	1.11036600	-4.14173500
C	0.59558200	2.79437200	0.08482400	H	-1.85738600	1.37000500	-4.13377300
C	1.74755700	3.14105800	-0.71850500	H	-0.91502700	1.64664000	-2.65809200
C	1.59331500	3.60136100	-2.04207000	C	-1.30194900	-1.38306100	-4.36178600
C	3.04643600	3.07916300	-0.17520900	H	-0.40253800	-1.28030700	-4.97819400
C	2.70225100	3.99473800	-2.79007700	H	-1.39918100	-2.43460500	-4.07395300
H	0.59855300	3.65628700	-2.47278000	H	-2.16489600	-1.12432700	-4.98470800
C	4.14852100	3.48332700	-0.92673700	C	-3.42153600	-2.05823700	1.27418500
H	3.18069000	2.71404700	0.83791200	H	-2.37216600	-2.22777600	1.53304400
C	3.98466500	3.94181900	-2.23702100	C	-4.01293100	-1.13432000	2.35681200
H	2.56203100	4.35100100	-3.80696100	H	-3.49113600	-0.17428100	2.37491900
H	5.14087500	3.43788800	-0.48651100	H	-5.07944300	-0.94996700	2.18755400
H	4.84602600	4.25382100	-2.82026200	H	-3.91159100	-1.60351300	3.34167600
C	-0.11698100	-0.72423100	0.12746600	C	-4.13890600	-3.42434300	1.28905700
C	0.70147600	-2.85037800	0.11069200	H	-4.03943500	-3.89015900	2.27533200
C	-0.53626700	-2.88868000	-0.44672000	H	-5.20861400	-3.30866800	1.08330200
N	-1.03424000	-1.58755500	-0.41883800	H	-3.72588000	-4.11049600	0.54529000
N	0.95594200	-1.51965500	0.43981100	C	3.16994100	-1.21857100	-1.46913200
Cl	-1.36244500	-4.22457500	-1.12803500	C	1.26123600	-1.04811700	3.32914600
Cl	1.78312000	-4.14212900	0.41712500	C	4.19535000	-2.29721900	-1.87477300
C	-2.41826000	-0.64713100	-2.21416500	H	4.03777400	-2.58999200	-2.91820200
C	-2.33768200	-1.20314400	-0.92057500	H	5.22122600	-1.92411400	-1.78801200
C	-3.47519800	-1.41968200	-0.11247600	H	4.10776300	-3.19223700	-1.25271500
C	-4.71604200	-1.03598000	-0.63673300	C	1.61095800	-2.27611700	4.19558800
C	-4.82407700	-0.46594300	-1.90218400	H	1.78214700	-3.16535200	3.58093700
C	-3.68639900	-0.27737000	-2.68090600	H	2.51578400	-2.09747100	4.78688700
H	-5.61105400	-1.18545600	-0.04100200	H	0.79327100	-2.49452700	4.89075100
H	-5.79808600	-0.17442600	-2.28455700	C	3.31088900	0.02351100	-2.36795100
H	-3.78267800	0.15527900	-3.67183200	H	4.29398100	0.49049700	-2.25204000
C	3.28522400	-0.87305800	0.01518300	H	3.19971300	-0.26440100	-3.41915800
C	4.50215900	-0.39293700	0.51503800	H	2.55588400	0.77748900	-2.13500500
C	4.66402700	-0.10268400	1.86721000	H	2.17471700	-1.63338000	-1.65093700
C	3.60996600	-0.29909300	2.75519000	Cu	-0.50006900	1.14039900	0.69226500

H	-1.69591700	1.00312300	1.67960800
C	0.96055200	0.17718700	4.21166800
H	0.12469300	-0.04442800	4.88343600
H	1.81925900	0.45185000	4.83346100
H	0.68490000	1.04409000	3.60420400
H	0.34477000	-1.28102100	2.78103900
TS26			
C	3.82527100	-0.06411900	2.26195700
C	4.23961000	1.41563100	2.30907700
H	4.71116600	-0.68736800	2.07460200
H	3.42628100	-0.35674900	3.24181500
C	5.24633900	1.72028700	3.42521000
H	4.66638400	1.70003900	1.33800000
H	3.33991900	2.02982600	2.44638400
C	5.65906500	3.19499500	3.47240400
H	4.81204900	1.42970300	4.39161700
H	6.13933000	1.09470600	3.29163300
H	6.37652700	3.38372900	4.27787700
H	6.12620800	3.50507200	2.53059700
H	4.79121800	3.84321100	3.64005600
C	2.82379300	-0.38634200	1.19987900
C	2.66629700	-1.03445300	0.09882200
C	3.39016100	-1.90696100	-0.80519300
C	4.11327700	-1.38640500	-1.90037700
C	3.38495900	-3.30727900	-0.62413500
C	4.80189300	-2.23108500	-2.76983000
H	4.13111000	-0.31219400	-2.05968300
C	4.07686800	-4.14486900	-1.49797500
H	2.83347700	-3.73012300	0.21065100
C	4.78870300	-3.61579700	-2.57847800
H	5.35427400	-1.80284200	-3.60243100
H	4.05967200	-5.21903300	-1.33185000
H	5.32395500	-4.27103000	-3.25937500
C	-0.84234400	0.17135600	0.00717100
C	-3.09328800	-0.04315800	-0.24806800
C	-2.71938900	1.09631300	-0.88656900
N	-1.34049400	1.21916400	-0.72341800
N	-1.93686200	-0.60355700	0.29320700
Cl	-3.68086600	2.21384400	-1.75615200
Cl	-4.65362000	-0.72802900	-0.08779900
C	0.02960700	2.15897100	-2.53084900
C	-0.53389500	2.30078400	-1.24613800
C	-0.34873100	3.45216500	-0.45264200
C	0.45797600	4.46990800	-0.97753400
C	1.04593600	4.34949700	-2.23396000
C	0.82840700	3.20881100	-3.00181700
H	0.62420000	5.37012300	-0.39413400
H	1.66931500	5.15123000	-2.61923100
H	1.28199600	3.13206500	-3.98510300
C	-1.72791400	-3.05027500	0.32107900
C	-1.67269300	-4.23581500	1.06478200
C	-1.77773400	-4.22182400	2.45307000
C	-1.94720700	-3.01711800	3.12995200
C	-2.00894900	-1.79924300	2.44043700
C	-1.88622300	-1.84466400	1.03616300
H	-1.54922400	-5.18237300	0.54788700
H	-1.73278200	-5.15381800	3.00912500
H	-2.03767500	-3.02045700	4.21163500
C	-0.21550600	0.94273200	-3.41945000
H	-0.84127400	0.23556200	-2.86795300
C	1.09531800	0.21282700	-3.76597800
H	0.88252100	-0.67291800	-4.37414700
H	1.77211800	0.85435900	-4.34062700
H	1.61853600	-0.11290900	-2.86314500
C	-0.98373600	1.33539000	-4.69789700
H	-1.20129000	0.44394400	-5.29557200
H	-1.93251400	1.82647400	-4.46111700
H	-0.39728600	2.01900000	-5.32104600
C	-1.00840700	3.64221400	0.91050200
H	-1.53479000	2.71877900	1.16806300
C	0.02539800	3.89961600	2.02278300
H	0.74553500	3.07902400	2.08560200
H	0.57656200	4.83075200	1.85356700
H	-0.48056100	3.98650100	2.99034200
C	-2.05611100	4.77365900	0.86271100
H	-2.55827700	4.86484200	1.83172800
H	-1.58788400	5.73796300	0.63746000
H	-2.81794000	4.58374100	0.10083500
C	-1.63945300	-3.11078000	-1.20111200
C	-2.23645300	-0.50513700	3.21666500
C	-2.85474000	-3.84739400	-1.80038400
H	-2.80104000	-3.83598400	-2.89417100

H	-2.88179200	-4.89415900	-1.47906700	C	-4.51046500	2.78416800	-3.04427000
H	-3.79688100	-3.37929800	-1.50041300	H	-5.13302500	1.10727800	-4.24991100
C	-3.65284400	-0.47089100	3.82701800	H	-3.74240200	4.22417500	-1.63256500
H	-4.42350600	-0.58449600	3.05866600	H	-4.93833000	3.53158300	-3.70660100
H	-3.78804200	-1.27369100	4.55987100	C	1.06517600	-0.06221000	0.08428500
H	-3.82048000	0.48201700	4.34018700	C	3.18042700	0.60967600	0.56758000
C	-0.32197700	-3.75295300	-1.67387900	C	3.24510200	-0.69363200	0.17967500
H	-0.25177800	-4.80053200	-1.36186500	N	1.94391500	-1.09120200	-0.11265700
H	-0.26545400	-3.73000200	-2.76742700	N	1.84055300	0.98280100	0.50431100
H	0.54692500	-3.22215400	-1.27665600	Cl	4.60916300	-1.71738800	0.04889100
H	-1.65433400	-2.08671700	-1.58456700	Cl	4.44314900	1.65607200	1.05439100
Cu	0.95396700	-0.07823000	0.61018400	C	1.52036500	-2.65075800	-1.96197600
H	1.52503300	0.56351900	1.91931300	C	1.55896400	-2.40955000	-0.57422500
C	-1.16523400	-0.28556300	4.30151000	C	1.23322500	-3.38983600	0.38419800
H	-1.33580200	0.67131200	4.80634400	C	0.84322300	-4.64782000	-0.09238900
H	-1.19474700	-1.07105400	5.06389100	C	0.78542200	-4.91475400	-1.45771300
H	-0.16248500	-0.26661600	3.86493700	C	1.12238400	-3.92711000	-2.37954100
H	-2.16004800	0.33139600	2.51662400	H	0.57984000	-5.42687300	0.61636000
72				H	0.47828000	-5.89702100	-1.80479400
C	-5.00326900	-1.34183500	0.15550800	H	1.07442100	-4.14847500	-3.44117800
C	-5.60473500	-1.40089800	1.57250600	C	1.24211300	3.26123900	-0.19451300
H	-5.24808100	-2.28630100	-0.35736600	C	0.74526300	4.52402700	0.15233100
H	-5.49018300	-0.54517800	-0.41716600	C	0.35459600	4.81194300	1.45724100
C	-7.11247900	-1.68291300	1.58924000	C	0.45511200	3.83966300	2.44882700
H	-5.08555800	-2.17635800	2.15446600	C	0.94920000	2.56071700	2.16284300
H	-5.40528200	-0.45031700	2.08702800	C	1.32991600	2.29879500	0.83131900
C	-7.70157400	-1.74036900	3.00254900	H	0.66246700	5.29045000	-0.61182100
H	-7.63170900	-0.90907100	1.00739800	H	-0.02945800	5.79784000	1.70251500
H	-7.30739700	-2.63295500	1.07250700	H	0.14550100	4.07574300	3.46210200
H	-8.77772400	-1.94325500	2.98155900	C	1.88084100	-1.59413800	-3.00188700
H	-7.22587400	-2.52871400	3.59765300	H	2.19355000	-0.68749000	-2.47613600
H	-7.55196500	-0.79232100	3.53223400	C	0.66001200	-1.21999200	-3.86494400
C	-3.50115800	-1.14763600	0.17079500	H	0.92749400	-0.43112800	-4.57601500
C	-2.75645700	-0.18256800	-0.42238100	H	0.29928300	-2.07990200	-4.43920900
C	-3.38888400	0.83076500	-1.31193200	H	-0.16566500	-0.85715500	-3.24473100
C	-4.06888700	0.46511100	-2.49254100	C	3.06618900	-2.04292100	-3.87872300
C	-3.27668700	2.20987600	-1.03757100	H	3.34017700	-1.24511600	-4.57691100
C	-4.61755800	1.42449000	-3.34645900	H	3.94486000	-2.28069100	-3.27108700
H	-4.15772900	-0.58922700	-2.74114600	H	2.81561300	-2.92958200	-4.47054600
C	-3.83748700	3.16977100	-1.88071300	C	1.28078000	-3.13295200	1.88692700
H	-2.73895300	2.52395200	-0.14601700	H	1.64098900	-2.11337500	2.04977500

C	-0.12472300	-3.22171000	2.51316400	H	5.88758100	1.58417100	5.17900600
H	-0.81278700	-2.51486000	2.03866900	H	6.57199700	1.01557900	3.64981400
H	-0.54607000	-4.22713100	2.40756000	H	5.63947500	2.51726100	3.69630400
H	-0.07798000	-2.98915900	3.58236300	C	2.54348200	-0.38786700	0.59360200
C	2.26677000	-4.08316800	2.59401300	C	2.92676300	-0.60392700	-0.59385900
H	2.32513600	-3.84014300	3.66012700	C	3.96437900	-0.91122800	-1.56701300
H	1.94921800	-5.12763300	2.50868900	C	3.75692800	-0.80313500	-2.95156300
H	3.27250900	-4.00147100	2.17037700	C	5.23223400	-1.32267000	-1.10569200
C	1.65811900	2.98492200	-1.63594300	C	4.78692200	-1.08515800	-3.84823000
C	1.04641500	1.52275400	3.27635800	H	2.77341400	-0.50440900	-3.29883000
C	2.85695200	3.85992800	-2.05275500	C	6.25698500	-1.60931400	-2.00518700
H	3.16874000	3.61236800	-3.07296300	H	5.40375800	-1.41969400	-0.03796200
H	2.60001100	4.92439500	-2.03215700	C	6.04022600	-1.48920600	-3.38112900
H	3.71325700	3.70762200	-1.38860200	H	4.60887200	-0.99286800	-4.91612900
C	1.97123600	1.99658000	4.41462800	H	7.22632000	-1.92726900	-1.63133200
H	2.97047200	2.24069100	4.04100400	H	6.84000900	-1.71208700	-4.08152000
H	1.57128200	2.88564700	4.91315900	C	-0.83422600	0.03587600	-0.02994100
H	2.07212600	1.21015500	5.16989200	C	-2.84305400	1.07326300	0.25199000
C	0.47582300	3.16412200	-2.60793300	C	-3.02950600	-0.24574300	0.51029400
H	0.13778100	4.20539300	-2.63958300	N	-1.79373300	-0.87227200	0.34201600
H	0.77714200	2.88282400	-3.62251900	N	-1.49755300	1.23662600	-0.07852200
H	-0.37738800	2.54397700	-2.31718700	Cl	-4.47514600	-1.05600200	0.94290300
H	1.97699300	1.94132000	-1.70660000	Cl	-3.98614100	2.34721600	0.31204700
Cu	-0.84881200	-0.10344500	-0.16970600	C	-1.25183300	-2.80337000	1.77333000
H	-2.98512300	-1.88739700	0.78988000	C	-1.58853200	-2.29934400	0.49768100
C	-0.34900000	1.14697200	3.81229600	C	-1.78902000	-3.13562400	-0.62191900
H	-0.26357200	0.36959000	4.57910700	C	-1.62977300	-4.51469500	-0.43196600
H	-0.84776500	2.01025900	4.26555300	C	-1.29598800	-5.03938200	0.81237100
H	-0.99096100	0.76848700	3.01061300	C	-1.11041800	-4.19110400	1.90024200
H	1.48723200	0.61314800	2.85909300	H	-1.77744300	-5.18609000	-1.27178700
73				H	-1.18265200	-6.11252900	0.93618600
C	2.82754400	-0.21978800	2.04254900	H	-0.85500100	-4.61332600	2.86652400
C	4.11960400	0.57590600	2.32080300	C	-0.32965800	3.31962500	0.52070300
H	2.92559900	-1.21956500	2.48849900	C	0.19851000	4.55188400	0.11518300
H	1.98475200	0.25508900	2.55454100	C	0.14940100	4.95585100	-1.21575500
C	4.41762800	0.71383800	3.81905000	C	-0.43676900	4.13341100	-2.17270500
H	4.96207700	0.08119200	1.82169500	C	-0.98522200	2.89098100	-1.82862900
H	4.03702000	1.57190400	1.86703200	C	-0.91078700	2.50275600	-0.47281700
C	5.70064100	1.50156000	4.10326900	H	0.64984500	5.20580700	0.85401800
H	3.56868300	1.20521900	4.31337900	H	0.56468000	5.91643800	-1.50663500
H	4.49409800	-0.28664200	4.26628400	H	-0.47707900	4.46227600	-3.20620100

C	-1.07050100	-1.91624300	3.00304100
H	-0.96219000	-0.88244400	2.66175200
C	0.20028100	-2.27252000	3.79675700
H	0.37784600	-1.52105300	4.57296200
H	0.10609700	-3.24132400	4.29814600
H	1.07969300	-2.31248400	3.15010500
C	-2.30231900	-1.98206500	3.93060000
H	-2.15921000	-1.32433500	4.79465700
H	-3.21834400	-1.67710600	3.41904500
H	-2.45033200	-3.00087500	4.30534500
C	-2.20243900	-2.61795900	-1.99762300
H	-2.15601300	-1.52574100	-1.98212500
C	-1.24234500	-3.09143200	-3.10509900
H	-0.21945100	-2.76612600	-2.89894600
H	-1.25083200	-4.18123000	-3.21221300
H	-1.54644400	-2.66379400	-4.06653000
C	-3.65427200	-3.02289300	-2.32829700
H	-3.94991500	-2.60663000	-3.29723100
H	-3.75586000	-4.11209800	-2.38778400
H	-4.35819200	-2.66099600	-1.57360000
C	-0.29217300	2.93862500	1.99825300
C	-1.66257200	2.05310000	-2.91081700
C	-1.34368600	3.73054600	2.80352500
H	-1.32674900	3.42273700	3.85459300
H	-1.13475300	4.80531000	2.76500800
H	-2.35447700	3.57146800	2.41867400
C	-2.96909400	2.72026200	-3.38995000
H	-3.66473200	2.89302300	-2.56436200
H	-2.76500000	3.68592800	-3.86529600
H	-3.46791200	2.08368400	-4.12852900
C	1.10608000	3.13250400	2.61326700
H	1.37942600	4.19093100	2.67559900
H	1.12495200	2.73152500	3.63210600
H	1.87404300	2.62130700	2.02722300
H	-0.53869400	1.87631300	2.08240800
Cu	0.98865800	-0.33531300	-0.70682800
H	0.78177900	-0.51599000	-2.24066300
C	-0.72896600	1.78256300	-4.10598300
H	-1.23635700	1.13995300	-4.83360800
H	-0.45271100	2.70831600	-4.62172100
H	0.18290700	1.27518300	-3.78202300
H	-1.92152900	1.08174600	-2.48049400

TS27

C	-3.36369800	0.13361900	-2.08619700
C	-4.29271100	1.32037400	-1.74977800
H	-3.97669300	-0.69224800	-2.48080900
H	-2.69597200	0.43629700	-2.90173800
C	-5.09386900	1.81427100	-2.96098100
H	-4.98138600	1.02550800	-0.94772200
H	-3.68857200	2.14416500	-1.34832000
C	-6.01337900	2.99456600	-2.63002600
H	-4.39873600	2.10351900	-3.76087100
H	-5.69242200	0.98508500	-3.36235500
H	-6.57332800	3.32510600	-3.51122900
H	-6.74002500	2.72410800	-1.85533800
H	-5.43909600	3.85133400	-2.25911100
C	-2.58013600	-0.33437900	-0.89922100
C	-2.78630800	-0.99207200	0.19893700
C	-3.82171900	-1.70676100	0.95281000
C	-3.61062900	-2.27659400	2.21767500
C	-5.10442200	-1.82952000	0.37683000
C	-4.63737000	-2.94049200	2.88839700
H	-2.62594300	-2.19116400	2.66835100
C	-6.12864900	-2.49603400	1.04603400
H	-5.29315100	-1.39996400	-0.60134600
C	-5.90224700	-3.05504400	2.30728800
H	-4.44741100	-3.37054000	3.86807900
H	-7.10726000	-2.57866000	0.58102600
H	-6.70164200	-3.57305600	2.82915100
C	0.95292500	0.07244700	0.06621300
C	2.89987100	1.22970300	0.29524400
C	3.21078700	0.01140100	-0.21845600
N	2.01353100	-0.69104800	-0.35206600
N	1.51573700	1.25873600	0.46328400
Cl	4.74117000	-0.61709100	-0.65857100
Cl	3.93647000	2.53356500	0.69009200
C	1.68290500	-2.22050500	-2.24427400
C	1.89589300	-2.03987200	-0.86205100
C	2.00824900	-3.11813200	0.04012600
C	1.88611300	-4.41088400	-0.48532000
C	1.66577200	-4.62020900	-1.84394400
C	1.56775300	-3.53594900	-2.71151800

H	1.96676300	-5.26458500	0.18025700
H	1.57415300	-5.63194000	-2.22842700
H	1.40207700	-3.71160300	-3.76991400
C	0.34566300	3.37455100	0.03760000
C	-0.39758400	4.45052900	0.53867300
C	-0.70300800	4.54689700	1.89368800
C	-0.26296000	3.56851700	2.78086000
C	0.48298200	2.46862900	2.33781300
C	0.76391000	2.39133400	0.95828900
H	-0.73951800	5.22309100	-0.14292800
H	-1.28136600	5.39005000	2.26027800
H	-0.49895300	3.65955400	3.83646100
C	1.58971500	-1.06143700	-3.23187300
H	1.67290600	-0.12634500	-2.67134000
C	0.22636900	-1.03798300	-3.94883400
H	0.16317400	-0.16613500	-4.60889700
H	0.08008700	-1.93196400	-4.56457000
H	-0.59233100	-0.98259900	-3.22575200
C	2.75073500	-1.09532500	-4.24565700
H	2.69524700	-0.22880500	-4.91320000
H	3.72216900	-1.07557000	-3.74219700
H	2.71210900	-1.99679300	-4.86655100
C	2.27361300	-2.93494500	1.53156000
H	2.27155800	-1.86363000	1.75072100
C	1.16730500	-3.57409200	2.39231400
H	0.18621700	-3.16498500	2.13506800
H	1.13230100	-4.66093300	2.26186800
H	1.35576000	-3.37423700	3.45265400
C	3.66087900	-3.48486400	1.92116700
H	3.85546100	-3.30177400	2.98325400
H	3.72080700	-4.56549600	1.75244900
H	4.45793000	-3.00968000	1.34166100
C	0.67649000	3.31806800	-1.45129000
C	0.97640400	1.43762300	3.34837300
C	1.54378900	4.51849800	-1.88038100
H	1.81698000	4.42709200	-2.93694900
H	1.00544100	5.46429400	-1.75719000
H	2.46559300	4.57717900	-1.29402700
C	2.01932100	2.05559600	4.30221900
H	2.86879000	2.47128700	3.75179200
H	1.58019700	2.86052500	4.90135400
H	2.39948900	1.29450400	4.99187500
C	-0.59818500	3.22416000	-2.31182700
H	-1.22667100	4.11354800	-2.19399000
H	-0.33235400	3.14293000	-3.37139200
H	-1.19126700	2.34751200	-2.03795600
H	1.25828200	2.41137600	-1.63919300
Cu	-0.88006000	-0.44074500	0.14206300
H	-1.48442600	-1.25644300	1.33526000
C	-0.18497600	0.80442900	4.13795900
H	0.19878400	0.03300800	4.81428600
H	-0.71087500	1.54655500	4.74805300
H	-0.90980500	0.33750200	3.46481400
H	1.47036500	0.63105500	2.79975400
74			
C	-3.33750800	1.36923000	-0.93183400
C	-3.22864500	2.60581500	-0.01832400
H	-4.38792700	1.23835400	-1.22881700
H	-2.78641800	1.59849200	-1.85597500
C	-3.74587000	3.89740100	-0.66428400
H	-3.78059600	2.42077100	0.91473400
H	-2.17838700	2.73956100	0.27603900
C	-3.61594400	5.12231600	0.24752100
H	-3.19610000	4.07797900	-1.59846900
H	-4.79798000	3.76495300	-0.95211100
H	-3.99229700	6.02874600	-0.23910600
H	-4.18045000	4.98523900	1.17731600
H	-2.56902600	5.29963400	0.52008900
C	-2.74206700	0.10835900	-0.31875600
C	-3.52423600	-0.92790100	0.09225100
C	-4.99972300	-1.09773800	0.08602500
C	-5.53099000	-2.37914800	-0.17022900
C	-5.91792200	-0.06803000	0.37595000
C	-6.90475900	-2.61518200	-0.17684800
H	-4.84487100	-3.19839100	-0.37404100
C	-7.29441300	-0.30147100	0.37153900
H	-5.55058800	0.91798200	0.63828400
C	-7.79808200	-1.57320100	0.08881200
H	-7.27954800	-3.61381000	-0.38655600
H	-7.97594200	0.51332100	0.60271500
H	-8.86945600	-1.75302600	0.08796600
C	1.09513900	-0.15181500	-0.01408100

C	3.29289500	0.39820100	0.15572400	H	2.30396500	-2.89767100	4.40305400
C	3.21277500	-0.96074300	0.13034200	H	1.70609900	-4.40381700	3.69842100
N	1.86242700	-1.28239000	0.02596300	H	3.10510000	-3.58957700	2.98097600
N	1.98990200	0.87922200	0.06631000	C	1.82835800	2.29109200	-2.50269300
Cl	4.46757600	-2.12052700	0.20914200	C	1.45759200	2.17083200	2.64276800
Cl	4.67427000	1.39995400	0.27437300	C	3.00331400	2.98151900	-3.22278800
C	1.14943800	-3.23891300	-1.27850500	H	3.24037700	2.45138700	-4.15118000
C	1.32704100	-2.62749300	-0.02149100	H	2.76037800	4.01679700	-3.48437900
C	1.00097300	-3.26253600	1.19363200	H	3.90224700	2.99417500	-2.59876500
C	0.46527700	-4.55426900	1.11803900	C	2.47708900	2.85001600	3.57806900
C	0.27062500	-5.18307400	-0.10910700	H	3.46408100	2.91847600	3.11033000
C	0.61068800	-4.53180800	-1.29186000	H	2.16181400	3.86292100	3.84920400
H	0.19530900	-5.07279100	2.03273100	H	2.57810500	2.27526200	4.50459000
H	-0.14649900	-6.18529300	-0.14357400	C	0.57698100	2.24387500	-3.40096800
H	0.45534100	-5.03300500	-2.24215500	H	0.22887000	3.25098400	-3.65409600
C	1.52599200	2.95594000	-1.16318600	H	0.80335700	1.72372000	-4.33775000
C	1.13904000	4.30163400	-1.12846100	H	-0.24456800	1.71603800	-2.90653100
C	0.85834100	4.94043000	0.07671500	H	2.12711400	1.25655600	-2.31202200
C	0.96449600	4.24555600	1.27908100	Cu	-0.82900500	-0.02614800	-0.16201200
C	1.34904400	2.89901400	1.30647800	H	-3.01723800	-1.82770000	0.45056600
C	1.61458300	2.27839600	0.06925800	C	0.08023400	2.03986700	3.32236300
H	1.05623700	4.85498300	-2.05857600	H	0.17284900	1.48090400	4.25968000
H	0.56004200	5.98475300	0.07946400	H	-0.34271400	3.02215100	3.55878900
H	0.74627500	4.75499700	2.21250000	H	-0.62979100	1.51197400	2.67795100
C	1.50367500	-2.55425800	-2.59500200	H	1.82033100	1.15671200	2.45268700
H	1.95529300	-1.58468400	-2.36694400	75			
C	0.24125700	-2.28095400	-3.43626400	C	0.20163200	2.63009500	0.82564300
H	0.50682300	-1.75097700	-4.35723900	C	0.41953700	3.77722500	0.13744300
H	-0.25840200	-3.21374200	-3.71860600	C	2.07651100	-0.62232100	-0.05889000
H	-0.47631200	-1.66766800	-2.88172100	C	2.57343700	-2.79800700	-0.47906000
C	2.54280900	-3.36316000	-3.39537500	C	3.70251800	-2.07133100	-0.70415700
H	2.82371100	-2.82000300	-4.30376000	N	3.38361700	-0.74219300	-0.44259200
H	3.45009400	-3.53826800	-2.80899900	N	1.58766800	-1.89876100	-0.08329700
H	2.14616500	-4.33692000	-3.70104000	Cl	5.24754000	-2.60159000	-1.21190200
C	1.19556300	-2.60189800	2.55489800	Cl	2.32400000	-4.48304500	-0.63476900
H	1.66938000	-1.62863300	2.39882200	C	5.06661100	0.73620500	0.56482700
C	-0.15704100	-2.34207300	3.24690700	C	4.30260900	0.37089600	-0.56146800
H	-0.80551200	-1.71696600	2.62486900	C	4.39493000	1.03690800	-1.80004600
H	-0.68540200	-3.27911400	3.45270400	C	5.28554200	2.11464400	-1.88342600
H	-0.00119000	-1.82913700	4.20195600	C	6.04996100	2.50430000	-0.78676000
C	2.13420000	-3.42490100	3.45845700	C	5.94070800	1.82118600	0.42152400

H	5.38037400	2.65569300	-2.81975800
H	6.73408600	3.34330200	-0.87438600
H	6.54291000	2.13453900	1.26852700
C	-0.07165300	-2.60175600	1.58748500
C	-1.39857800	-2.93867800	1.88255500
C	-2.38079400	-2.93088700	0.89575100
C	-2.05607000	-2.58919400	-0.41446500
C	-0.74497500	-2.24698500	-0.76968100
C	0.22434000	-2.25656300	0.25331800
H	-1.66500000	-3.20659400	2.90032400
H	-3.40681400	-3.18529400	1.14434200
H	-2.83491900	-2.58050100	-1.17007400
C	4.97524800	0.01255300	1.90484900
H	4.25652300	-0.80574400	1.80579600
C	4.44721300	0.94714900	3.01094600
H	4.34150700	0.39673900	3.95192500
H	5.13165600	1.78345300	3.18802700
H	3.46990100	1.36114200	2.74365800
C	6.32660700	-0.61259100	2.30346700
H	6.22126600	-1.17286100	3.23841700
H	6.69107500	-1.29989300	1.53381400
H	7.09264300	0.15417800	2.46031400
C	3.56863600	0.64240300	-3.02032900
H	2.98892000	-0.25020300	-2.76834000
C	2.56092100	1.74906900	-3.38911800
H	1.94395900	1.43332500	-4.23727700
H	1.89694500	1.97441100	-2.54846800
H	3.07295600	2.67462000	-3.67351400
C	4.46209500	0.27972400	-4.22224400
H	3.84520700	-0.06327400	-5.05938400
H	5.04066200	1.14220300	-4.56923300
H	5.16645800	-0.51858300	-3.96897200
C	0.97647100	-2.62244900	2.69593300
C	-0.42587200	-1.88284200	-2.21639700
C	1.17795300	-4.04557000	3.25381900
H	1.96591400	-4.04498200	4.01445600
H	0.26252800	-4.42168200	3.72286200
H	1.46523400	-4.74869600	2.46620600
C	-0.70800100	-3.06132400	-3.16905500
H	-0.14835100	-3.95475600	-2.87495200
H	-1.77208600	-3.31909800	-3.18218900
H	-0.41709400	-2.79779600	-4.19146800
C	0.62560900	-1.63383700	3.82496400
H	-0.30141900	-1.92017700	4.33292700
H	1.42443300	-1.62100500	4.57425600
H	0.49609900	-0.61732500	3.44186400
H	1.93138400	-2.29976700	2.27130900
Cu	1.13303200	1.00055200	0.39318500
H	1.13247000	3.75444800	-0.69166600
C	-1.18723600	-0.61703900	-2.65732700
H	-0.91206100	-0.34988000	-3.68344800
H	-2.27061700	-0.77123500	-2.62946800
H	-0.94934400	0.23133600	-2.00763400
H	0.64231000	-1.65765200	-2.28691400
C	-7.96940700	0.16439000	-1.26762200
C	-6.45312100	0.32570800	-1.02467000
H	-8.17677800	-0.18120400	-2.28492000
H	-8.41731600	-0.53808400	-0.56208900
H	-8.44828900	1.13912500	-1.13548800
C	-6.18628500	0.79011400	0.42362800
C	-5.85488000	1.33335100	-2.02730700
H	-5.11510600	0.88861800	0.62328000
H	-6.65047400	1.77121400	0.56285300
H	-6.61498900	0.09996100	1.15271600
H	-6.33384300	2.30571300	-1.88228100
H	-4.77890600	1.45283900	-1.87643000
H	-6.02415100	1.01595800	-3.05950900
C	-5.75598600	-1.01432500	-1.26603000
O	-4.91608800	-1.28261000	-2.05937300
Br	-6.38640400	-2.52377800	-0.03685900
C	-0.78242800	2.59239100	1.94355500
C	-0.37340700	2.30560900	3.26261000
C	-2.16294400	2.78646500	1.72886200
C	-1.28882600	2.23803600	4.31354100
H	0.68328800	2.13844700	3.45796300
C	-3.08316300	2.70651300	2.77683500
H	-2.51212000	2.99862500	0.72170300
C	-2.65279700	2.43475700	4.07791400
H	-0.93657800	2.02577200	5.32013900
H	-4.14055400	2.86170700	2.57568000
H	-3.36762700	2.37317500	4.89369200
C	-0.18206900	5.14827200	0.36425200

C	-1.02798800	5.64723900	-0.82364500
H	0.63298500	5.87167700	0.52619000
H	-0.79299600	5.15563000	1.27355600
C	-1.54358500	7.08134900	-0.64830800
H	-0.43129300	5.58680500	-1.74543700
H	-1.87921100	4.96751300	-0.96827400
C	-2.40094200	7.56452400	-1.82295000
H	-2.12675000	7.14464500	0.28071600
H	-0.68814000	7.75809300	-0.51603800
H	-2.75022900	8.59136900	-1.67026000
H	-1.83517800	7.54148100	-2.76168000
H	-3.28418200	6.92883700	-1.95522200

TS28

C	-2.30432100	-0.45902300	0.41050500
C	-3.12244300	0.30614100	-0.34532700
C	1.18507900	0.55520700	0.12606500
C	3.16462000	1.41531200	0.86200400
C	2.36991000	2.46343100	0.52658700
N	1.15671900	1.93008400	0.09584200
N	2.44512800	0.25386200	0.59025000
Cl	2.75872600	4.13035900	0.53293100
Cl	4.73792100	1.44569400	1.53788100
C	-0.77030800	3.44043500	0.44083600
C	0.08233900	2.74472300	-0.44343000
C	-0.02202300	2.85936100	-1.84758600
C	-1.03813500	3.67977300	-2.35412600
C	-1.89803300	4.37169100	-1.50694600
C	-1.75865100	4.25497000	-0.12761200
H	-1.14529100	3.78902900	-3.42844300
H	-2.67332800	5.00892700	-1.92241700
H	-2.42841700	4.80676000	0.52406000
C	2.86076800	-1.93377000	1.66689900
C	3.49587900	-3.18221000	1.62192200
C	4.30630500	-3.54328300	0.55086100
C	4.51277100	-2.65069500	-0.49624400
C	3.91179300	-1.38610300	-0.50613100
C	3.06985100	-1.05950700	0.58242400
H	3.35752000	-3.87817600	2.44227700
H	4.78571000	-4.51781100	0.53668600
H	5.15752600	-2.93661400	-1.32128300
C	-0.66980700	3.36262000	1.96337900
H	0.08442600	2.61184000	2.22047500
C	-2.00206900	2.91773100	2.59739300
H	-1.87148600	2.76592200	3.67403300
H	-2.77751800	3.67980600	2.46548300
H	-2.36164400	1.98458100	2.16216900
C	-0.23073700	4.70914200	2.57659800
H	-0.13624200	4.61198200	3.66343500
H	0.72806000	5.05024100	2.18095200
H	-0.97443400	5.48808700	2.37662300
C	0.94913500	2.19512300	-2.82071300
H	1.55595400	1.47604000	-2.26594500
C	0.22885300	1.40468400	-3.92842600
H	0.96606600	0.88997400	-4.55370000
H	-0.44567100	0.65280500	-3.51060500
H	-0.35313400	2.06129500	-4.58401000
C	1.90651600	3.24240500	-3.42742000
H	2.63496500	2.75495200	-4.08418700
H	1.35656100	3.97857000	-4.02375700
H	2.45625900	3.78436000	-2.65154800
C	2.03451300	-1.55880200	2.89268400
C	4.23091000	-0.43609000	-1.66253000
C	2.95537500	-1.17511500	4.07022500
H	2.35887600	-0.86505500	4.93501800
H	3.57389500	-2.02640600	4.37543500
H	3.62622400	-0.35221200	3.80599500
C	5.73510200	-0.09155800	-1.70318700
H	6.08390300	0.32629400	-0.75577900
H	6.33803000	-0.97923500	-1.92221800
H	5.92887800	0.64290600	-2.49208100
C	1.06154900	-2.67730600	3.30606000
H	1.59303900	-3.57138800	3.64797400
H	0.42720000	-2.33822700	4.12942200
H	0.40827600	-2.96441700	2.47705100
H	1.43500900	-0.67929800	2.64142600
Cu	-0.42936100	-0.65935800	-0.21874500
H	-2.81997700	0.50776700	-1.37669500
C	3.78454700	-0.99792100	-3.02614500
H	4.00035000	-0.27035200	-3.81611900
H	4.32180200	-1.92032900	-3.27219600
H	2.71543900	-1.21771500	-3.03672600
H	3.68724700	0.49979700	-1.50647200

C	-2.01405000	-4.48054500	-2.58171400
C	-2.33328400	-3.43829000	-1.47935700
H	-2.25258100	-4.09273500	-3.57620800
H	-0.96339300	-4.77451900	-2.56095400
H	-2.62977600	-5.36764800	-2.40236800
C	-1.95174900	-3.98788000	-0.10301000
C	-3.83679000	-3.09193000	-1.54070000
H	-2.17431300	-3.26988900	0.68720300
H	-2.53094800	-4.89807900	0.08341200
H	-0.89133300	-4.24272900	-0.05989600
H	-4.41396200	-3.98240500	-1.27405600
H	-4.08013700	-2.28842400	-0.84611700
H	-4.12709200	-2.77844200	-2.54672800
C	-1.57665300	-2.15093600	-1.87602900
O	-1.84319400	-1.36670800	-2.72629900
Br	0.64711900	-2.56207900	-1.70021400
C	-2.67216200	-0.85855500	1.79374200
C	-1.81294200	-0.60787300	2.88352000
C	-3.88726500	-1.51888700	2.08237800
C	-2.16221900	-0.95505700	4.18838500
H	-0.86371200	-0.11517300	2.69474600
C	-4.23083100	-1.88707100	3.38439600
H	-4.57064100	-1.74650500	1.27022700
C	-3.37344500	-1.60207400	4.44922500
H	-1.48349000	-0.72404700	5.00562500
H	-5.17479400	-2.39477000	3.56628200
H	-3.64119900	-1.88302500	5.46378400
C	-4.40864000	1.00888600	0.03831500
C	-5.61713300	0.60828200	-0.82903000
H	-4.25198300	2.09234800	-0.08199900
H	-4.64428900	0.84390000	1.09490800
C	-6.87870500	1.42773600	-0.52770000
H	-5.35588400	0.72161700	-1.89092900
H	-5.83429700	-0.45885800	-0.68285700
C	-8.08132100	1.02611800	-1.38803500
H	-7.13558400	1.31838900	0.53492200
H	-6.65968100	2.49379300	-0.67859500
H	-8.96420700	1.62930900	-1.15073800
H	-7.86563100	1.15700500	-2.45483300
H	-8.34580500	-0.02622000	-1.23213900
C	-4.53824600	-0.67026900	-0.46490300
C	-4.46098400	0.59650800	-0.92622200
C	2.31675500	0.31991400	0.04974500
C	4.33510200	1.07902700	-0.64966700
C	3.52228400	2.16053400	-0.49333800
N	2.28683100	1.67985000	-0.06800000
N	3.58302700	-0.04162500	-0.31297700
Cl	3.87211400	3.81617900	-0.73539300
Cl	5.96787700	1.01603000	-1.15119300
C	0.92950100	2.96231600	1.52860200
C	1.12567800	2.50189600	0.21099100
C	0.24923800	2.80906500	-0.84953700
C	-0.86060000	3.60916900	-0.54905300
C	-1.08707600	4.07370300	0.74384800
C	-0.20229400	3.75127600	1.76929000
H	-1.55646500	3.87076000	-1.34005700
H	-1.95558300	4.69153000	0.95277500
H	-0.39023100	4.11918300	2.77303800
C	4.67113600	-1.93199700	0.81788700
C	5.09908100	-3.26456600	0.76976300
C	4.93102600	-4.03470200	-0.37802400
C	4.33280600	-3.48577500	-1.50896100
C	3.88376100	-2.15909800	-1.52042700
C	4.06030600	-1.40998600	-0.33998100
H	5.56763600	-3.70461100	1.64439300
H	5.26917200	-5.06667500	-0.39148600
H	4.20980700	-4.09608900	-2.39814600
C	1.88362200	2.64405400	2.67570500
H	2.70180000	2.03325300	2.28417800
C	1.18577800	1.81805700	3.77408700
H	1.89914000	1.56316700	4.56490900
H	0.36373600	2.37731500	4.23322700
H	0.77514200	0.88738400	3.37016600
C	2.51082800	3.92572000	3.25912000
H	3.23392100	3.66872400	4.04023900
H	3.03165800	4.50199300	2.48825400
H	1.75165500	4.57378800	3.70928800
C	0.46599200	2.32748400	-2.28097900
H	1.33492700	1.66321200	-2.29271300
C	-0.73444900	1.51389100	-2.80128900
H	-0.51313700	1.12221900	-3.79992000

76

H	-0.97626900	0.66941200	-2.15046000	C	-3.83280900	-1.71191700	-1.31546700
H	-1.63089200	2.13788500	-2.88608300	O	-2.80432000	-1.39316200	-1.90248800
C	0.77472000	3.50866500	-3.22377200	Br	-0.58068600	-2.31047800	1.49093700
H	0.97447600	3.14160600	-4.23599000	C	-5.23942200	-1.00605100	0.81342600
H	-0.07317600	4.19968500	-3.28046000	C	-4.50537200	-1.46518700	1.92067700
H	1.64824500	4.07495000	-2.88750700	C	-6.62345100	-0.81380700	0.96167500
C	4.86982700	-1.11969000	2.09412400	C	-5.14083900	-1.73111500	3.13501500
C	3.23408400	-1.59333300	-2.77964200	H	-3.43229300	-1.61145200	1.82797100
C	6.35810400	-1.02746900	2.48365400	C	-7.25861900	-1.08124100	2.17620300
H	6.47630800	-0.38971900	3.36584400	H	-7.20407200	-0.45626300	0.11600900
H	6.77155500	-2.01131700	2.72832000	C	-6.51894000	-1.54226900	3.26713900
H	6.95772800	-0.60230300	1.67297500	H	-4.55600500	-2.08406600	3.97980400
C	4.20666600	-1.61554300	-3.97533100	H	-8.33032700	-0.92877900	2.26836800
H	5.12818800	-1.06922600	-3.75156200	H	-7.01146600	-1.75115800	4.21247800
H	4.48032700	-2.63952800	-4.25041700	C	-5.01316800	1.84495300	-0.30671600
H	3.73844900	-1.15111800	-4.84947500	C	-6.06326500	2.54602400	-1.19285300
C	4.02601600	-1.68523500	3.25345200	H	-4.17184700	2.53820400	-0.15443200
H	4.32924700	-2.70691800	3.50553600	H	-5.43856700	1.64019500	0.68000600
H	4.15197900	-1.06777000	4.14921000	C	-6.54934400	3.87599600	-0.60367100
H	2.96219800	-1.70360400	2.99692600	H	-5.64063400	2.72103100	-2.19194300
H	4.52161100	-0.09943000	1.90993500	H	-6.91984500	1.87387800	-1.33699000
Cu	0.95056800	-0.85113000	0.66331000	C	-7.60277500	4.56922400	-1.47364900
H	-3.91746600	0.74028700	-1.85878600	H	-6.96069700	3.69785300	0.39897500
C	1.92401100	-2.33229900	-3.11509100	H	-5.68883400	4.54465300	-0.46525600
H	1.45154900	-1.88263800	-3.99466600	H	-7.92947600	5.51455700	-1.02796200
H	2.10766200	-3.38877000	-3.33724400	H	-7.20887800	4.79023500	-2.47238500
H	1.21464700	-2.28117900	-2.28343900	H	-8.48907100	3.93707600	-1.60069800
H	2.97526800	-0.54720800	-2.59342400	77			
C	-3.71563500	-3.76092700	-2.75130100	C	2.24260200	-0.40753300	-0.97945100
C	-4.42039900	-3.13046200	-1.53499000	C	3.24902200	-1.00804600	0.02309700
H	-3.86630300	-3.16198600	-3.65458100	H	2.19248500	0.67746900	-0.85031200
H	-2.63957300	-3.84804600	-2.58542500	H	2.62125500	-0.59119400	-1.99629200
H	-4.12310300	-4.76133400	-2.93089200	C	4.66703600	-0.45030600	-0.14841600
C	-4.15245700	-4.02395300	-0.29847700	H	2.89949300	-0.81416100	1.04602400
C	-5.93668500	-3.05380500	-1.81461400	H	3.26967700	-2.10046500	-0.09114400
H	-4.72017100	-3.70340900	0.57595000	C	5.66769100	-1.03702600	0.85155200
H	-4.44450300	-5.05363000	-0.53351100	H	5.01072800	-0.64982800	-1.17232800
H	-3.08978700	-4.02424300	-0.03525800	H	4.64082200	0.64260400	-0.04336200
H	-6.31807400	-4.05722100	-2.03350200	H	6.66963600	-0.62121400	0.70364400
H	-6.49556200	-2.66589900	-0.96076700	H	5.36772300	-0.82359000	1.88381200
H	-6.14946400	-2.41947900	-2.68212600	H	5.74004000	-2.12556800	0.74693900

C	0.88066000	-1.02665800	-0.88326700
C	-0.28918100	-0.43181600	-0.56740300
C	-0.39214600	1.02962900	-0.26798500
C	-1.10721700	1.87376300	-1.13425400
C	0.25805700	1.60603800	0.83580000
C	-1.17609700	3.24779800	-0.90077300
H	-1.60390500	1.44975200	-2.00243600
C	0.18946000	2.98037100	1.07080400
H	0.81520200	0.96904300	1.51633400
C	-0.52903000	3.80579300	0.20404500
H	-1.73175900	3.88232800	-1.58499300
H	0.69784100	3.40451100	1.93176500
H	-0.58290500	4.87489100	0.38634900
H	0.83809900	-2.09198700	-1.10632700
C	-1.98631100	-1.02887800	1.90033400
C	-2.60291700	-1.26547700	0.50624700
H	-1.25694400	-1.80684200	2.14995700
H	-1.49210500	-0.05856200	1.97600900
H	-2.77708500	-1.05836100	2.65767100
C	-3.60358700	-0.13212100	0.17040600
C	-3.36628800	-2.60383900	0.51302500
H	-4.02778900	-0.26639900	-0.83013700
H	-4.42866700	-0.15781600	0.89070000
H	-3.14352700	0.85605100	0.21946900
H	-4.15008600	-2.57424200	1.27663800
H	-3.83001200	-2.80157000	-0.45549400
H	-2.69924800	-3.44109200	0.74010600
C	-1.50435500	-1.34240700	-0.58614900
O	-1.57792100	-2.20368400	-1.45478400

78

C	-0.83884600	3.89825700	0.77898600
C	-1.47696100	4.38043800	-0.53823000
H	-0.20563700	4.70216400	1.18110300
H	-1.65480900	3.76176000	1.50412500
C	-2.31723200	5.65457000	-0.38516900
H	-0.68816000	4.55202700	-1.28518700
H	-2.10531600	3.57592700	-0.94483800
C	-2.96586900	6.11265800	-1.69577400
H	-3.09913600	5.48058300	0.36719500
H	-1.68694900	6.46170900	0.01318600
H	-3.56069900	7.02161200	-1.55437400
H	-2.20865700	6.32641400	-2.45927400
H	-3.63012500	5.33853800	-2.09752800
C	-0.09304400	2.57777800	0.64534300
C	1.26492400	2.50613800	0.72300100
C	2.29044200	3.56402700	0.90675800
C	3.43822400	3.26543900	1.67134700
C	2.22525500	4.84320500	0.31812200
C	4.45040300	4.20346500	1.87054600
H	3.52306100	2.27938400	2.12316800
C	3.23805800	5.78402500	0.51460000
H	1.38887600	5.09321600	-0.32537000
C	4.35363500	5.47429600	1.29598700
H	5.31613900	3.94294600	2.47417400
H	3.15949900	6.76080200	0.04394600
H	5.14097300	6.20759500	1.44614400
C	-1.99775500	-0.74029100	0.16660200
C	-3.56498400	-2.31169500	-0.31700400
C	-2.44658900	-2.96575100	0.10234400
N	-1.49702200	-1.99174700	0.39519900
N	-3.27514200	-0.95089200	-0.27302900
Cl	-2.17322500	-4.64607500	0.26882000
Cl	-5.07077700	-2.95183000	-0.81679000
C	0.05793900	-2.32979800	2.26583700
C	-0.15341800	-2.24548400	0.87518400
C	0.88489800	-2.37764800	-0.06844100
C	2.17961300	-2.57936000	0.42696800
C	2.42298600	-2.65372400	1.79597300
C	1.37258500	-2.53581700	2.70251400
H	3.01011700	-2.67078500	-0.26577800
H	3.43831300	-2.79816400	2.15184100
H	1.57524100	-2.59761600	3.76722000
C	-5.01846100	0.66632600	0.34216900
C	-5.86442700	1.71375800	-0.04397200
C	-5.88080200	2.18033600	-1.35597600
C	-5.05295800	1.60298900	-2.31549600
C	-4.18671600	0.55203100	-1.98786300
C	-4.18458000	0.11174900	-0.64932400
H	-6.51689400	2.17061800	0.69372500
H	-6.54415600	2.99467800	-1.63251900
H	-5.07857500	1.97286100	-3.33568600
C	-1.06553300	-2.18952700	3.28815600

H	-2.01274700	-2.10015300	2.74864500
C	-0.89742300	-0.90656200	4.12626400
H	-1.73551700	-0.79546700	4.82272600
H	0.02594000	-0.93458400	4.71474200
H	-0.86291100	-0.01921400	3.48596800
C	-1.17419900	-3.43407800	4.19040300
H	-2.02545900	-3.33205800	4.87170600
H	-1.31847700	-4.34350100	3.59893400
H	-0.27562900	-3.56881300	4.80154700
C	0.65544200	-2.30293300	-1.57475300
H	-0.41340900	-2.15455200	-1.75249800
C	1.39068600	-1.09919700	-2.19661200
H	1.16263600	-1.02982600	-3.26581200
H	1.08584300	-0.16162000	-1.72075200
H	2.47630100	-1.19660100	-2.09222600
C	1.05551500	-3.61836800	-2.27154500
H	0.82961100	-3.56179100	-3.34168900
H	2.12746000	-3.81546500	-2.16779600
H	0.51343000	-4.47261600	-1.85400000
C	-5.02502500	0.18170600	1.78840200
C	-3.29824500	-0.06025500	-3.06643400
C	-6.41760900	-0.32611900	2.20996900
H	-6.37952200	-0.72728700	3.22816000
H	-7.16024600	0.47846700	2.19850700
H	-6.77061200	-1.11963800	1.54407000
C	-4.13481200	-0.66668400	-4.21003800
H	-4.84017200	-1.41471400	-3.83515500
H	-4.70822500	0.10147200	-4.73941300
H	-3.47850900	-1.15247000	-4.93974100
C	-4.51632200	1.27580600	2.74750500
H	-5.17048900	2.15415100	2.73367200
H	-4.48776300	0.89574200	3.77423800
H	-3.50710900	1.60107200	2.47513800
H	-4.33544900	-0.66323600	1.86939400
Cu	-1.07486800	0.94068600	0.40556400
H	1.71562700	1.51066400	0.69632100
C	-2.28050400	0.96448000	-3.60389000
H	-1.62843100	0.49465200	-4.34777700
H	-2.78244300	1.81046700	-4.08565500
H	-1.65307300	1.35686800	-2.79748200
H	-2.72616200	-0.87646300	-2.61647100
C	8.31802700	-0.33221800	-0.92282900
C	7.00148300	0.07395900	-0.22632800
H	8.84805700	-1.10503900	-0.35797100
H	8.14114900	-0.69952900	-1.93546500
H	8.96393700	0.54875000	-0.98302000
C	6.25967900	1.14375700	-1.05674300
C	7.28993200	0.60576500	1.19248900
H	5.32220500	1.44317700	-0.57894900
H	6.89934600	2.02819700	-1.13105600
H	6.04243900	0.78970000	-2.06622600
H	7.93333300	1.48675300	1.11703300
H	6.36795400	0.89511100	1.70321900
H	7.80078700	-0.14371800	1.80258200
C	6.10650100	-1.15670500	-0.06889500
O	5.67481600	-1.64255900	0.92180200
Br	5.60987200	-2.06251900	-1.84168900
TS29			
C	2.94446300	0.71670200	-0.81650500
C	4.32546200	0.35378100	-1.40502600
H	3.05000700	1.62393300	-0.20381900
H	2.30497900	1.02752100	-1.65068200
C	4.99552000	1.53854000	-2.11426500
H	4.98941300	-0.01796100	-0.61699700
H	4.21252200	-0.46951100	-2.12020700
C	6.34388900	1.17988900	-2.74770900
H	4.31893200	1.92816000	-2.88754000
H	5.13556600	2.35821700	-1.39575200
H	6.79819700	2.04510100	-3.24254700
H	7.05192200	0.81863700	-1.99290600
H	6.23091400	0.38908500	-3.49850900
C	2.23764100	-0.36761800	-0.00270600
C	2.73554100	-0.91777300	1.13486700
C	3.93375900	-0.65414200	1.96440900
C	4.29576500	-1.63685700	2.91271700
C	4.72190000	0.51677100	1.92993800
C	5.39153600	-1.47842000	3.75826000
H	3.69790300	-2.54303600	2.97749400
C	5.81485600	0.68105400	2.78171600
H	4.47365000	1.31685300	1.24454400
C	6.16329700	-0.31487000	3.69721700
H	5.64158900	-2.26236900	4.46844300

H	6.39688500	1.59771700	2.72985200	H	-3.36772600	-1.88184600	-2.48695900
H	7.01747200	-0.18388400	4.35534700	H	-4.88327000	-2.74665100	-2.20194600
C	-1.29021700	0.54722100	0.08063600	C	-6.12260400	-0.78723000	-0.65628600
C	-2.51551100	2.43271700	0.46544200	H	-6.56930400	-0.20995500	-1.47276700
C	-3.20881300	1.38720500	0.98409100	H	-6.64501600	-1.74861500	-0.60740300
N	-2.46606700	0.23684700	0.72324800	H	-6.30864500	-0.25496800	0.27908300
N	-1.34008200	1.91112500	-0.06757600	C	0.44982600	3.39799600	1.73587900
Cl	-4.67860400	1.42166400	1.86144700	C	-1.18493900	2.11084900	-2.99922500
Cl	-2.95643300	4.08576200	0.40571700	C	0.22208200	4.79476400	2.34793400
C	-2.37632900	-1.73768100	2.18945700	H	0.07885000	4.70922800	3.43018700
C	-2.92733200	-1.09813900	1.05854400	H	1.08353600	5.44965900	2.18057100
C	-3.93717600	-1.68645800	0.26445800	H	-0.66034400	5.28268000	1.92523700
C	-4.35827600	-2.97502400	0.61709400	C	-2.08099000	3.11554700	-3.75119000
C	-3.81347200	-3.64219100	1.70954100	H	-2.64427400	3.74641500	-3.05651700
C	-2.83957800	-3.02519100	2.48936100	H	-1.48830100	3.77285500	-4.39661200
H	-5.12735500	-3.46111000	0.02506000	H	-2.79733200	2.58237400	-4.38521700
H	-4.15601600	-4.64189900	1.96070300	C	1.69120700	2.73097200	2.35848800
H	-2.43777500	-3.54832000	3.35045000	H	2.59961700	3.30278700	2.13988600
C	0.54686400	3.45907400	0.21177400	H	1.58384100	2.68409300	3.44770200
C	1.51926500	4.27447800	-0.38053100	H	1.82886900	1.71367200	1.98415500
C	1.63306700	4.37597800	-1.76450500	H	-0.41179600	2.78021500	2.00321200
C	0.76812900	3.66413200	-2.59043400	Cu	0.31903900	-0.61584600	-0.39167100
C	-0.22560700	2.83237800	-2.05703600	H	2.15601000	-1.74401600	1.55118800
C	-0.30447700	2.73732400	-0.65277300	C	-0.43831200	1.19142000	-3.98399800
H	2.19450400	4.84101600	0.25305100	H	-1.15568600	0.63992100	-4.60076800
H	2.39330500	5.01775500	-2.20024400	H	0.20898000	1.76201700	-4.65858200
H	0.85662300	3.76263600	-3.66779500	H	0.18282200	0.46407500	-3.45286800
C	-1.36822400	-1.06069700	3.11555300	H	-1.84023900	1.47369000	-2.40006400
H	-0.89541400	-0.24356800	2.56498300	C	1.71702500	-4.75422400	-2.45734000
C	-0.24146900	-2.00547600	3.56954100	C	2.14051100	-3.35543600	-1.93948100
H	0.52632500	-1.43498000	4.10190100	H	1.71340700	-5.49068900	-1.64892900
H	-0.60641500	-2.77691700	4.25596700	H	0.72576100	-4.72712200	-2.91406400
H	0.23037300	-2.50226100	2.71792400	H	2.44130200	-5.07466500	-3.21281900
C	-2.08559100	-0.44845100	4.33772600	C	2.15258000	-2.34727100	-3.09134200
H	-1.36499200	0.06559600	4.98294000	C	3.53148300	-3.46651500	-1.27722600
H	-2.85141400	0.27426100	4.04044200	H	2.30171700	-1.33170500	-2.72202100
H	-2.57465300	-1.22849000	4.93176300	H	2.97305800	-2.59665100	-3.77135700
C	-4.61448600	-0.99097700	-0.91825800	H	1.21852700	-2.37564000	-3.65447900
H	-4.16226900	-0.00312600	-1.04659000	H	4.25674800	-3.77411400	-2.03676300
C	-4.42394700	-1.75326100	-2.24388600	H	3.84408300	-2.51315100	-0.85197900
H	-4.90203300	-1.20204000	-3.06080700	H	3.52641300	-4.21613400	-0.48176300

C	1.14330500	-3.00983300	-0.81451000
O	1.06585500	-3.46784100	0.27657000
Br	-0.86012500	-2.58385500	-1.75976700

79

C	4.95367300	0.81800400	0.25550400
C	4.23973400	0.96980800	-1.10362400
H	5.74304100	1.56992100	0.34724500
H	4.22683700	1.00682600	1.05237700
C	3.63504700	2.36407500	-1.30971400
H	4.94466300	0.75196200	-1.91816300
H	3.44312100	0.21877100	-1.18202600
C	2.94590400	2.51717500	-2.66967300
H	2.91060900	2.56358200	-0.50886700
H	4.42357600	3.12292400	-1.20711400
H	2.50062700	3.51149200	-2.78235200
H	3.65681800	2.37518700	-3.49221500
H	2.14854400	1.77516700	-2.78838000
C	5.52215200	-0.56509800	0.48639100
C	6.83424800	-0.89441000	0.42959600
C	8.00612600	-0.06146200	0.10881200
C	9.22777100	-0.37272700	0.73978900
C	7.99652600	0.99565500	-0.82217300
C	10.38146700	0.36568400	0.48640000
H	9.26217400	-1.19911600	1.44510800
C	9.15457700	1.72818300	-1.08327400
H	7.09128700	1.22442400	-1.37195600
C	10.34872400	1.42411300	-0.42559000
H	11.30709700	0.11153000	0.99479900
H	9.12474900	2.53364700	-1.81149100
H	11.24784900	1.99746800	-0.63125500
C	-2.62375800	0.22036400	0.07314300
C	-3.93696100	1.50686300	1.39867500
C	-4.63915700	0.37906200	1.09795900
N	-3.82164100	-0.39980000	0.28490300
N	-2.70379800	1.39541700	0.76325400
Cl	-6.21593700	-0.07451500	1.57708500
Cl	-4.39816200	2.84546600	2.35610800
C	-3.88762800	-2.84954800	0.46207000
C	-4.18182200	-1.68615900	-0.27654500
C	-4.80845200	-1.71466900	-1.53885000
C	-5.13180000	-2.97193100	-2.06430900
C	-4.84888700	-4.14080500	-1.36266400
C	-4.23533400	-4.07779900	-0.11443300
H	-5.61062800	-3.03509200	-3.03645300
H	-5.10817400	-5.10488300	-1.79024400
H	-4.02019400	-4.99639700	0.42217600
C	-0.68739200	2.29079800	1.84127300
C	0.32981200	3.25348500	1.85659000
C	0.38339000	4.26114000	0.89696000
C	-0.58345500	4.32933500	-0.10315700
C	-1.62364800	3.39407800	-0.17063200
C	-1.64568400	2.38437900	0.81280700
H	1.08940100	3.21106400	2.63063600
H	1.18044100	4.99811000	0.93006400
H	-0.53090400	5.12039700	-0.84458900
C	-3.21568800	-2.82205800	1.83159500
H	-3.05213800	-1.77816000	2.11415400
C	-1.83412600	-3.50387800	1.79064500
H	-1.34880100	-3.43287900	2.76975300
H	-1.92109400	-4.56558500	1.53668300
H	-1.18015200	-3.03278500	1.05044200
C	-4.11376600	-3.45126100	2.91490000
H	-3.63454000	-3.36735400	3.89585100
H	-5.08629400	-2.95221300	2.96686200
H	-4.29056600	-4.51460500	2.72180700
C	-5.13597100	-0.45597900	-2.33670500
H	-4.83216200	0.41400300	-1.74742200
C	-4.34492000	-0.40935900	-3.65860400
H	-4.55902000	0.52109000	-4.19517100
H	-3.26660100	-0.45967000	-3.47818700
H	-4.61555600	-1.24336900	-4.31460700
C	-6.65076200	-0.32504600	-2.59006300
H	-6.86538500	0.61387300	-3.11095400
H	-7.02618500	-1.14355500	-3.21304000
H	-7.21375400	-0.33042100	-1.65170100
C	-0.71380200	1.20330900	2.91082500
C	-2.66684100	3.50178600	-1.27831100
C	-0.84069100	1.80394700	4.32478900
H	-0.91420300	1.00280900	5.06765200
H	0.03150000	2.41435700	4.58133900
H	-1.73111400	2.43413100	4.41370300
C	-3.45214800	4.82515800	-1.18628200

H	-3.93335900	4.93628800	-0.20971600
H	-2.79852300	5.69014200	-1.34025100
H	-4.23060000	4.85572700	-1.95576800
C	0.51906000	0.28528300	2.80454000
H	1.44829000	0.83751500	2.97632200
H	0.46143800	-0.51150000	3.55357400
H	0.58795100	-0.17925700	1.81693000
H	-1.59676400	0.57918900	2.74512100
Cu	-1.16844700	-0.42236600	-0.96737600
H	7.10555400	-1.90371800	0.72492000
C	-2.02919400	3.32990300	-2.67085900
H	-2.80233700	3.35969300	-3.44595900
H	-1.31245800	4.12998100	-2.88388200
H	-1.50072600	2.37491000	-2.75126000
H	-3.38806100	2.68907700	-1.15207500
C	3.09724300	-3.60787000	0.60357600
C	4.54908200	-3.08238400	0.57636900
H	2.64341500	-3.46230300	1.58527000
H	2.47621000	-3.09099900	-0.13526300
H	3.09187100	-4.67722500	0.36845200
C	5.12632400	-3.32388600	-0.83377800
C	5.36319300	-3.85815500	1.64297900
H	6.18787700	-3.08290400	-0.91137200
H	5.00429600	-4.38002500	-1.09764600
H	4.59258600	-2.73149200	-1.58444500
H	5.29883500	-4.93238000	1.43833300
H	6.42290900	-3.58828700	1.65189000
H	4.95894800	-3.67950200	2.64434700
C	4.50763800	-1.57643700	0.96638300
O	3.59475600	-1.17640100	1.68225600
Br	0.55038900	-1.21112100	-2.22250000

80

C	-0.38980300	0.92051900	0.58786400
C	-0.60181700	2.14618200	-0.32700400
H	0.54478400	1.04009400	1.14468200
H	-1.18547800	0.91259000	1.33740800
C	-0.62149100	3.47012300	0.44655800
H	0.18790600	2.17514600	-1.08908600
H	-1.54380600	2.03129100	-0.87930200
C	-0.82729000	4.68973100	-0.45667400
H	-1.41739200	3.43512700	1.20280100
H	0.31992200	3.57887500	1.00196800
H	-0.83587500	5.61818000	0.12340400
H	-0.02804100	4.76994000	-1.20214100
H	-1.77819500	4.62585200	-0.99757200
C	-0.36361100	-0.39051000	-0.16692600
C	0.76176500	-1.06788500	-0.50260400
C	2.17746000	-0.78904200	-0.21490500
C	3.03770600	-1.89587200	-0.06012400
C	2.74232300	0.49841100	-0.12450500
C	4.39188400	-1.72808800	0.21604600
H	2.62692900	-2.89794400	-0.14992200
C	4.10095000	0.66610200	0.14271900
H	2.13048200	1.37417400	-0.30218900
C	4.92966400	-0.44287200	0.32326100
H	5.02903700	-2.59865200	0.34064200
H	4.51460300	1.66870500	0.19931300
H	5.98674900	-0.30748500	0.53135300
H	0.60268000	-2.00959100	-1.02416700
C	-3.78880500	-2.29954300	-0.26869400
C	-2.88523000	-1.18560700	0.29537100
H	-4.11489100	-2.07060100	-1.28521500
H	-3.26564300	-3.25991400	-0.29543700
H	-4.67399700	-2.40866100	0.36615900
C	-2.47182300	-1.56858000	1.73333300
C	-3.69470400	0.13520100	0.28850800
H	-1.85099000	-0.81258400	2.21864600
H	-3.36878200	-1.70202400	2.34752300
H	-1.91860700	-2.51342400	1.74299100
H	-4.61900400	-0.00726500	0.85857700
H	-3.15737500	0.97168400	0.73939200
H	-3.97149400	0.41724800	-0.73247100
C	-1.64206900	-1.06018900	-0.62689200
O	-1.66802200	-1.57740600	-1.73866800

81

C	5.35010800	1.47489400	-0.46311500
C	6.58772900	1.77756500	-1.33191400
H	5.63824300	1.42655800	0.59098800
H	4.64628800	2.31520100	-0.56229600
C	7.26952000	3.10135400	-0.96400200
H	7.30863800	0.95456600	-1.23418400
H	6.29301300	1.80044400	-2.39027400

C	8.50042400	3.40177000	-1.82517700
H	6.54369900	3.92011000	-1.06169900
H	7.55944600	3.07654200	0.09507100
H	8.96587200	4.35069200	-1.53903500
H	9.25684100	2.61526300	-1.72237600
H	8.23465600	3.46756000	-2.88651600
C	4.63087700	0.22679900	-0.88313100
C	4.41432100	-0.89567100	-0.16654600
C	4.87116700	-1.06706800	1.24584700
C	3.92183000	-1.25447700	2.26602700
C	6.22989500	-1.00430800	1.59919500
C	4.32209900	-1.37565800	3.59783700
H	2.86453100	-1.29451900	2.01549100
C	6.62924300	-1.12697600	2.93151900
H	6.97644600	-0.86655800	0.82236100
C	5.67648300	-1.31368700	3.93530400
H	3.57292800	-1.51625500	4.37187900
H	7.68492400	-1.07825000	3.18337200
H	5.98682400	-1.40965200	4.97180800
H	4.22924300	0.24351900	-1.89577200
C	3.61512100	-4.16753100	0.40835100
C	4.10124000	-3.45364100	-0.87738100
H	4.07270400	-3.75437600	1.30897100
H	2.52765600	-4.09473200	0.51035300
H	3.87940000	-5.22942900	0.34926200
C	3.47821400	-4.16112200	-2.09623400
C	5.63873100	-3.53451600	-0.97390000
H	3.79375200	-3.69154700	-3.03341900
H	3.79722100	-5.20846400	-2.11447200
H	2.38758100	-4.12919400	-2.05793000
H	5.94500300	-4.58369600	-1.04746100
H	6.01057800	-3.01458000	-1.86337800
H	6.12954100	-3.10687100	-0.09723400
C	3.62118600	-1.97872400	-0.87413000
O	2.62418800	-1.66375300	-1.51363300
C	-2.16160800	0.23275900	0.12693800
C	-3.47526200	1.85736600	-0.76284700
C	-4.17173300	0.68920200	-0.82603800
N	-3.35578900	-0.29567700	-0.27768900
N	-2.24511700	1.56188800	-0.18227200
Cl	-5.74177400	0.39855300	-1.43990900
Cl	-3.95162000	3.42455400	-1.25613900
C	-4.38220600	-2.10560100	1.02837900
C	-3.71418100	-1.69307100	-0.14220500
C	-3.37930000	-2.57810200	-1.18636500
C	-3.72806400	-3.92463000	-1.02122900
C	-4.38334300	-4.36464700	0.12565300
C	-4.70661100	-3.46364600	1.13676300
H	-3.48147800	-4.63696800	-1.80239000
H	-4.64375700	-5.41373800	0.23165700
H	-5.21788300	-3.81877000	2.02611900
C	-1.12930700	3.14727500	1.32661000
C	-0.08914800	4.06040400	1.54156600
C	0.84058000	4.34138000	0.54429300
C	0.74865600	3.71469300	-0.69558900
C	-0.26721300	2.78988300	-0.96866300
C	-1.18810900	2.52190500	0.06476500
H	-0.00846000	4.55805900	2.50291200
H	1.63852700	5.05359700	0.73324600
H	1.47703800	3.94662700	-1.46639500
C	-4.74967800	-1.14975600	2.15904100
H	-4.43184600	-0.14260200	1.87469300
C	-4.00544600	-1.50978800	3.45980600
H	-4.24313700	-0.78359200	4.24444300
H	-4.29474900	-2.50129100	3.82412200
H	-2.92136100	-1.50892100	3.30842500
C	-6.27337300	-1.10005100	2.38540200
H	-6.51536300	-0.36746700	3.16252500
H	-6.80303500	-0.81477400	1.47129100
H	-6.66227000	-2.07052400	2.71112100
C	-2.66627800	-2.13475000	-2.45992300
H	-2.50049300	-1.05536800	-2.40376700
C	-1.28189900	-2.79920500	-2.58951000
H	-0.64862600	-2.57038200	-1.72694500
H	-1.36791100	-3.88828000	-2.66812000
H	-0.77363500	-2.43797600	-3.48960300
C	-3.52946500	-2.39880900	-3.70950300
H	-3.02270000	-2.02127000	-4.60381400
H	-3.70658900	-3.46960300	-3.85547700
H	-4.50282000	-1.90391900	-3.63510100
C	-2.13522200	2.87556100	2.44098400
C	-0.34404700	2.14156100	-2.34791200

C	-2.92149600	4.14865600	2.81197500	C	-5.95520100	-1.96100100	-2.26149100
H	-3.67236700	3.91841100	3.57511800	H	-5.63431700	-2.03718000	-0.13492200
H	-2.26227300	4.92350400	3.21750300	C	-5.42629800	-1.59714000	-3.50204600
H	-3.43730300	4.56673300	1.94186300	H	-3.74398200	-0.71224500	-4.52053200
C	-0.65609200	3.18986700	-3.43600500	H	-6.94397600	-2.40733300	-2.19930700
H	-1.58400600	3.72855900	-3.22259000	H	-5.99891900	-1.76012100	-4.41074500
H	0.14970700	3.92735000	-3.51785600	H	-2.99866800	0.12337300	1.90199900
H	-0.76126000	2.70176600	-4.41070400	C	-2.31874500	-3.88050800	-0.94200100
C	-1.45217400	2.26331100	3.67918800	C	-1.94395200	-3.29423600	0.43055400
H	-0.72644200	2.95556300	4.11905000	H	-3.34421900	-3.65649300	-1.23586400
H	-2.19899800	2.03129600	4.44598100	H	-1.64962800	-3.50693500	-1.72261400
H	-0.92487300	1.33883000	3.42296000	H	-2.21638100	-4.97139000	-0.90090300
H	-2.86112900	2.14266300	2.07795900	C	-0.55589300	-3.83603800	0.81665000
Cu	-0.72321900	-0.69670500	1.03927900	C	-2.97601000	-3.76904600	1.48505300
H	0.36445700	-1.43174400	1.81273600	H	-0.25643500	-3.50323100	1.81135800
C	0.94035300	1.36388800	-2.69246600	H	-0.56928400	-4.93153200	0.80209300
H	0.82904800	0.87766400	-3.66771900	H	0.20302900	-3.49869700	0.10115900
H	1.80514600	2.03339300	-2.75673000	H	-2.98821600	-4.86375500	1.52725400
H	1.16704700	0.59058400	-1.95380500	H	-2.72002500	-3.39106100	2.47947300
H	-1.16650200	1.42050200	-2.34364300	H	-3.98787200	-3.43155600	1.24040200
TS30				C	-1.92553300	-1.72841500	0.53314400
C	-4.76189500	0.94512400	0.86853500	O	-1.25456300	-1.25262400	1.52538100
C	-5.80330300	0.74601200	1.98781400	C	1.56271400	0.35755500	-0.02966700
H	-5.24605500	0.84215900	-0.10728900	C	3.04221200	2.08294600	-0.09804400
H	-4.38622600	1.97817200	0.92968500	C	3.75259200	0.94716400	0.13500900
C	-6.95734100	1.75485400	1.92787300	N	2.83631900	-0.10190000	0.17629400
H	-6.20569200	-0.27433500	1.92735400	N	1.70383100	1.70936000	-0.19700500
H	-5.30508200	0.81945000	2.96462700	Cl	5.43955900	0.75038400	0.34452500
C	-7.99281100	1.55054200	3.03836600	Cl	3.59689900	3.69409000	-0.25609600
H	-6.54973900	2.77327000	1.98875700	C	3.44424100	-2.30848000	-0.71304500
H	-7.45037300	1.68256100	0.94890900	C	3.16911100	-1.49198500	0.40291200
H	-8.80197500	2.28539000	2.97119300	C	3.20096000	-1.97048900	1.72856100
H	-8.44321400	0.55295700	2.98056100	C	3.50743700	-3.32469700	1.91439800
H	-7.53477300	1.64873800	4.02933800	C	3.77438600	-4.15886400	0.83214800
C	-3.58952600	0.01434200	0.99529200	C	3.74440400	-3.65396500	-0.46528000
C	-3.17316200	-0.92696500	0.12399800	H	3.53749200	-3.72874900	2.92152400
C	-3.93126600	-1.18015300	-1.14158100	H	4.00960500	-5.20583900	1.00038600
C	-3.42117300	-0.80440200	-2.39528000	H	3.95944500	-4.31318400	-1.30053800
C	-5.21613500	-1.75072900	-1.09583200	C	0.21727700	2.86831500	-1.77014200
C	-4.15918700	-1.01282700	-3.56223100	C	-0.88387000	3.71036200	-1.97048900
H	-2.44114700	-0.34450300	-2.44911900	C	-1.56391500	4.27571500	-0.89482100

C	-1.14806100	4.02042700	0.40944600	Cu	-0.03873300	-0.67533500	-0.12454700
C	-0.05424600	3.18542200	0.67176000	H	-1.03213800	-1.49161000	-1.04365400
C	0.59774800	2.61024800	-0.43752600	C	-0.69297000	2.24035900	2.94091900
H	-1.20977000	3.92749900	-2.98300000	H	-0.33324900	2.07155400	3.96187800
H	-2.41605200	4.92492200	-1.07407700	H	-1.60464700	2.84437400	3.00733600
H	-1.67804300	4.47902300	1.23843700	H	-0.95195100	1.27168400	2.50430300
C	3.43586800	-1.78986500	-2.14811800	H	1.26768200	2.29787600	2.09801600
H	3.18126000	-0.72652900	-2.12712600	82			
C	2.36136600	-2.49562700	-2.99804000	C	4.40193000	1.35744000	-0.21698800
H	2.35127500	-2.08122600	-4.01191300	C	5.49407800	1.79239400	-1.21466700
H	2.55714300	-3.57020100	-3.07959400	H	4.86789600	1.08548400	0.73581400
H	1.36644500	-2.36077100	-2.56273800	H	3.76106400	2.23021600	-0.01741500
C	4.82875700	-1.91439900	-2.79679000	C	6.31130400	2.99705100	-0.73127200
H	4.81551900	-1.48344800	-3.80344200	H	6.16866600	0.94628900	-1.40636600
H	5.59003600	-1.38981400	-2.21120900	H	5.02817400	2.03287300	-2.18072900
H	5.13611700	-2.96164600	-2.88752300	C	7.39693100	3.42779800	-1.72287900
C	2.93190000	-1.08552300	2.94226500	H	5.63239600	3.83994600	-0.54186400
H	2.70579700	-0.07611300	2.58741700	H	6.77300800	2.75603100	0.23610200
C	1.70457400	-1.56941800	3.73945700	H	7.96183400	4.28898900	-1.35037400
H	0.80808400	-1.59399900	3.11359700	H	8.11029200	2.61593400	-1.90621300
H	1.86630000	-2.57225400	4.15004200	H	6.96137100	3.70773900	-2.68909700
H	1.51823900	-0.89441300	4.58197200	C	3.53301700	0.24308500	-0.73549800
C	4.17711400	-0.98553500	3.84598000	C	3.37413800	-1.00590100	-0.25802400
H	3.98273200	-0.30491900	4.68166100	C	4.11743900	-1.50712200	0.93634700
H	4.44423400	-1.96081300	4.26680900	C	3.42798400	-2.04108100	2.04130200
H	5.04372200	-0.60858100	3.29413200	C	5.52218700	-1.45799700	1.00874300
C	0.95831700	2.29555400	-2.97536200	C	4.11064100	-2.49596600	3.17087400
C	0.39266500	2.95374400	2.11241900	H	2.34297600	-2.08604300	2.02285500
C	1.57023800	3.41846800	-3.83696000	C	6.20801400	-1.91347900	2.13582000
H	2.14663700	2.98781700	-4.66255300	H	6.08044600	-1.07342300	0.16025500
H	0.79415400	4.05775000	-4.27089900	C	5.50511300	-2.43545300	3.22417100
H	2.23950000	4.05384000	-3.24892900	H	3.55085200	-2.89623200	4.01208100
C	0.82372600	4.27490800	2.78059100	H	7.29347500	-1.86607000	2.16032600
H	1.61721400	4.77075600	2.21296100	H	6.03712400	-2.79280600	4.10129700
H	-0.01600400	4.97269600	2.86553300	H	2.90949700	0.50073600	-1.59024500
H	1.19778200	4.08066300	3.79131000	C	4.09264300	-3.79665900	-1.32524000
C	0.05335200	1.37940100	-3.82107200	C	2.96134500	-2.96108300	-1.95276600
H	-0.81096500	1.92335700	-4.21671300	H	4.97294000	-3.19254400	-1.09168700
H	0.61388000	0.97863800	-4.67245700	H	3.76756600	-4.28310400	-0.39808800
H	-0.31292800	0.53697900	-3.22705100	H	4.40707800	-4.58496000	-2.02033600
H	1.78477100	1.67947700	-2.61022100	C	1.84296100	-3.92521500	-2.39720100

C	3.50089700	-2.21389800	-3.18381500
H	1.01458000	-3.37504400	-2.84810700
H	2.22254500	-4.65040900	-3.12758800
H	1.45005400	-4.49018900	-1.54219400
H	3.89350800	-2.92281700	-3.92292500
H	2.70800300	-1.62819200	-3.65647400
H	4.31052200	-1.52967500	-2.91009100
C	2.33214000	-1.94893100	-0.91262500
O	1.29132800	-1.25729600	-1.53646500
C	-1.69034800	0.30804200	0.00173000
C	-3.19138100	1.80165400	0.82033700
C	-3.82559400	0.60168700	0.71563900
N	-2.89520100	-0.30357400	0.21438700
N	-1.88478500	1.60752200	0.38101900
Cl	-5.44170800	0.19453700	1.09782400
Cl	-3.80049700	3.30217400	1.36904100
C	-2.95162400	-2.63398900	0.98704400
C	-3.15867700	-1.70309600	-0.05068900
C	-3.61167700	-2.07195900	-1.33306700
C	-3.84978000	-3.43322100	-1.56117900
C	-3.65105500	-4.37810500	-0.55814100
C	-3.20807700	-3.98078600	0.70065700
H	-4.19398700	-3.75615600	-2.53865300
H	-3.84255200	-5.42830400	-0.75810700
H	-3.05647300	-4.72733200	1.47399000
C	-0.06474200	2.84669500	1.46894700
C	0.91361000	3.84592800	1.38890900
C	1.08037200	4.60053600	0.23041600
C	0.26746100	4.37249500	-0.87687100
C	-0.72789400	3.38750300	-0.85534300
C	-0.86651700	2.63677400	0.32919400
H	1.55220500	4.03450700	2.24613500
H	1.84487800	5.37099600	0.19153300
H	0.40538600	4.96831100	-1.77360400
C	-2.45610800	-2.23880000	2.37485100
H	-2.35345600	-1.15053000	2.40688300
C	-1.06272200	-2.83457300	2.65639200
H	-0.69857300	-2.50195500	3.63431300
H	-1.09132000	-3.92927500	2.66407300
H	-0.34018300	-2.52189200	1.89574500
C	-3.46212000	-2.63300200	3.47370100
H	-3.10846700	-2.28507900	4.44986600
H	-4.44624100	-2.19092300	3.29068300
H	-3.58659700	-3.71917300	3.53402000
C	-3.83717100	-1.06715400	-2.45867400
H	-3.63277600	-0.06514600	-2.07086500
C	-2.85912600	-1.30965500	-3.62502000
H	-1.82001000	-1.26679000	-3.28375000
H	-3.02264200	-2.28971400	-4.08569100
H	-2.99801400	-0.54843400	-4.40015200
C	-5.29939300	-1.07697200	-2.94532400
H	-5.44626400	-0.30787100	-3.71080600
H	-5.56960000	-2.04119900	-3.38843300
H	-5.99469900	-0.87728200	-2.12410600
C	-0.22031900	2.04384200	2.75684700
C	-1.60288900	3.17253000	-2.08658300
C	-0.61718800	2.94822500	3.94056900
H	-0.77803800	2.34359400	4.83930000
H	0.16793600	3.67729300	4.16699000
H	-1.53870200	3.50009400	3.73143200
C	-2.42194600	4.43437200	-2.42334300
H	-3.04363900	4.74426500	-1.57767200
H	-1.77159200	5.27442100	-2.68914100
H	-3.07964900	4.24014900	-3.27703500
C	1.05595100	1.24177700	3.07708700
H	1.90521700	1.90478700	3.27288100
H	0.90104500	0.62743100	3.97042500
H	1.33039900	0.58139200	2.24919700
H	-1.02920500	1.32098600	2.61554000
Cu	-0.13467800	-0.48189000	-0.70746300
H	1.95516600	-2.59411100	-0.09658100
C	-0.76508600	2.71545600	-3.29693900
H	-1.41673500	2.52062300	-4.15531500
H	-0.04217700	3.48247700	-3.59440900
H	-0.21090100	1.79886600	-3.07210800
H	-2.31550700	2.37260500	-1.86649200
83			
H	-0.39552700	-1.81711700	-1.27448600
C	-4.54540200	0.26007000	0.83926200
C	-4.45549200	-0.96574300	0.28115000
C	-3.89251100	-2.04952500	1.18301500
O	-2.99932600	-1.75690900	1.97062000

C	2.16582700	0.19101000	-0.09065200	C	2.05634900	4.27683900	-2.74865700
C	4.23738300	0.89446000	0.51914800	H	2.71805800	4.15546000	-3.61267900
C	3.40490500	1.96974300	0.58543000	H	1.24647700	4.95222100	-3.04406000
N	2.13975400	1.52390500	0.21208600	H	2.62506400	4.76205500	-1.94939900
N	3.46531600	-0.18639200	0.10487100	C	3.39071500	-2.04228500	2.37494600
Cl	3.76404400	3.58603500	1.01541200	C	4.50505400	-0.92428200	-2.53807700
Cl	5.91189500	0.80010300	0.85506200	C	4.46849900	-2.21050000	3.46386300
C	0.15510800	2.46540500	1.31548600	H	4.08231600	-1.87169800	4.43088700
C	0.95234700	2.35368700	0.15819900	H	4.76750500	-3.25807300	3.57511600
C	0.65460300	3.02356700	-1.04575800	H	5.36508400	-1.62728100	3.23190500
C	-0.49410700	3.82427300	-1.06758300	C	5.94252600	-0.74127600	-3.06294400
C	-1.29911000	3.96004400	0.06023200	H	6.61636700	-0.39935800	-2.27130000
C	-0.97574500	3.28831600	1.23624600	H	6.34520600	-1.67538900	-3.46837300
H	-0.75903100	4.34996400	-1.97960300	H	5.95699200	0.00207100	-3.86692300
H	-2.18096700	4.59307500	0.02291500	C	2.11660500	-2.83523900	2.72594400
H	-1.61055300	3.40327000	2.10900100	H	2.32128700	-3.90927800	2.78985300
C	3.91957400	-2.42904400	0.99721700	H	1.72420800	-2.51086700	3.69553500
C	4.38656600	-3.73047900	0.77403800	H	1.33612800	-2.68435100	1.97364900
C	4.87245000	-4.11841300	-0.47174900	H	3.11683200	-0.98357400	2.35316600
C	4.90626700	-3.20807700	-1.52472300	Cu	0.71395900	-0.92618600	-0.73028900
C	4.45369900	-1.89288700	-1.36081400	H	-4.21804000	0.34810800	1.87434800
C	3.95840700	-1.53475300	-0.09109000	C	3.55317000	-1.36786800	-3.66636700
H	4.36627300	-4.44925100	1.58720800	H	3.57218400	-0.64077400	-4.48522400
H	5.22765000	-5.13369900	-0.62211800	H	3.84672100	-2.34058400	-4.07513900
H	5.28900100	-3.52208700	-2.49077600	H	2.52330900	-1.45046200	-3.30449200
C	0.47870700	1.75276900	2.62511700	H	4.16158800	0.05470700	-2.19248300
H	1.31895000	1.07573700	2.44699900	C	-5.02832600	1.53239800	0.20981800
C	-0.69954700	0.89143200	3.11828800	C	-6.26605200	2.12079900	0.91711400
H	-0.40020700	0.32756300	4.00823400	H	-5.24047500	1.38905300	-0.85358900
H	-1.55837900	1.51106200	3.39858300	H	-4.21069000	2.26621600	0.27567300
H	-1.03552900	0.17903200	2.35997600	C	-6.70059300	3.47306300	0.33817900
C	0.91300800	2.75725700	3.71221800	H	-7.09721400	1.40652100	0.84332300
H	1.18429600	2.22639800	4.63091900	H	-6.05463600	2.23346400	1.98952000
H	1.77542000	3.35060300	3.39412600	C	-7.93547000	4.05486500	1.03351700
H	0.09985300	3.45010700	3.95454900	H	-5.86611300	4.18332900	0.41602300
C	1.51521600	2.90540800	-2.29970900	H	-6.90334600	3.35832700	-0.73512700
H	2.38031600	2.27926600	-2.06480600	H	-8.22076400	5.01888700	0.59959500
C	0.74728400	2.20937400	-3.44043400	H	-8.79514100	3.38112800	0.94224100
H	0.39643900	1.21872100	-3.13425200	H	-7.75104300	4.21201600	2.10248600
H	-0.12460900	2.79560400	-3.74956900	C	-4.84442400	-1.22604700	-1.13979100
H	1.39632500	2.08856700	-4.31435000	C	-6.17245100	-1.08788300	-1.57707000

C	-3.86028600	-1.56363700	-2.08516600	H	0.10671900	5.27281100	-0.61503200
C	-6.51052900	-1.29066400	-2.91687300	H	-0.62649500	5.55077000	1.72607400
H	-6.94456300	-0.82373600	-0.85999100	H	-0.03154700	3.86487200	3.42696800
C	-4.19872300	-1.76523200	-3.42458900	C	2.55409300	-3.11132700	0.13773300
H	-2.82420700	-1.65927100	-1.76970000	C	2.42745700	-4.42260000	-0.33821400
C	-5.52461500	-1.63225200	-3.84481500	C	2.34784100	-4.68952300	-1.70231800
H	-7.54397500	-1.18153200	-3.23368200	C	2.39755500	-3.64652400	-2.62334200
H	-3.42329000	-2.02380100	-4.14022800	C	2.51945000	-2.31484400	-2.20643800
H	-5.78659600	-1.79090500	-4.88697700	C	2.58652300	-2.07603900	-0.81845100
C	-4.48113200	-3.48425400	1.20256300	H	2.39314000	-5.24451300	0.37016800
C	-6.02439100	-3.43628000	1.19032600	H	2.25152600	-5.71432900	-2.04920100
C	-3.96933600	-4.29828100	-0.01129100	H	2.34232400	-3.86797000	-3.68460000
C	-4.00852900	-4.18301200	2.49163100	C	1.41043700	1.58390100	3.14885500
H	-6.41138700	-2.85175400	2.03210600	H	1.95729000	0.76063700	2.68100100
H	-6.41652400	-3.00787800	0.26584500	C	0.16111400	0.97556200	3.81430500
H	-6.42089500	-4.45349700	1.28038500	H	0.46186200	0.24210100	4.57039200
H	-2.87506600	-4.30470600	-0.04842300	H	-0.43755800	1.74205600	4.31821800
H	-4.30879600	-5.33557800	0.08714200	H	-0.47171800	0.46813300	3.08094200
H	-4.34225600	-3.90989200	-0.95988500	C	2.34518100	2.21802500	4.19876700
H	-4.42400200	-5.19538200	2.53150800	H	2.64549300	1.46775700	4.93779600
H	-2.91913800	-4.25282900	2.52939700	H	3.25090000	2.62321000	3.73711500
H	-4.33854000	-3.64139700	3.38333800	H	1.84746200	3.03307700	4.73508300
TS31				C	1.57339900	3.28147000	-1.72588200
H	-1.49302300	-0.15400700	-1.34700200	H	2.11973300	2.34088000	-1.83612700
C	-2.88682600	0.59004500	-0.31052200	C	0.37749800	3.22335400	-2.69557600
C	-3.52086100	-0.52202800	0.25137800	H	-0.27639300	2.37745500	-2.46269100
C	-2.72102200	-1.28978600	1.17543300	H	-0.21928000	4.14085400	-2.65386900
O	-1.47109200	-1.07941100	1.23164500	H	0.73376200	3.10552400	-3.72454600
C	1.63129200	0.10245500	-0.07946700	C	2.53927700	4.42179000	-2.10670900
C	3.90317900	-0.04767400	-0.11345500	H	2.89836200	4.28561800	-3.13229600
C	3.58571000	1.20241000	0.31708000	H	2.04499900	5.39773400	-2.05367400
N	2.19512800	1.28263300	0.33270100	H	3.40809600	4.44855300	-1.44215100
N	2.70113800	-0.71045400	-0.35227300	C	2.65783200	-2.86075800	1.63907600
Cl	4.62392400	2.48384000	0.77739800	C	2.59488300	-1.20355000	-3.24948800
Cl	5.44647700	-0.75283500	-0.34112200	C	3.88898600	-3.56406700	2.24418900
C	1.04067500	2.59077600	2.06344700	H	3.97850800	-3.31692700	3.30727900
C	1.43395400	2.45191300	0.71650900	H	3.80973600	-4.65330300	2.16277700
C	1.12003200	3.40546100	-0.27399000	H	4.81225200	-3.25530500	1.74412500
C	0.36854200	4.51950700	0.12158300	C	3.88372900	-1.31736500	-4.08878900
C	-0.04516200	4.67839300	1.44170200	H	4.77656300	-1.29871800	-3.45630200
C	0.29062000	3.72539800	2.39966000	H	3.90058100	-2.24754300	-4.66689800

H	3.94918800	-0.48378200	-4.79609300	H	-5.08590900	-1.36701200	2.70877900
C	1.36538300	-3.27475800	2.36840500	H	-5.36034700	-2.64630500	1.51844000
H	1.17334700	-4.34771400	2.25785200	H	-5.00309500	-3.06583600	3.19433600
H	1.45416500	-3.06240300	3.43966300	H	-1.79649700	-3.84142700	1.32007600
H	0.49948600	-2.72929500	1.98208200	H	-3.14592700	-4.58476400	2.19930600
H	2.78825600	-1.78684900	1.79902500	H	-3.39719600	-3.95725600	0.56356900
Cu	-0.24725800	-0.27029600	-0.35056800	H	-2.83267400	-3.06019600	4.14828300
H	-2.10741200	1.04602300	0.29461400	H	-1.44527400	-2.27959800	3.35746900
C	1.34736800	-1.18001800	-4.15298500	H	-2.79357900	-1.30045600	3.95219200
H	1.41084900	-0.34404700	-4.85783200	84			
H	1.25636800	-2.10097000	-4.73864600	H	-3.24813700	1.58830800	-0.68866800
H	0.43530400	-1.05958300	-3.56109400	C	-3.10898600	0.93616300	0.18606800
H	2.62861800	-0.24437200	-2.72545100	C	-3.55798100	-0.47472000	-0.18030600
C	-3.50106800	1.53234400	-1.31618700	C	-2.75598000	-1.55236100	0.07475300
C	-4.14711800	2.76175800	-0.64189400	O	-1.58742000	-1.42042600	0.72896000
H	-4.24342000	1.01412600	-1.93084100	C	1.65594700	0.20093700	-0.08984300
H	-2.71628100	1.88874600	-1.99128600	C	3.88910000	0.51538200	-0.34589600
C	-4.71796400	3.76156000	-1.65655000	C	3.27231100	1.68580900	-0.66649300
H	-4.94535100	2.43742300	0.03732400	N	1.90558000	1.48031300	-0.50241700
H	-3.39629100	3.26571200	-0.01735600	N	2.88768100	-0.38666800	0.00183800
C	-5.35183400	4.99015700	-0.99622700	Cl	3.95834600	3.16440500	-1.18152600
H	-3.91725300	4.08155700	-2.33699300	Cl	5.55743900	0.14195600	-0.33502800
H	-5.46488500	3.25404800	-2.28168000	C	0.56112900	3.35208600	0.34338300
H	-5.75301900	5.68329400	-1.74311500	C	0.88472800	2.48508300	-0.71989500
H	-6.17543200	4.70194500	-0.33285100	C	0.26390600	2.55323700	-1.98309800
H	-4.61850100	5.53780800	-0.39309400	C	-0.72865000	3.52651100	-2.15623200
C	-4.78328500	-1.03923700	-0.36761000	C	-1.07948800	4.39066400	-1.12243000
C	-6.02699600	-0.42168800	-0.15273200	C	-0.44026400	4.30334300	0.11171300
C	-4.73787900	-2.13977400	-1.24174600	H	-1.23264000	3.60815000	-3.11423200
C	-7.18504000	-0.89564100	-0.77172000	H	-1.85290800	5.13669100	-1.27974800
H	-6.08652900	0.42656500	0.52296400	H	-0.72247100	4.98419600	0.90864100
C	-5.89456500	-2.61937300	-1.86112800	C	3.22971500	-2.06178000	1.76731800
H	-3.78267300	-2.61716700	-1.44251700	C	3.41445500	-3.40555800	2.11675600
C	-7.12391400	-1.99969300	-1.62606200	C	3.47964000	-4.40097700	1.14551000
H	-8.13628300	-0.40507700	-0.58368800	C	3.36874200	-4.07216900	-0.20301100
H	-5.83368900	-3.47331200	-2.53045700	C	3.18251200	-2.74620300	-0.61341700
H	-8.02502000	-2.37084300	-2.10605700	C	3.10570300	-1.76433700	0.39534600
C	-3.24974400	-2.40827800	2.11537200	H	3.51019900	-3.67391700	3.16411000
C	-4.76566100	-2.36352000	2.38700000	H	3.62221700	-5.43648400	1.44031000
C	-2.87235500	-3.77998100	1.50713100	H	3.42770700	-4.85674200	-0.95086200
C	-2.52868400	-2.25104600	3.47538400	C	1.23921000	3.28636200	1.70888900

H	2.03351400	2.53601800	1.66336500	C	-3.86143300	1.58366900	1.37014400
C	0.25049800	2.83433600	2.80132000	C	-3.63964400	0.89255300	2.72030200
H	0.76206400	2.75722200	3.76667600	H	-4.93733700	1.60261200	1.14822800
H	-0.57144200	3.54915900	2.91381100	H	-3.54773200	2.63470400	1.44770900
H	-0.18236000	1.85761200	2.56432300	C	-4.44437400	1.51846000	3.86681500
C	1.90305800	4.62641600	2.08148900	H	-3.89925200	-0.17032800	2.62907700
H	2.43039200	4.53089500	3.03630600	H	-2.57035100	0.92228600	2.97286200
H	2.62693000	4.93791300	1.32235000	C	-4.21285000	0.82979100	5.21612500
H	1.16345200	5.42643300	2.19054600	H	-4.18814500	2.58395000	3.95231000
C	0.62346700	1.62651500	-3.14028400	H	-5.51442700	1.48458700	3.61858700
H	1.42411600	0.95842000	-2.81058900	H	-4.80127500	1.29625700	6.01376300
C	-0.57065300	0.73858700	-3.54146200	H	-4.49234800	-0.22926600	5.17168700
H	-0.93317100	0.15279300	-2.69079600	H	-3.15743100	0.87874500	5.50885000
H	-1.40543300	1.33912200	-3.91848900	C	-4.91733100	-0.48341200	-0.80867100
H	-0.27468300	0.04419000	-4.33500500	C	-6.07682700	-0.75330700	-0.05908500
C	1.15995900	2.41619400	-4.35050200	C	-5.09214800	-0.09267100	-2.14931000
H	1.46709600	1.72657200	-5.14365900	C	-7.34994700	-0.67336900	-0.62972300
H	0.39600000	3.08135000	-4.76644900	H	-5.97140100	-1.03990900	0.98384000
H	2.02520500	3.02774500	-4.07647700	C	-6.36087200	-0.01111300	-2.72622300
C	3.18301800	-0.99808800	2.85979400	H	-4.21378600	0.13751300	-2.74754300
C	3.08057800	-2.42486500	-2.10163500	C	-7.49790600	-0.30430100	-1.96842700
C	4.51537800	-0.93072300	3.63239400	H	-8.22629000	-0.89680000	-0.02651600
H	4.48228100	-0.12262500	4.37061900	H	-6.46237700	0.27989200	-3.76877800
H	4.71409100	-1.86408900	4.16956000	H	-8.48647300	-0.24154000	-2.41491700
H	5.35791000	-0.74358300	2.95950100	C	-3.02685200	-3.04919500	-0.25066000
C	4.37819200	-2.79811300	-2.84586600	C	-4.26984300	-3.37054400	-1.10123200
H	5.24731000	-2.29620900	-2.41037000	C	-1.80241700	-3.60372000	-1.01890500
H	4.56062900	-3.87740800	-2.81313400	C	-3.15145700	-3.80821700	1.09232600
H	4.30653900	-2.50474300	-3.89843600	H	-5.20386300	-3.12548700	-0.59415600
C	1.99656200	-1.22060800	3.81774800	H	-4.26103500	-2.84420100	-2.05953400
H	2.08823800	-2.17003900	4.35573000	H	-4.28011800	-4.44714900	-1.31158300
H	1.95806500	-0.41833100	4.56214700	H	-0.88264700	-3.46528500	-0.44880600
H	1.04562100	-1.23072300	3.27617100	H	-1.93267300	-4.67452600	-1.21572700
H	3.03509600	-0.02446900	2.38433100	H	-1.68776800	-3.09887400	-1.98568900
Cu	-0.01637400	-0.58745500	0.27488200	H	-3.25624300	-4.88593900	0.91736600
H	-2.03743400	0.93596400	0.40985600	H	-2.26819700	-3.64060100	1.71271100
C	1.85910500	-3.10680400	-2.74726100	H	-4.03204500	-3.47049700	1.65066200
H	1.78315400	-2.82182700	-3.80203600	85			
H	1.94037800	-4.19803100	-2.70286800	C	6.20567500	0.06252100	-1.33986800
H	0.93064000	-2.81786700	-2.24650400	C	7.20308300	-0.33870800	-0.23710500
H	2.94203300	-1.34549900	-2.21218800	H	6.05690100	1.14727900	-1.32902600

H	6.66451000	-0.17188600	-2.31398200
C	8.57402400	0.33195000	-0.38864800
H	6.77916400	-0.08775900	0.74460800
H	7.33046800	-1.43072800	-0.24305500
C	9.56874000	-0.07311300	0.70406400
H	8.99037100	0.08219900	-1.37433000
H	8.44583800	1.42298400	-0.38111200
H	10.53574900	0.42335800	0.57037300
H	9.19293200	0.19218900	1.69897300
H	9.74590700	-1.15489300	0.69647200
C	4.88904100	-0.65997400	-1.22399400
C	3.63789800	-0.16357700	-1.28536200
C	3.38609100	1.28796900	-1.53523300
C	3.88112400	1.90803400	-2.69806200
C	2.66995700	2.07780700	-0.61829800
C	3.66592100	3.26573000	-2.94273500
H	4.43289500	1.31435500	-3.42158400
C	2.45902100	3.43721700	-0.86187400
H	2.31771700	1.61469800	0.29500500
C	2.95092000	4.03707200	-2.02398800
H	4.05758800	3.71884600	-3.84974300
H	1.90902000	4.03029800	-0.13666400
H	2.78398700	5.09482800	-2.20913800
H	4.98591600	-1.73333300	-1.04974200
C	0.94646000	-0.29539400	-3.07223100
C	1.72878000	-1.48569600	-2.48899200
H	0.19584800	0.07985600	-2.36547300
H	1.60066300	0.53831400	-3.33463000
H	0.41807800	-0.60615900	-3.98093600
C	2.76483900	-1.95097900	-3.53420900
C	0.75771100	-2.65830600	-2.24045300
H	3.45935200	-1.15216100	-3.80672200
H	3.35676500	-2.79413200	-3.15993700
H	2.25411500	-2.28090100	-4.44634700
H	0.26593200	-2.95034000	-3.17536500
H	1.28994100	-3.53235300	-1.84907100
H	-0.02272700	-2.39576300	-1.51988600
C	2.47132000	-1.15856000	-1.14295200
O	1.56877700	-0.82429400	-0.08085100
C	-2.15613500	0.15905600	0.10240100
C	-4.06024800	1.25722400	0.68705700
C	-4.40993800	-0.01402700	0.35819500
N	-3.24015600	-0.67581200	-0.00543600
N	-2.67973900	1.35257600	0.52806400
Cl	-5.96088700	-0.73493700	0.37092600
Cl	-5.06393100	2.54679400	1.19227500
C	-2.94945800	-3.09552400	0.37484400
C	-3.20717700	-2.03339600	-0.51698600
C	-3.48042900	-2.23429700	-1.88729300
C	-3.44950900	-3.55171900	-2.36173900
C	-3.17587800	-4.61863600	-1.51115500
C	-2.93569800	-4.39073400	-0.15912400
H	-3.64845600	-3.74278200	-3.41150900
H	-3.15867300	-5.63221100	-1.90097900
H	-2.74045300	-5.23293700	0.49626300
C	-1.44375700	2.88371100	2.01199600
C	-0.80656200	4.11977300	2.18190500
C	-0.67860500	5.01830100	1.12647400
C	-1.17954300	4.69469600	-0.13143000
C	-1.82474000	3.47363100	-0.36381000
C	-1.94149900	2.58563700	0.72643600
H	-0.41418500	4.38474400	3.15832300
H	-0.18936300	5.97489000	1.28569500
H	-1.07485700	5.40332300	-0.94684800
C	-2.74834700	-2.89613000	1.87442800
H	-2.56812900	-1.83293000	2.05701100
C	-1.52768500	-3.66308600	2.41386300
H	-1.37165800	-3.41241000	3.46797000
H	-1.67071000	-4.74708900	2.35502600
H	-0.61722700	-3.40696500	1.86657200
C	-4.02075400	-3.29769700	2.65076900
H	-3.88313400	-3.11667200	3.72209700
H	-4.89570700	-2.73167900	2.31884400
H	-4.23888700	-4.36266600	2.51460200
C	-3.83258800	-1.10393300	-2.85233000
H	-3.77803600	-0.15570300	-2.30999100
C	-2.83420300	-1.01349700	-4.02084400
H	-1.81276300	-0.87782700	-3.65966900
H	-2.85757100	-1.91629900	-4.64023700
H	-3.08618400	-0.16387900	-4.66436500
C	-5.27409200	-1.24965500	-3.38199200
H	-5.52441100	-0.40080000	-4.02698900

H	-5.38759800	-2.16304300	-3.97544600
H	-6.00211000	-1.28480600	-2.56701800
C	-1.59698100	1.94811500	3.20786300
C	-2.38134700	3.17654600	-1.75356300
C	-2.60996600	2.50916200	4.22731600
H	-2.74149500	1.80457100	5.05534900
H	-2.25821100	3.45765800	4.64755500
H	-3.58818400	2.68641100	3.77175900
C	-3.52143900	4.14819400	-2.11997500
H	-4.33056300	4.11363400	-1.38457200
H	-3.16001500	5.18056900	-2.17442000
H	-3.93818500	3.88887200	-3.09887300
C	-0.24591500	1.66438500	3.89055400
H	0.17178500	2.56771400	4.34741400
H	-0.38145900	0.92682500	4.68828000
H	0.48675800	1.26875100	3.18279700
H	-1.98409000	0.99099500	2.84637200
Cu	-0.31183900	-0.31671800	-0.02641600
H	2.93591700	-2.10532500	-0.85271700
C	-1.27577500	3.20153800	-2.82665200
H	-1.69212900	2.91812500	-3.79913800
H	-0.84073400	4.20085000	-2.93151000
H	-0.46577200	2.50838700	-2.58467000
H	-2.80161600	2.16693200	-1.74919100
Si	1.85811700	-1.31537700	1.81709700
H	0.37808600	-0.94725700	1.80435500
O	2.38933800	-2.81181800	1.20421800
O	2.94863300	-0.01467600	1.88244200
C	3.83610000	0.27328600	2.95399300
C	4.56607300	1.57970300	2.66732000
H	4.56830000	-0.53898300	3.07681100
H	3.29409700	0.35887000	3.90520000
H	5.26827400	1.81061400	3.47624200
H	5.12515100	1.51505900	1.72900000
H	3.85576800	2.40814300	2.57977400
C	3.00668700	-3.85624700	1.94130100
C	3.41166100	-4.97105800	0.98491300
H	2.32209300	-4.25508900	2.70258000
H	3.89546100	-3.48781300	2.47366900
H	3.88471300	-5.79398300	1.53217200
H	2.53589100	-5.36547900	0.45919200
H	4.12077300	-4.60266200	0.23661400
C	1.77043500	-1.78280900	3.70412000
H	1.38259000	-0.93173200	4.27773800
H	1.05598800	-2.60464900	3.84134300
H	2.71112800	-2.09063200	4.17674700

TS32

C	-6.19361500	0.76237800	1.48358600
C	-7.49980100	0.16460700	0.93152200
H	-5.99358500	1.72559100	1.00283400
H	-6.34935100	0.98509300	2.55156400
C	-8.71692600	1.07161600	1.15135600
H	-7.38430900	-0.03689500	-0.14123400
H	-7.68322400	-0.80991800	1.40653700
C	-10.01968200	0.47712400	0.60656600
H	-8.82712400	1.27372400	2.22583400
H	-8.53241300	2.04518900	0.67703300
H	-10.86882300	1.14711400	0.77836600
H	-9.95133800	0.29635800	-0.47237900
H	-10.24893900	-0.48097100	1.08737100
C	-5.00914500	-0.15995900	1.34023800
C	-3.75337800	0.13524500	0.95511300
C	-3.39288200	1.52950900	0.54904400
C	-3.45877600	2.59313600	1.46554100
C	-3.07008300	1.82891000	-0.78629700
C	-3.20840300	3.90866600	1.06800000
H	-3.72064800	2.38695000	2.49951300
C	-2.82109100	3.14323400	-1.18551000
H	-3.05261000	1.02428700	-1.51112500
C	-2.88609600	4.18859200	-0.26085400
H	-3.27200900	4.71264700	1.79645800
H	-2.58358600	3.35255100	-2.22502600
H	-2.69375200	5.21043400	-0.57488200
H	-5.22224500	-1.20076000	1.58939600
C	-1.26432000	0.03749500	2.82478100
C	-1.99880800	-1.22097200	2.33538100
H	-0.50306800	0.36370200	2.10829800
H	-1.95478400	0.86955700	2.98336900
H	-0.76405900	-0.16122700	3.77899500
C	-3.04146200	-1.62374200	3.39913200
C	-1.00420900	-2.39163300	2.20370800
H	-3.76279300	-0.82620600	3.59189500

H	-3.59853600	-2.51843500	3.09706300
H	-2.53399500	-1.85384100	4.34285500
H	-0.57510400	-2.63289100	3.18266300
H	-1.50266200	-3.28690900	1.81873800
H	-0.18097200	-2.15994800	1.52299400
C	-2.70267500	-0.99267800	0.94687000
O	-1.71786900	-0.82741300	-0.08935000
C	2.14838100	0.27351100	0.02651100
C	4.07158500	1.47045800	-0.21666100
C	4.42213200	0.21642200	0.16748400
N	3.24161100	-0.50661900	0.32269000
N	2.68100000	1.49701200	-0.29833000
Cl	5.98900600	-0.42400000	0.41860300
Cl	5.08440700	2.80623800	-0.56114800
C	3.13040800	-2.90386600	-0.23085100
C	3.19631400	-1.89151100	0.75080200
C	3.27042200	-2.17091600	2.13233600
C	3.22634600	-3.51650900	2.51897100
C	3.13282800	-4.53546100	1.57595900
C	3.09400100	-4.23002800	0.21838600
H	3.27461200	-3.76793700	3.57388600
H	3.10133500	-5.57193500	1.89911200
H	3.04113300	-5.03479700	-0.50707500
C	1.70209400	2.91377000	-2.05363600
C	1.04602000	4.10255500	-2.39866100
C	0.65355900	5.01825800	-1.42702500
C	0.90202300	4.76070500	-0.08190100
C	1.55005500	3.58817400	0.32509500
C	1.93619200	2.67934000	-0.68277600
H	0.84915400	4.31616400	-3.44457800
H	0.15372800	5.93723700	-1.71923000
H	0.59277800	5.48368300	0.66608800
C	3.16280100	-2.61647100	-1.72993400
H	2.93958400	-1.55625300	-1.87869000
C	2.10464600	-3.41623100	-2.51137000
H	2.09299200	-3.08666800	-3.55585800
H	2.33020400	-4.48831700	-2.51499600
H	1.10418100	-3.27731200	-2.09437400
C	4.57132900	-2.88446400	-2.30235600
H	4.59843300	-2.64067000	-3.36987400
H	5.33744200	-2.28930800	-1.79735400
H	4.84082600	-3.94067700	-2.19171400
C	3.43207000	-1.09378600	3.20291600
H	3.43020000	-0.11591300	2.71270500
C	2.26568400	-1.10129300	4.20729000
H	1.30773700	-0.96712300	3.70192400
H	2.22486900	-2.04193300	4.76671000
H	2.38807400	-0.28959400	4.93249500
C	4.77789300	-1.23853500	3.94327200
H	4.90053900	-0.42175400	4.66241100
H	4.82352800	-2.18078100	4.49957900
H	5.62445200	-1.21430200	3.25220200
C	2.15179300	1.95932700	-3.15633700
C	1.83535600	3.36329800	1.80737500
C	3.23053100	2.60476000	-4.04986700
H	3.57536900	1.88779900	-4.80246000
H	2.83641800	3.47938500	-4.57840500
H	4.09655100	2.92771100	-3.46478200
C	2.90498800	4.34687300	2.32521600
H	3.83801500	4.26565100	1.76044900
H	2.55487200	5.38200200	2.24858200
H	3.12512600	4.14555500	3.37903200
C	0.96178300	1.46847600	-4.00193100
H	0.47617100	2.29605800	-4.52995100
H	1.30651700	0.75166500	-4.75474000
H	0.21335100	0.97194800	-3.37900500
H	2.59790200	1.07792100	-2.68717700
Cu	0.34968500	-0.33400200	-0.28272900
H	-3.24751100	-1.91820700	0.73572800
C	0.55639700	3.45860500	2.66037600
H	0.77913600	3.18867800	3.69817100
H	0.15144900	4.47591200	2.66556800
H	-0.22388500	2.78935400	2.29009300
H	2.22955800	2.35046100	1.92936500
Si	-1.74899800	-1.70302900	-1.68030800
H	-0.27216900	-1.02056400	-1.70313200
O	-1.38778400	-3.27256800	-1.14707100
O	-3.46236500	-1.52496300	-1.69109700
C	-4.34733300	-1.82746300	-2.75380100
C	-5.78745500	-1.65551600	-2.28620300
H	-4.20543000	-2.85806000	-3.11297600
H	-4.16459400	-1.16721000	-3.61434400

H	-6.48507700	-1.87702000	-3.10183900
H	-6.00768000	-2.32755800	-1.45075200
H	-5.96129000	-0.62937200	-1.94907900
C	-2.02613600	-4.42555300	-1.67862600
C	-1.42398100	-5.67690600	-1.05350900
H	-1.90869500	-4.46741600	-2.77223800
H	-3.10623000	-4.39172100	-1.47160200
H	-1.90718500	-6.57640300	-1.45069700
H	-0.35223600	-5.73669400	-1.26765700
H	-1.55418200	-5.66690000	0.03352400
C	-1.49918800	-1.72623000	-3.60337400
H	-1.63712800	-0.71562600	-4.01134200
H	-0.46543200	-2.01789100	-3.81847100
H	-2.16775600	-2.39116100	-4.16209900

86

C	6.16385500	3.42112300	0.30250700
C	5.64442000	3.80654700	1.70074800
H	5.41354000	3.67222900	-0.45345600
H	7.04696800	4.04035100	0.08021200
C	5.31981800	5.29965500	1.83240300
H	4.74611700	3.21613500	1.92723800
H	6.39248000	3.52887000	2.45683000
C	4.80429100	5.68334200	3.22311100
H	6.21969000	5.88571300	1.59995000
H	4.57306000	5.57531800	1.07565800
H	4.58499000	6.75437100	3.28690800
H	3.88436200	5.14004900	3.46788800
H	5.54309700	5.44782500	3.99796900
C	6.54761700	1.96893200	0.21486400
C	6.17286100	1.04729900	-0.69478800
C	5.30288400	1.39375200	-1.86136200
C	5.70965900	2.38451500	-2.77363900
C	4.06644100	0.76126700	-2.08271800
C	4.91402600	2.73138000	-3.86722000
H	6.66548900	2.87911000	-2.62703100
C	3.26938800	1.10945000	-3.17419200
H	3.73309900	-0.00649100	-1.39620300
C	3.68849900	2.09447500	-4.07185500
H	5.25393800	3.49763600	-4.55860400
H	2.31635600	0.60864000	-3.32120400
H	3.06655100	2.36246900	-4.92125300
H	7.19894100	1.63017400	1.02282600
C	6.85613100	-1.29849800	-2.91083600
C	7.60307400	-0.98360900	-1.60107100
H	5.98973700	-1.93776800	-2.72133100
H	6.50803000	-0.39395100	-3.41397700
H	7.52542200	-1.82780900	-3.59889300
C	8.75258400	0.00368500	-1.87973300
C	8.20147200	-2.29520100	-1.04856300
H	8.38950800	0.93291200	-2.32832800
H	9.29176200	0.26163200	-0.96077000
H	9.47267200	-0.44402800	-2.57355100
H	8.88682600	-2.73894500	-1.77911100
H	8.76489600	-2.11764300	-0.12500500
H	7.41807100	-3.02569400	-0.83062400
C	6.67559400	-0.38573900	-0.49534900
O	5.56963800	-1.28730100	-0.28688500
C	-3.82152200	-0.02291800	0.02334300
C	-6.02136000	0.53281400	-0.07181400
C	-5.93011400	-0.81015500	-0.27750900
N	-4.57817300	-1.13551600	-0.21697600
N	-4.72331600	1.00068000	0.11049900
Cl	-7.17526800	-1.94782700	-0.56101500
Cl	-7.41135800	1.52837600	-0.02850400
C	-3.89278900	-3.29075100	0.74305800
C	-4.03471900	-2.46747000	-0.39172100
C	-3.66960800	-2.87958000	-1.68899500
C	-3.13219600	-4.16574100	-1.82545900
C	-2.97234400	-5.00062900	-0.72281100
C	-3.35034200	-4.56682100	0.54501000
H	-2.83352700	-4.51549400	-2.80871900
H	-2.55211700	-5.99373400	-0.85211800
H	-3.21968700	-5.22737900	1.39648300
C	-4.31860800	2.83838500	1.68948300
C	-3.95945500	4.17574800	1.89822900
C	-3.66586900	5.01824600	0.82933100
C	-3.72703100	4.53981400	-0.47670700
C	-4.08030100	3.21171400	-0.74715100
C	-4.36531900	2.38313000	0.35649800
H	-3.90767000	4.55999200	2.91213500
H	-3.38844500	6.05177100	1.01487300
H	-3.49498000	5.20654600	-1.30117500

C	-4.28881400	-2.84858600	2.14810400	H	-4.45014100	1.67789700	-2.19022600
H	-4.71961800	-1.84547500	2.08416000	Si	4.85305400	-1.63900900	1.16626100
C	-3.05722400	-2.75577100	3.07019000	H	-0.38045800	0.16832200	0.36917700
H	-3.35134900	-2.38785300	4.05894000	O	4.14249300	-3.12833600	1.01853400
H	-2.58523500	-3.73485000	3.20439400	O	6.09782400	-1.65048200	2.27106100
H	-2.30648900	-2.07319500	2.65941900	C	5.91152600	-1.82049200	3.68087900
C	-5.36769800	-3.76963700	2.75048200	C	7.26554800	-1.78409900	4.37075900
H	-5.67092600	-3.39985100	3.73555700	H	5.41001900	-2.77749300	3.87829900
H	-6.25688100	-3.81211900	2.11383400	H	5.26569300	-1.02261300	4.07171400
H	-4.99694400	-4.79183200	2.87974200	H	7.14539800	-1.91379500	5.45122900
C	-3.82378400	-1.99153000	-2.91985900	H	7.91114400	-2.58416400	3.99578200
H	-4.30249900	-1.05759800	-2.61223800	H	7.76424600	-0.82662200	4.19095300
C	-2.45039400	-1.62367200	-3.51493300	C	4.82181600	-4.30828600	0.57049700
H	-1.82014500	-1.12250300	-2.77333600	C	3.94502800	-5.52100200	0.83828700
H	-1.91676400	-2.51383900	-3.86441000	H	5.78302900	-4.41044000	1.09169600
H	-2.57616800	-0.95084900	-4.36989500	H	5.03400600	-4.21825500	-0.50225200
C	-4.73547100	-2.64029300	-3.97938900	H	4.44067900	-6.43244700	0.48813800
H	-4.87687600	-1.95664400	-4.82301000	H	3.74498800	-5.62572900	1.90916300
H	-4.30178100	-3.56588000	-4.37224800	H	2.98743200	-5.42653200	0.31702300
H	-5.72005800	-2.87896800	-3.56556400	C	3.48828200	-0.46744000	1.65044600
C	-4.62580800	1.94306500	2.88560100	H	3.86395200	0.55763200	1.72473500
C	-4.13331100	2.72456700	-2.19193800	H	2.68336100	-0.47966500	0.90890300
C	-5.79542600	2.49352400	3.72477000	H	3.05160900	-0.74263900	2.61599200
H	-6.03261900	1.80050400	4.53869000	87			
H	-5.54831600	3.46071400	4.17478200	C	3.00733400	-0.08838800	-0.77619500
H	-6.69534200	2.62528400	3.11622800	C	3.41428400	1.39383100	-0.68032000
C	-5.16879700	3.51188800	-3.01856400	H	3.61761900	-0.56257400	-1.56075600
H	-6.16631800	3.44910800	-2.57276300	H	3.25907500	-0.60102700	0.15772900
H	-4.90044800	4.57072100	-3.09574700	C	4.90232200	1.59172100	-0.36976700
H	-5.22378100	3.10871600	-4.03520000	H	3.16766300	1.90064700	-1.62374400
C	-3.37108200	1.72632500	3.75437500	H	2.80767100	1.88239700	0.09349700
H	-3.01778900	2.66912300	4.18541400	C	5.30740000	3.06554100	-0.27128300
H	-3.59571500	1.04368700	4.58089400	H	5.14590500	1.08174200	0.57219600
H	-2.55297400	1.29678600	3.16753400	H	5.50233600	1.09763500	-1.14633000
H	-4.93231100	0.96247300	2.51068200	H	6.37317600	3.17354400	-0.04414500
Cu	-1.89249700	0.08271400	0.21199100	H	5.11221100	3.59417200	-1.21133800
H	7.28074400	-0.36874800	0.41889600	H	4.74536400	3.57811200	0.51780900
C	-2.74013000	2.77567300	-2.84881900	C	1.54954000	-0.25998500	-1.10632800
H	-2.78666300	2.37322600	-3.86630700	C	0.63092700	-1.02396300	-0.48745000
H	-2.36596900	3.80293200	-2.91246500	C	0.95212200	-1.91418700	0.66787400
H	-2.01360200	2.18718100	-2.27968400	C	0.23298000	-1.80557500	1.87270200

C	1.97514300	-2.87561700	0.59537400
C	0.53460100	-2.62013900	2.96430400
H	-0.55489000	-1.06248500	1.95945400
C	2.27497000	-3.69349900	1.68582700
H	2.52868500	-2.99151500	-0.33154500
C	1.55604200	-3.56897800	2.87596800
H	-0.02778300	-2.51086200	3.88742100
H	3.06733400	-4.43202200	1.60221300
H	1.78725000	-4.20582400	3.72479300
H	1.19172300	0.36924300	-1.91962500
C	-0.50515600	-1.60117900	-3.39576800
C	-1.22696100	-1.95744400	-2.08505800
H	-0.72788200	-0.57474600	-3.70039000
H	0.57944100	-1.70127100	-3.29621200
H	-0.83205900	-2.27196100	-4.19803300
C	-0.87867700	-3.40254500	-1.68148000
C	-2.75084600	-1.86247600	-2.30452000
H	0.19961000	-3.55044600	-1.58055300
H	-1.34618700	-3.67860000	-0.72968700
H	-1.24135900	-4.09905700	-2.44534700
H	-3.06922400	-2.57603800	-3.07244400
H	-3.29863700	-2.09704700	-1.38400800
H	-3.04332000	-0.86097100	-2.62945400
C	-0.83845700	-0.97722800	-0.92714800
O	-1.22206300	0.34809200	-1.32969300
H	-1.45196900	-1.26638200	-0.06655000
Si	-1.82930400	1.52620000	-0.34637300
O	-2.43626300	0.78943700	1.01459700
O	-0.56661000	2.52702800	0.06512500
C	-0.66440700	3.51646500	1.09710800
C	0.58544000	4.38039400	1.08831400
H	-0.77849200	3.02045000	2.06993000
H	-1.55250000	4.14558500	0.94009000
H	0.52641700	5.14006500	1.87450700
H	1.47711900	3.77120200	1.26353900
H	0.69803500	4.88682700	0.12508600
C	-3.57866100	1.19327300	1.77791200
C	-4.02997100	0.03974200	2.65801700
H	-4.39363700	1.49868500	1.10912700
H	-3.31764800	2.06129600	2.39787500
H	-4.89789500	0.33721800	3.25538400
H	-4.30909900	-0.82503400	2.04857900
H	-3.22955400	-0.26188300	3.34027700
C	-3.13323300	2.46057400	-1.30059800
H	-2.72132600	2.78758600	-2.26060500
H	-4.00169900	1.82697900	-1.50670100
H	-3.48215700	3.35107800	-0.76794100

88

Si	0.45437500	-0.42416700	0.00956800
O	-0.29260300	-0.92653600	-1.45532800
O	0.59857800	-1.47555900	1.35633600
C	-0.31346300	-1.63079200	2.42429800
C	0.33260500	-2.47406500	3.51845600
H	-1.23657300	-2.12205600	2.08078400
H	-0.61628700	-0.65885900	2.83772300
H	-0.35865500	-2.61820900	4.35693100
H	0.61550400	-3.45954900	3.13381000
H	1.23698200	-1.98776700	3.89895100
C	0.35431300	-1.40820900	-2.62016400
C	-0.65872800	-1.49454900	-3.75733100
H	0.79581600	-2.39799600	-2.44219600
H	1.18228300	-0.74965400	-2.91021300
H	-0.18018900	-1.86008300	-4.67312500
H	-1.47623300	-2.17857600	-3.50500700
H	-1.09219500	-0.51062100	-3.96762800
C	0.92282900	1.41655400	0.17699700
H	0.05524800	2.08300000	0.19623900
H	1.47919300	1.56890800	1.11038200
H	1.59432100	1.71923000	-0.63167500
N	-4.34647500	0.01101900	-0.53441100
C	-3.50730700	1.13448800	-1.16907400
C	-4.08421800	2.54839600	-1.22286700
H	-3.33200700	0.80109800	-2.19484300
H	-2.55188100	1.08906300	-0.64271500
C	-3.05925000	3.49069900	-1.87906000
H	-5.00610500	2.56808900	-1.81466900
H	-4.32759400	2.93116300	-0.22928300
C	-3.57697700	4.92665200	-1.99933400
H	-2.13179200	3.48055800	-1.29311100
H	-2.79777800	3.10947800	-2.87452300
H	-2.82947400	5.57500500	-2.46644100
H	-4.48609400	4.97165700	-2.60931400

H	-3.81456500	5.34641000	-1.01564700
C	-3.71702600	-1.28150300	-1.10769700
C	-4.15807200	-2.60560700	-0.48493500
H	-2.63809200	-1.14977100	-0.99342600
H	-3.96328300	-1.26740700	-2.17277600
C	-3.52496300	-3.77541400	-1.25933400
H	-3.84056000	-2.66576500	0.56046800
H	-5.24801900	-2.72447100	-0.49707800
C	-3.88592400	-5.13734700	-0.66016800
H	-3.85034300	-3.73696400	-2.30708600
H	-2.43531900	-3.65241700	-1.26779400
H	-3.42693800	-5.95058400	-1.23051900
H	-3.53836900	-5.21890700	0.37542800
H	-4.96993100	-5.29787400	-0.66228500
C	-4.17311400	-0.05457400	0.98810900
C	-4.18521700	1.24795300	1.78687600
H	-3.19395200	-0.51148400	1.12702700
H	-4.94894700	-0.73496800	1.34484500
C	-4.04598600	0.92932900	3.28565600
H	-3.33839400	1.87095300	1.48429900
H	-5.09847600	1.82670300	1.63042300
C	-4.01166500	2.19305900	4.14966600
H	-4.88026700	0.28987700	3.60256100
H	-3.12990400	0.34785200	3.44808800
H	-3.91340500	1.94145700	5.21007700
H	-3.16581000	2.83405300	3.87880100
H	-4.92838900	2.78088100	4.02902100
C	-9.23909900	1.64413500	-0.11502900
C	-8.18502900	0.82864800	-0.86909000
H	-10.21697500	1.56374200	-0.59921300
H	-9.34737800	1.29386400	0.91724600
H	-8.96964100	2.70535800	-0.08059100
C	-6.79516800	0.91784000	-0.21575200
H	-8.49904600	-0.22197800	-0.91756000
H	-8.12156700	1.17989700	-1.90691600
C	-5.80332800	0.05022400	-0.99063000
H	-6.48208600	1.96400600	-0.18710800
H	-6.86953500	0.57148700	0.82034400
H	-6.15494900	-0.98115700	-0.95506100
H	-5.77058500	0.34568300	-2.04233100
F	-1.20400800	-0.04384200	0.52065400
C	5.43633700	1.80122600	-1.15394900
C	6.48451900	1.50904900	-2.24416100
H	5.94517500	2.08532000	-0.22727700
H	4.85616700	2.68395400	-1.46806500
C	7.40463300	2.70119200	-2.53229300
H	7.09073200	0.64469900	-1.93963800
H	5.97353200	1.21195000	-3.17091000
C	8.44990900	2.41143400	-3.61370200
H	6.79382900	3.56299900	-2.83459900
H	7.91118400	2.99929500	-1.60426300
H	9.08972700	3.28129600	-3.79590700
H	9.09812900	1.57649100	-3.32387000
H	7.97324600	2.14402400	-4.56380100
C	4.50770400	0.63654800	-0.92633400
C	4.12604000	0.05437600	0.22772200
C	4.46202100	0.63829000	1.56101500
C	4.30583700	2.02033600	1.79265400
C	4.88333200	-0.14845700	2.65007300
C	4.58599100	2.59082200	3.03449200
H	3.93255000	2.64896800	0.99184300
C	5.16753700	0.41935100	3.89269800
H	5.00617800	-1.21638600	2.52344000
C	5.02467800	1.79343300	4.09299200
H	4.45052700	3.65969600	3.17633800
H	5.50135600	-0.21757900	4.70746000
H	5.24211600	2.23434100	5.06158700
H	4.11139100	0.20148700	-1.84132700
C	4.22325900	-2.47233000	-1.82075300
C	3.87826400	-2.52681300	-0.32104200
H	3.35800100	-2.14580600	-2.40284100
H	5.05720200	-1.79510200	-2.02563300
H	4.51768000	-3.46869700	-2.17306900
C	5.16011400	-2.85307600	0.46619100
C	2.87088100	-3.67350700	-0.09947800
H	5.89402300	-2.04292000	0.40543000
H	4.94677000	-3.04812600	1.52343300
H	5.63030200	-3.75786700	0.06295800
H	3.31123500	-4.63435600	-0.39306400
H	2.57567300	-3.74015200	0.95266100
H	1.96473000	-3.51074700	-0.68603800
C	3.20128100	-1.19606800	0.19755200

O	2.04651500	-0.95157700	-0.56662200
H	2.92169300	-1.40431100	1.23816300

TS33

Si	0.20100500	-0.59845300	1.14218900
O	-0.13929100	-1.32439600	-0.30783600
O	0.36949100	-1.62915000	2.41596500
C	1.55622200	-2.16925100	3.02114000
C	1.94242200	-1.36892600	4.25727500
H	2.34764300	-2.17789300	2.26617400
H	1.31678400	-3.20183600	3.30584200
H	2.80748000	-1.82786400	4.74927100
H	2.21102000	-0.34155600	3.99071200
H	1.11898400	-1.33141800	4.97881600
C	0.26786800	-2.65422900	-0.68414200
C	0.06843400	-2.82834700	-2.18056200
H	-0.34755900	-3.38141200	-0.13484800
H	1.31896600	-2.77664400	-0.40978500
H	0.33047900	-3.84974500	-2.47815000
H	-0.97173400	-2.64638200	-2.47331200
H	0.70894800	-2.13764100	-2.73764000
C	1.14212100	1.00573000	1.11536900
H	0.87088800	1.61151000	1.98698200
H	2.21562700	0.82992600	1.09527800
H	0.87078800	1.57138400	0.21675300
N	-4.29974100	-0.16960900	-0.41299900
C	-3.24203900	0.76655800	-1.02515000
C	-3.64969700	2.18273300	-1.42875300
H	-2.89055700	0.24439000	-1.91763100
H	-2.42448700	0.77237700	-0.30363700
C	-2.42369900	2.92445400	-1.99184500
H	-4.42594900	2.15557700	-2.20086400
H	-4.04880500	2.74935400	-0.58475600
C	-2.76390500	4.34348400	-2.45547700
H	-1.63964200	2.96489300	-1.22543600
H	-2.00526500	2.35391900	-2.83057800
H	-1.87739500	4.84929200	-2.84936100
H	-3.52136700	4.33094500	-3.24695100
H	-3.15422100	4.94788500	-1.62935700
C	-3.72623600	-1.58701800	-0.64881800
C	-4.41107000	-2.74441300	0.07784500
H	-2.67382900	-1.52423900	-0.36248100
H	-3.77927300	-1.73800600	-1.73006200
C	-3.82272400	-4.08417900	-0.39938100
H	-4.26821600	-2.66159800	1.15933000
H	-5.49183300	-2.75426600	-0.10386300
C	-4.44587900	-5.28276700	0.32138500
H	-3.97563500	-4.18390900	-1.48149500
H	-2.73781500	-4.08308600	-0.23790300
H	-4.01496100	-6.22202500	-0.03788200
H	-4.27392600	-5.22814000	1.40171600
H	-5.52819200	-5.32649200	0.15672700
C	-4.42599700	0.01438100	1.10504600
C	-4.43188600	1.43189600	1.67574000
H	-3.56164500	-0.50336300	1.51916700
H	-5.32944000	-0.52416100	1.39690600
C	-4.58993600	1.36512400	3.20494600
H	-3.48449100	1.92881200	1.44687700
H	-5.23725500	2.04189100	1.26015400
C	-4.57389600	2.75220600	3.85292800
H	-5.52883900	0.85368000	3.45365300
H	-3.78139100	0.75394700	3.62473500
H	-4.68854200	2.67839300	4.93854500
H	-3.63121700	3.27236600	3.65153800
H	-5.38869300	3.37805000	3.47246100
C	-8.98136700	1.87196800	-1.25592400
C	-7.90296400	0.85413400	-1.63780500
H	-9.85699600	1.77599500	-1.90477200
H	-9.31401500	1.72840200	-0.22214500
H	-8.60822700	2.89777100	-1.34715800
C	-6.65189500	0.96505400	-0.74874400
H	-8.31412100	-0.16098400	-1.56605200
H	-7.61700700	0.99816500	-2.68754900
C	-5.63360300	-0.09861200	-1.15841700
H	-6.24282400	1.97397900	-0.83650000
H	-6.94814600	0.82258700	0.29569100
H	-6.09640800	-1.07756200	-1.03187300
H	-5.36894700	0.00210500	-2.21400400
F	-1.33187400	-0.04045800	1.48238500
C	5.47082600	2.40875000	0.37354200
C	4.89531400	3.40271100	1.39967900
H	5.14302100	2.69281300	-0.63195100
H	6.56805200	2.51376700	0.37646600

C	5.31284600	4.85548500	1.14302500	C	1.43966500	0.47209600	1.34328900
H	3.79913500	3.33022600	1.39376400	C	1.50127700	1.98696400	1.53028600
H	5.21314700	3.10719600	2.40998800	H	1.46954000	0.01097100	2.33465300
C	4.73344900	5.84164300	2.16201400	H	0.52548800	0.12530700	0.84020000
H	6.40959300	4.92293700	1.15112900	C	0.27813100	2.44575100	2.34460800
H	4.99926800	5.14883400	0.13172300	H	2.40928500	2.27955700	2.07025500
H	5.04896800	6.86906100	1.95134900	H	1.50718000	2.51865100	0.57622100
H	3.63753700	5.82161400	2.15259400	C	0.26124200	3.95916700	2.57683700
H	5.05822200	5.59594800	3.17971400	H	-0.63789100	2.14052900	1.82368700
C	5.09365400	0.98007900	0.67622600	H	0.26873500	1.92598200	3.31148300
C	4.53328900	0.04994200	-0.12373400	H	-0.61447500	4.25793300	3.16118500
C	4.25392300	0.32442400	-1.56207700	H	1.15379700	4.28827100	3.12085800
C	5.27063200	0.77504600	-2.42505500	H	0.23081300	4.50506300	1.62716600
C	2.96711500	0.13650100	-2.10392900	C	2.43418700	-1.70982900	0.98745400
C	5.01630900	1.03817300	-3.77289400	C	3.26502200	-2.73198400	0.21243200
H	6.27597100	0.90541300	-2.03473400	H	1.37052500	-1.93472600	0.86281000
C	2.71460600	0.40168000	-3.45073400	H	2.70727800	-1.72504100	2.04620300
H	2.19765900	-0.24552400	-1.44467100	C	3.12979700	-4.11547400	0.87273800
C	3.73341900	0.85579500	-4.29319100	H	2.91409800	-2.80126200	-0.82163000
H	5.82224700	1.38303100	-4.41573700	H	4.32788500	-2.46479100	0.17455800
H	1.71191600	0.25521400	-3.84601300	C	3.89831000	-5.20353100	0.11765400
H	3.53136900	1.06312900	-5.34068500	H	3.48993100	-4.06200600	1.90830400
H	5.26875000	0.68603500	1.71453000	H	2.06823300	-4.38649200	0.92778200
C	4.72751000	-2.91436200	-1.44876900	H	3.78433100	-6.17623500	0.60602500
C	4.99087400	-2.53965800	0.01878400	H	3.53562000	-5.30220900	-0.91127200
H	3.65108900	-2.99538000	-1.62076900	H	4.96927700	-4.97569500	0.07312600
H	5.12387600	-2.16493500	-2.13966900	C	2.29638100	-0.19608200	-0.95168100
H	5.19544500	-3.87648400	-1.69696400	C	1.89022400	1.12511300	-1.60492600
C	6.48578800	-2.23993100	0.22096000	H	1.45381000	-0.89167800	-1.06058300
C	4.60311600	-3.74013300	0.90222000	H	3.19901900	-0.59458000	-1.42008300
H	6.82689500	-1.42540000	-0.42598400	C	1.79356600	0.92962700	-3.12802800
H	6.69439800	-1.94737300	1.25779100	H	0.90754800	1.43089700	-1.23245300
H	7.09925800	-3.12278900	-0.00236700	H	2.59053100	1.93776100	-1.39759900
H	5.17048700	-4.63854500	0.62681600	C	1.32205600	2.19326000	-3.85292900
H	4.80309600	-3.53075900	1.96108000	H	2.77324900	0.62572500	-3.52015500
H	3.53604400	-3.95213600	0.79927800	H	1.10390400	0.10377200	-3.34311600
C	4.08902000	-1.31407900	0.49341200	H	1.26616600	2.03014100	-4.93373900
O	2.75460800	-1.54349800	0.33464200	H	0.32723100	2.49807500	-3.50971600
H	4.38656100	-1.20947300	1.57194400	H	2.00608600	3.03110700	-3.67666500
89				C	6.61140500	2.97608600	0.19951800
N	2.56416900	-0.22738700	0.55965300	C	5.93611000	1.78363900	0.88268800

H	7.58802200	3.18397000	0.64707500	H	-3.16432600	-3.44056500	0.17720500
H	6.76668900	2.78501800	-0.86791600	H	-2.38837600	-4.80960900	-0.63289500
H	6.00243800	3.88214400	0.29056700	C	-3.08775200	-2.76903900	-2.47489100
C	4.55595700	1.46734300	0.28182300	C	-0.70933100	-3.52737300	-2.26370000
H	6.58224100	0.89991300	0.80106900	H	-3.97649100	-2.37941600	-1.96768800
H	5.82739800	1.98780600	1.95569100	H	-2.86544600	-2.09914600	-3.31507300
C	3.95097100	0.24824700	0.97818500	H	-3.34757100	-3.74975900	-2.89441300
H	3.91624500	2.34763800	0.37964800	H	-0.94884900	-4.55048600	-2.57978500
H	4.67433900	1.26805300	-0.78844700	H	-0.44339300	-2.95383700	-3.16132100
H	4.62099400	-0.59692900	0.81885100	H	0.16780500	-3.55677700	-1.61139300
H	3.88928900	0.41245100	2.05747800	C	-1.38994400	-1.43616900	-1.06446300
C	-3.66326900	1.80791300	-0.91819600	O	-0.35413800	-1.47801500	-0.17459600
C	-2.92923000	3.15917400	-1.00495800	H	-1.09233300	-0.97521200	-2.04440400
H	-4.08898800	1.68869100	0.08360300	3b			
H	-4.51949100	1.84048300	-1.61139000	H	-0.36470200	-2.06973800	-1.93395200
C	-3.82834600	4.36501400	-0.70817900	C	2.12498400	-0.41491000	0.67528300
H	-2.08322100	3.15326200	-0.30318000	C	3.30705100	-1.01218000	-0.11179000
H	-2.49112300	3.27117700	-2.00751700	H	2.25952800	-0.66326600	1.73932100
C	-3.09222100	5.70545400	-0.79524000	H	2.15232200	0.67722700	0.60940100
H	-4.67439900	4.36580600	-1.40928600	C	4.67223200	-0.52223900	0.38519100
H	-4.26530200	4.25196500	0.29333000	H	3.26873700	-2.10882200	-0.04903200
H	-3.76057100	6.54572100	-0.57941400	H	3.19391300	-0.76291600	-1.17571300
H	-2.26268400	5.74852900	-0.07974100	C	5.84673000	-1.11508000	-0.39896400
H	-2.67275500	5.86246400	-1.79574400	H	4.70697600	0.57389700	0.32431300
C	-2.76856600	0.64389300	-1.26276200	H	4.77886000	-0.77102900	1.44987800
C	-2.52278200	-0.48765400	-0.57089800	H	6.80631500	-0.74728500	-0.02105900
C	-3.23761100	-0.79369800	0.70106600	H	5.85804000	-2.20876700	-0.32819300
C	-4.64399500	-0.78851300	0.75987700	H	5.78530000	-0.85373300	-1.46158500
C	-2.53367700	-1.10722800	1.88004100	C	0.80004400	-0.95094400	0.20629200
C	-5.32227800	-1.07063300	1.94755000	C	-0.29771000	-0.27249700	-0.17985900
H	-5.20962800	-0.57506600	-0.14248600	C	-0.38689800	1.21733300	-0.14065400
C	-3.21132700	-1.38861300	3.06631700	C	-0.72607300	1.95156400	-1.29125300
H	-1.45360400	-1.15871200	1.81124200	C	-0.13146400	1.93173100	1.04326400
C	-4.60832800	-1.36728000	3.11022700	C	-0.79959100	3.34457700	-1.26079000
H	-6.40911100	-1.06134400	1.96204900	H	-0.91458200	1.43106000	-2.22575900
H	-2.64603000	-1.62661700	3.96428700	C	-0.20716100	3.32451100	1.07658100
H	-5.13347700	-1.58394000	4.03651900	H	0.11243400	1.38423700	1.94861300
H	-2.20922300	0.77610500	-2.19279000	C	-0.54215700	4.03761000	-0.07614200
C	-2.24619300	-3.76733600	-0.31816700	H	-1.05498400	3.88873500	-2.16558000
C	-1.88916900	-2.87544700	-1.51772700	H	-0.00941300	3.85156300	2.00561400
H	-1.43403500	-3.73013700	0.41288200	H	-0.60309200	5.12157400	-0.05151700

H	0.75065400	-2.03628400	0.12590700
C	-3.18985900	-0.10138200	0.92587200
C	-2.64119100	-1.38348200	0.27352000
H	-2.45141000	0.38137600	1.57068300
H	-3.50670600	0.62990500	0.17386800
H	-4.06248500	-0.34486200	1.54183000
C	-3.78631500	-2.06306700	-0.50713400
C	-2.13079400	-2.34004500	1.36513400
H	-3.44906700	-2.98659600	-0.98266900
H	-4.61496800	-2.30383100	0.16791400
H	-4.17582500	-1.40102200	-1.28969300
H	-2.94674400	-2.59963800	2.04868900
H	-1.74545000	-3.26514000	0.92836200
H	-1.33088400	-1.88230100	1.95475100
C	-1.50583300	-1.03377200	-0.74545900
O	-1.11326600	-2.26674400	-1.35417300
H	-1.97261300	-0.38674400	-1.50556900

91

C	4.02370900	1.79119100	-0.67950000
C	4.11305600	2.33203200	-2.12107400
H	4.98374400	1.92537200	-0.17162800
H	3.28368300	2.39598200	-0.13386800
C	4.46201100	3.82442300	-2.17871100
H	4.86480700	1.75696000	-2.67852500
H	3.15603500	2.16063700	-2.63198300
C	4.55324900	4.36477100	-3.60930900
H	3.70531300	4.39139400	-1.61960000
H	5.41568800	3.99454600	-1.66052200
H	4.79976000	5.43174200	-3.61870500
H	5.32577000	3.83945300	-4.18258000
H	3.60335800	4.23684900	-4.14094500
C	3.56997000	0.36239500	-0.61480800
C	4.24497300	-0.70883000	-0.14715600
C	5.62387000	-0.63356100	0.42173200
C	5.85228000	-1.02621900	1.75227200
C	6.71027800	-0.14088800	-0.32167800
C	7.12337000	-0.93020100	2.32068900
H	5.02285200	-1.39862800	2.34727400
C	7.98213200	-0.04401400	0.24605600
H	6.55600200	0.15706800	-1.35443800
C	8.19350100	-0.43904200	1.56881500
H	7.27639000	-1.23574700	3.35184000
H	8.80814300	0.33720200	-0.34762900
H	9.18319900	-0.36518500	2.00996800
H	2.56308300	0.18034800	-0.99007700
C	5.05682400	-2.97081300	-1.95734800
C	4.11788000	-3.30333100	-0.78080600
H	4.53178700	-2.41125900	-2.73848100
H	5.92396000	-2.38686800	-1.64184600
H	5.42620300	-3.90079100	-2.40300700
C	4.90016900	-4.05630900	0.32446500
C	2.97856100	-4.21193600	-1.28317600
H	4.25344500	-4.27790200	1.17987800
H	5.26559100	-5.00779200	-0.07770300
H	5.76097100	-3.48734600	0.68185600
H	3.40048800	-5.13246600	-1.70013100
H	2.29543500	-4.47638700	-0.47377800
H	2.39440000	-3.71843700	-2.06644300
C	3.48638600	-2.02146700	-0.17638200
O	2.33204500	-2.05049000	0.23612400
C	-2.05755100	0.16371300	-0.04501700
C	-4.01833200	0.04316500	1.09558700
C	-3.38271200	1.17868800	1.49568300
N	-2.18226600	1.23677500	0.79364100
N	-3.19523900	-0.56807100	0.15469300
Cl	-3.89475400	2.36565600	2.61620900
Cl	-5.53218500	-0.58057300	1.59116800
C	-1.23704400	3.38739800	0.07178000
C	-1.18278600	2.27606500	0.93705900
C	-0.19992200	2.12955700	1.93747400
C	0.76533100	3.13974900	2.03827800
C	0.74911100	4.24191000	1.18713100
C	-0.24285400	4.36326400	0.21767000
H	1.53820800	3.06277900	2.79653300
H	1.50827800	5.01257000	1.28464000
H	-0.24842700	5.23070300	-0.43492100
C	-4.17749500	-1.77804800	-1.74514900
C	-4.42107500	-3.00029400	-2.38412600
C	-4.00018300	-4.20313700	-1.82334400
C	-3.32853100	-4.21017000	-0.60374500
C	-3.05475700	-3.01934800	0.08094500
C	-3.48370400	-1.81813800	-0.51906600

H	-4.94707000	-3.00849200	-3.33375100	H	-0.44184300	-3.70270800	2.28286600
H	-4.19913300	-5.13905300	-2.33728600	H	-0.98878100	-4.73612600	0.95719800
H	-3.01079400	-5.15508600	-0.17415000	H	-0.29870600	-3.14067000	0.61084400
C	-2.31872500	3.56581200	-0.98892600	H	-2.20054300	-2.04703200	1.78341100
H	-3.00572400	2.71753700	-0.92464000	TS34			
C	-1.72130800	3.55893000	-2.40929100	C	4.44854700	1.25386300	-0.60884300
H	-2.51912800	3.64006100	-3.15523900	C	5.20886600	1.50276800	-1.92663600
H	-1.03697600	4.40073900	-2.55957100	H	5.15217600	0.94341800	0.16941900
H	-1.16716000	2.63406100	-2.59860900	H	4.01440100	2.21052500	-0.28082200
C	-3.14696000	4.84151500	-0.73881100	C	6.28432000	2.58977800	-1.80536900
H	-3.95360600	4.91755300	-1.47556600	H	5.67256100	0.56483100	-2.26195000
H	-3.59654100	4.83636000	0.25898200	H	4.49291400	1.78517500	-2.71118100
H	-2.53159700	5.74307600	-0.82616700	C	7.03535500	2.84304100	-3.11652400
C	-0.16459300	0.95578200	2.91246100	H	5.81533600	3.52303900	-1.46458300
H	-0.95820300	0.25561100	2.63628000	H	6.99924400	2.30500000	-1.02155000
C	1.16618300	0.18272400	2.84400600	H	7.79283300	3.62533800	-2.99990600
H	1.36315200	-0.21282600	1.84402300	H	7.54426100	1.93614100	-3.46297200
H	2.01124400	0.81731700	3.13233000	H	6.34893700	3.15954300	-3.91041800
H	1.13813900	-0.66180500	3.54133800	C	3.32329800	0.26525400	-0.75713500
C	-0.44829500	1.42814900	4.35356700	C	3.16347300	-0.91895300	-0.13988000
H	-0.47779400	0.56951700	5.03267700	C	4.19198800	-1.46562200	0.80553100
H	0.33421100	2.10728000	4.70867000	C	3.87140800	-1.78487400	2.13681000
H	-1.40590300	1.95220100	4.42537100	C	5.51476300	-1.67381600	0.37411500
C	-4.65498900	-0.48066000	-2.39040000	C	4.84350400	-2.28224300	3.00592400
C	-2.33615800	-3.07176000	1.42602500	H	2.85245500	-1.64444700	2.47787000
C	-6.18384700	-0.47223300	-2.58422300	C	6.48637700	-2.17267700	1.24380900
H	-6.50496900	0.48969800	-2.99745100	H	5.77782600	-1.45223700	-0.65597300
H	-6.50531600	-1.25513000	-3.27896900	C	6.15478000	-2.47803600	2.56559600
H	-6.70771200	-0.62753400	-1.63597400	H	4.57463800	-2.51703500	4.03239900
C	-3.18481600	-3.81372600	2.47845100	H	7.50062200	-2.32651200	0.88554000
H	-4.17077900	-3.35313600	2.59398900	H	6.90895800	-2.86723500	3.24371100
H	-3.33395600	-4.86309500	2.20283700	H	2.52465800	0.57659200	-1.42738100
H	-2.68219200	-3.79315700	3.45115800	C	2.75556800	-2.80670000	-2.49151500
C	-3.92333300	-0.21693700	-3.72114000	C	1.98777700	-3.06774700	-1.18735800
H	-4.13625700	-1.00098900	-4.45563100	H	2.26215800	-2.03296800	-3.08806100
H	-4.24725400	0.73842100	-4.14771500	H	3.78251400	-2.48234600	-2.29926700
H	-2.83927000	-0.17791400	-3.57354900	H	2.79900300	-3.72397600	-3.08966800
H	-4.41051400	0.34687900	-1.71852300	C	2.71633500	-4.17098800	-0.37577400
Cu	-0.67194000	-0.17263100	-1.36489800	C	0.57231200	-3.57706000	-1.50912500
H	0.34999600	-0.39237500	-2.47317700	H	2.22013600	-4.33506100	0.58494500
C	-0.93400100	-3.69869000	1.30439000	H	2.69408300	-5.11067700	-0.93898000

H	3.76183000	-3.91970800	-0.18445400	C	-0.43034900	1.62369600	3.16407100
H	0.63123600	-4.51027800	-2.08040800	H	-1.31210200	1.06985700	2.82953100
H	0.00638500	-3.77043500	-0.59456400	C	0.63785600	0.58366800	3.55473400
H	0.02027600	-2.84483200	-2.10706100	H	0.88637100	-0.06497600	2.70979600
C	1.90136600	-1.79344400	-0.28175400	H	1.55783700	1.06916300	3.89850600
O	1.16080800	-1.87004300	0.76915600	H	0.26784600	-0.04482600	4.37242900
C	-1.55567500	0.34907000	0.03580200	C	-0.85883900	2.46852600	4.38037700
C	-3.74656600	0.83266800	0.40520500	H	-1.25657800	1.81971600	5.16779100
C	-3.02469000	1.93475800	0.74160900	H	-0.01380400	3.02255000	4.80269800
N	-1.68569100	1.62649400	0.51150700	H	-1.63483200	3.19193700	4.11130200
N	-2.83664000	-0.13089200	-0.02535000	C	-3.46101700	-0.54302300	-2.86483200
Cl	-3.56605700	3.44393600	1.33896900	C	-2.95974800	-2.27957800	1.97245300
Cl	-5.43885000	0.58685400	0.46748200	C	-4.85790700	-0.34473100	-3.48665000
C	-0.15290600	3.36653700	-0.29996800	H	-4.84379000	0.50040900	-4.18295500
C	-0.57259700	2.52113800	0.74709100	H	-5.17586000	-1.23101600	-4.04587500
C	0.04444700	2.50747900	2.01444700	H	-5.61210300	-0.14226800	-2.72007700
C	1.13681500	3.36311200	2.20540100	C	-4.22227900	-2.56178300	2.81167100
C	1.58492100	4.19930700	1.18612100	H	-5.06624500	-1.94669800	2.48430100
C	0.94290700	4.20234000	-0.04980600	H	-4.52306800	-3.61243500	2.73851900
H	1.64045600	3.37405600	3.16685400	H	-4.02977200	-2.34346200	3.86742900
H	2.43267100	4.85626400	1.35792500	C	-2.39846100	-0.77726800	-3.95581700
H	1.29470000	4.86562900	-0.83384100	H	-2.60065600	-1.69185700	-4.52345100
C	-3.46925000	-1.66837100	-1.83377800	H	-2.39586100	0.05927000	-4.66279400
C	-3.78608400	-2.97232700	-2.23541500	H	-1.39844400	-0.85899300	-3.51993500
C	-3.82471400	-4.01961000	-1.31865200	H	-3.19684200	0.38748800	-2.35457800
C	-3.55241200	-3.78346700	0.02623600	Cu	0.05823300	-0.53625800	-0.48724400
C	-3.22766200	-2.50089500	0.48680200	H	1.08534600	-0.78837200	-1.65121900
C	-3.18445600	-1.46439000	-0.46813500	C	-1.76355200	-3.11571700	2.46722100
H	-4.00811200	-3.16795400	-3.27994600	H	-1.57478000	-2.90534600	3.52574900
H	-4.07358100	-5.02275700	-1.65268700	H	-1.96249100	-4.18921700	2.37569100
H	-3.59477900	-4.60668400	0.73259100	H	-0.85614500	-2.88300000	1.90293000
C	-0.83925500	3.41084000	-1.66216600	H	-2.69983200	-1.22773200	2.12120200
H	-1.67500300	2.70571900	-1.64805600	92			
C	0.11163500	2.96352200	-2.78927500	C	4.68694000	1.18529900	-0.03167500
H	-0.41334800	2.97185500	-3.75060400	C	5.96700900	1.50274500	-0.82955600
H	0.97369300	3.63386700	-2.87474900	H	4.95724200	0.79750300	0.95557500
H	0.48173300	1.94965000	-2.60991400	H	4.14702700	2.12940700	0.13728000
C	-1.42438700	4.80751700	-1.95166000	C	6.85732200	2.55573800	-0.15748700
H	-1.95979500	4.80087600	-2.90692900	H	6.54167700	0.57774200	-0.97593100
H	-2.12541000	5.11725200	-1.17052700	H	5.69128700	1.84954300	-1.83570700
H	-0.63721400	5.56597200	-2.01750700	C	8.13011200	2.86567100	-0.95202400

H	6.27906200	3.47927600	-0.01623400	C	-0.13750800	3.07115700	-1.11012800
H	7.12851100	2.21058700	0.84958000	C	-0.52402600	2.54717800	0.14022700
H	8.74316000	3.62091800	-0.44879400	C	0.17390700	2.81904800	1.33409200
H	8.74588400	1.96777000	-1.07875800	C	1.30174600	3.64454400	1.24362600
H	7.88981200	3.24427100	-1.95233500	C	1.71221000	4.17359900	0.02275800
C	3.76274300	0.23718400	-0.74936200	C	1.00045400	3.88695800	-1.13925600
C	3.35918300	-0.99871000	-0.39238300	H	1.86442500	3.87541400	2.14259600
C	3.85757600	-1.66055400	0.85158400	H	2.58852200	4.81363700	-0.02290400
C	2.97539300	-2.11891300	1.84793900	H	1.33057100	4.30568400	-2.08484100
C	5.23690100	-1.84857800	1.05972900	C	-3.85513300	-1.86009300	-1.23879000
C	3.45688900	-2.73078300	3.00638100	C	-4.28252100	-3.18985200	-1.33971900
H	1.91120700	-1.99964700	1.68678600	C	-4.31786900	-4.02224300	-0.22408700
C	5.71879700	-2.46229300	2.21791100	C	-3.93008800	-3.53906600	1.02265400
H	5.93701600	-1.52185600	0.29621900	C	-3.49523600	-2.21764500	1.18532600
C	4.82975100	-2.90548900	3.19929000	C	-3.45911000	-1.40461000	0.03507600
H	2.75522400	-3.07379500	3.76263000	H	-4.58866100	-3.57828000	-2.30594200
H	6.78921900	-2.59663200	2.35015300	H	-4.65082700	-5.05094000	-0.32637200
H	5.20186500	-3.38300900	4.10155800	H	-3.96434800	-4.19725900	1.88518700
H	3.35380900	0.63610100	-1.68039000	C	-0.89463400	2.78688000	-2.40353500
C	4.15529700	-2.72233200	-2.74274900	H	-1.76371400	2.16797900	-2.16380600
C	2.83176300	-3.01255800	-2.01069400	C	-0.02785700	1.98703800	-3.39576100
H	4.05641400	-1.86631000	-3.42131400	H	-0.60395700	1.75220800	-4.29714800
H	4.96628700	-2.49893400	-2.04288400	H	0.85538000	2.55709100	-3.70278400
H	4.46028400	-3.58832700	-3.34253700	H	0.31401800	1.04597400	-2.95342000
C	3.02021300	-4.20158200	-1.05093400	C	-1.42423300	4.08298500	-3.04772000
C	1.76564400	-3.39809400	-3.05756000	H	-2.01394700	3.84634500	-3.93955100
H	2.11344600	-4.36845400	-0.46375100	H	-2.06286900	4.64014500	-2.35539100
H	3.23339900	-5.11517600	-1.62008000	H	-0.60656400	4.74278000	-3.35660200
H	3.84903000	-4.04114700	-0.35721600	C	-0.24291400	2.26071800	2.69131900
H	2.07285200	-4.29102100	-3.61543500	H	-1.13698800	1.64701600	2.55091100
H	0.80712600	-3.60507900	-2.57512300	C	0.84775500	1.34670100	3.28322100
H	1.61269500	-2.58860900	-3.78259300	H	1.09651600	0.52815300	2.60142700
C	2.32058500	-1.71132900	-1.28522300	H	1.76787000	1.90403600	3.48791600
O	1.13218800	-1.97695900	-0.58719400	H	0.50352200	0.91388300	4.22858600
C	-1.68719100	0.34484400	0.02873000	C	-0.61296800	3.38805700	3.67573200
C	-3.80552300	1.06269300	0.41979800	H	-0.95781200	2.96188800	4.62369200
C	-2.99367100	2.15486300	0.44152400	H	0.24863200	4.02817900	3.89325300
N	-1.69896600	1.70147200	0.20204500	H	-1.41087900	4.02171900	3.27685800
N	-2.99362000	-0.03882800	0.16517300	C	-3.82556400	-0.98015200	-2.48445300
Cl	-3.39708500	3.79647200	0.69956900	C	-3.08279400	-1.72468400	2.56858100
Cl	-5.49671000	0.96701900	0.65375200	C	-5.22343100	-0.84627000	-3.11981800

H	-5.18508200	-0.15952100	-3.97184200	H	-0.09084900	3.53164500	-1.90268100
H	-5.59209200	-1.80961600	-3.48746000	C	2.53295000	5.61186200	-2.49418200
H	-5.95261500	-0.45823900	-2.40203200	H	3.73707800	6.52483800	-0.95549800
C	-4.23800900	-1.84588100	3.58159100	H	1.16044200	4.54481900	-3.77227000
H	-5.12550500	-1.30343300	3.24140100	H	3.09196400	6.05291400	-3.31465000
H	-4.52339100	-2.89055000	3.74371500	H	-1.49507600	3.21335500	1.58743800
H	-3.93488700	-1.43121700	4.54868000	C	1.57274200	4.99236000	3.34147100
C	-2.79702300	-1.49798900	-3.50901000	C	1.10880600	3.52644600	3.27782500
H	-3.06536200	-2.49556200	-3.87274600	H	2.60365600	5.10516200	2.98571700
H	-2.75355400	-0.82709900	-4.37373100	H	0.92850500	5.64831500	2.74668700
H	-1.79640600	-1.55709000	-3.06968100	H	1.54914500	5.35397500	4.37656300
H	-3.50915200	0.02391700	-2.18804600	C	-0.27613600	3.41465200	3.94108600
Cu	-0.21226900	-0.77505200	-0.31287100	C	2.10590000	2.66779800	4.08390100
H	2.14591100	-1.00183900	-2.11546300	H	-0.98513900	4.13724900	3.52717300
C	-1.82342800	-2.45839200	3.07003700	H	-0.68743500	2.41035700	3.80902000
H	-1.52138600	-2.06705600	4.04736800	H	-0.19542900	3.61448100	5.01661900
H	-2.00542300	-3.53263200	3.18057900	H	2.18001800	3.02579000	5.11803100
H	-0.98799300	-2.32785600	2.37496000	H	1.79158300	1.62178000	4.09955700
H	-2.82934200	-0.66351000	2.49457100	H	3.10955100	2.71258700	3.64270500
93				C	1.11831700	2.97822200	1.79391100
C	-2.02593400	4.55154900	-0.05811800	O	0.68784100	1.64462300	1.79774100
C	-2.97924900	3.61448200	-0.82631300	C	1.70618500	-1.27205700	-0.22758500
H	-1.52037700	5.22265600	-0.75987100	C	1.59836600	-3.21601300	-1.39404900
H	-2.63995700	5.19069400	0.59615000	C	2.88467700	-3.06235200	-0.97594100
C	-4.07986000	4.36066600	-1.59122700	N	2.93703400	-1.86815300	-0.26296900
H	-2.39960700	2.99780000	-1.52673600	N	0.88835200	-2.11096500	-0.93432900
H	-3.44167700	2.91066400	-0.12041100	Cl	4.23476200	-4.08090400	-1.23155300
C	-5.00722200	3.42616100	-2.37541700	Cl	0.90326000	-4.48610800	-2.30455000
H	-4.67160800	4.95506900	-0.88147700	C	4.40933100	-1.68166400	1.69584500
H	-3.61891800	5.08177400	-2.28026100	C	4.12522300	-1.32408900	0.36253200
H	-5.79410700	3.98427500	-2.89430700	C	4.94640200	-0.46210600	-0.39183400
H	-4.44946400	2.85840800	-3.12926800	C	6.08506200	0.05419200	0.23954400
H	-5.49233100	2.70024900	-1.71258800	C	6.39225400	-0.27833600	1.55622400
C	-1.03636400	3.81571900	0.80659500	C	5.56326200	-1.13685000	2.27333000
C	0.31004800	3.81136100	0.75738600	H	6.73823100	0.72613400	-0.30823700
C	1.07262700	4.46464300	-0.34819600	H	7.28123700	0.13306300	2.02539900
C	2.17959000	5.30318000	-0.11567200	H	5.81320900	-1.38703100	3.29968600
C	0.73432300	4.20348200	-1.69147100	C	-1.45444300	-2.25156200	-0.19792800
C	2.89433000	5.87308400	-1.17078500	C	-2.80171700	-1.95522900	-0.44342800
H	2.47726900	5.52694000	0.90140900	C	-3.19570000	-1.30551200	-1.61043400
C	1.44838700	4.76962600	-2.74861600	C	-2.24828200	-0.95026600	-2.56731600

C	-0.88767500	-1.22063700	-2.37708600
C	-0.51862500	-1.85987600	-1.17593300
H	-3.55285500	-2.22551500	0.29243100
H	-4.24473600	-1.07019600	-1.76390200
H	-2.56785000	-0.44883000	-3.47574400
C	3.52249400	-2.61215200	2.51702600
H	2.67924400	-2.92229500	1.89340300
C	2.93598800	-1.88687900	3.74416700
H	2.25174600	-2.55062100	4.28332200
H	3.72340400	-1.58231100	4.44187700
H	2.38260700	-0.99051600	3.44692300
C	4.27586100	-3.89056000	2.93414500
H	3.60342300	-4.56464800	3.47508400
H	4.66663000	-4.42621900	2.06346200
H	5.11874100	-3.66169800	3.59482600
C	4.63904600	-0.07006700	-1.83361700
H	3.74914300	-0.61793100	-2.15558200
C	4.31337000	1.43246100	-1.94381600
H	3.47013600	1.70491900	-1.30167700
H	5.17153300	2.04767100	-1.65301700
H	4.05219800	1.68925100	-2.97580700
C	5.78382900	-0.46306600	-2.78747600
H	5.50931900	-0.22777000	-3.82107000
H	6.70523000	0.08220000	-2.55756400
H	6.00261200	-1.53375600	-2.72865400
C	-1.06774500	-2.98025000	1.08507000
C	0.11808600	-0.81923100	-3.45243100
C	-1.64027200	-4.41204700	1.10347000
H	-1.31516800	-4.93869300	2.00711700
H	-2.73547600	-4.40081200	1.09837300
H	-1.30678800	-4.98850400	0.23478100
C	-0.19258100	-1.49973400	-4.80015200
H	-0.22302200	-2.58885200	-4.69972900
H	-1.15657500	-1.17124700	-5.20256900
H	0.57751600	-1.24649000	-5.53641800
C	-1.50194600	-2.19368900	2.33702900
H	-2.59099300	-2.09541700	2.39129200
H	-1.16696100	-2.71182600	3.24211500
H	-1.07167400	-1.18746100	2.33886000
H	0.02212900	-3.06661800	1.11863500
Cu	1.22657100	0.28479100	0.71568300
H	2.17512500	3.05959400	1.48110000
C	0.19251500	0.71143800	-3.60998300
H	0.94265300	0.97859700	-4.36219300
H	-0.76853700	1.12514000	-3.93395300
H	0.46744000	1.19308500	-2.66748400
H	1.11042700	-1.15836700	-3.14153500
Si	-6.19909600	-0.32286200	1.16624600
H	-4.97943400	0.50217800	1.27227300
O	-6.55014300	-0.33689000	-0.46398600
O	-5.73069000	-1.81888700	1.73656600
C	-6.60574200	-2.91273200	2.03626100
C	-5.91446200	-3.86631500	2.99763100
H	-6.86650500	-3.43520300	1.10598900
H	-7.53995300	-2.54441300	2.48100200
H	-6.56700900	-4.71621600	3.22298900
H	-4.98714800	-4.25039400	2.56162700
H	-5.66967100	-3.35873300	3.93555500
C	-7.77295600	-0.79540000	-1.05244700
C	-7.81841200	-0.37379900	-2.51221600
H	-8.63302500	-0.37622700	-0.51305600
H	-7.83435400	-1.88950200	-0.97382900
H	-8.74864900	-0.71719600	-2.97653800
H	-7.76869100	0.71573400	-2.60039500
H	-6.97799600	-0.80339000	-3.06593300
C	-7.62704900	0.37277200	2.16579500
H	-7.34897100	0.43770500	3.22310700
H	-7.86894900	1.38353100	1.81993400
H	-8.53915300	-0.22843400	2.09724800

TS35

C	5.92985400	1.04744200	-1.46208500
C	7.31710900	0.40811400	-1.29098000
H	5.79633100	1.84944500	-0.72723400
H	5.89812300	1.54128600	-2.44630000
C	8.46721200	1.41419700	-1.41865400
H	7.37325900	-0.08718200	-0.31267600
H	7.44510200	-0.38540700	-2.04144100
C	9.85024700	0.77495600	-1.25718800
H	8.40515000	1.91177600	-2.39640000
H	8.33969400	2.20567300	-0.66747500
H	10.64912200	1.51799200	-1.35255100
H	9.95390000	0.29902400	-0.27519600

H	10.02078200	0.00336300	-2.01693000	C	-2.47287600	-4.59800800	-1.84159100
C	4.80077400	0.04507700	-1.36640900	C	-2.71444800	-4.36469500	-0.49039800
C	3.54026900	0.29013700	-0.97299100	H	-2.30241900	-3.73882000	-3.80060400
C	3.16603400	1.70608900	-0.62930600	H	-2.28717000	-5.60941100	-2.19126300
C	2.98159400	2.63972800	-1.66234300	H	-2.72204200	-5.20009400	0.20223600
C	3.06034300	2.15440500	0.69720400	C	-2.16142200	2.87336800	2.01476900
C	2.71040600	3.98132900	-1.38292700	C	-1.57858500	4.09365700	2.38090600
H	3.07085900	2.31131900	-2.69479800	C	-1.15231200	5.00680300	1.42054800
C	2.78637400	3.49509800	0.97837500	C	-1.30905800	4.72404200	0.06618900
H	3.22167300	1.44367100	1.49917400	C	-1.88451100	3.52116300	-0.36056600
C	2.61168800	4.41414500	-0.05927200	C	-2.28401700	2.60685900	0.63633400
H	2.58369100	4.68738900	-2.19931500	H	-1.46474400	4.33305400	3.43353300
H	2.71837800	3.82406500	2.01210000	H	-0.70459800	5.94706800	1.72908500
H	2.40636800	5.45777100	0.16198300	H	-0.98468900	5.44978600	-0.67291100
H	5.07459000	-0.95795600	-1.67206200	C	-3.27391200	-2.85902500	1.46878400
C	2.97647600	-2.05718700	-3.08814000	H	-3.28124300	-1.78306500	1.66460000
C	2.58593400	-2.15207100	-1.59281100	C	-2.21295000	-3.48112700	2.39516700
H	2.23372600	-1.47780600	-3.65005600	H	-2.43882800	-3.22896500	3.43701300
H	3.95042300	-1.59540400	-3.25674200	H	-2.20573800	-4.57417300	2.31968400
H	3.00480600	-3.06224800	-3.52420500	H	-1.20835000	-3.11855700	2.16208900
C	3.60473300	-3.02254000	-0.82737100	C	-4.67832800	-3.40187100	1.80676000
C	1.22635000	-2.88564100	-1.53922500	H	-4.91564700	-3.20828300	2.85831000
H	4.62613900	-2.64032500	-0.86799400	H	-5.45174900	-2.93360600	1.19088100
H	3.32077300	-3.10513800	0.22072200	H	-4.72958400	-4.48414200	1.64511800
H	3.61366700	-4.02985000	-1.26197200	C	-2.76143800	-1.10041500	-3.35777500
H	1.31109500	-3.85318500	-2.04865200	H	-3.00363700	-0.16841100	-2.83938500
H	0.91328100	-3.06198100	-0.50999600	C	-1.39902300	-0.89198200	-4.04573000
H	0.44389000	-2.31462700	-2.04947300	H	-0.62135500	-0.63846300	-3.31963600
C	2.36840500	-0.70429900	-1.02090600	H	-1.08004500	-1.79081700	-4.58388600
O	1.58535000	-0.67730900	0.20253700	H	-1.46540600	-0.07427400	-4.77140600
C	-2.20923900	0.19986500	-0.05101800	C	-3.87031300	-1.34144400	-4.40209700
C	-4.24942200	1.21243900	-0.05046500	H	-3.93587100	-0.48705600	-5.08384300
C	-4.42934700	-0.06059700	-0.48920200	H	-3.66576000	-2.23207400	-5.00539700
N	-3.17700600	-0.66943400	-0.48922500	H	-4.84616600	-1.47352200	-3.92569900
N	-2.89044000	1.36176200	0.21423200	C	-2.66684100	1.92413300	3.09723700
Cl	-5.87437200	-0.83664800	-0.97650200	C	-2.08422400	3.26661600	-1.85252300
Cl	-5.40854400	2.45352000	0.15749300	C	-3.86234500	2.53766800	3.85531500
C	-2.95480800	-3.07143800	-0.00848500	H	-4.24746900	1.82517400	4.59258600
C	-2.93278300	-2.02061200	-0.94803500	H	-3.56637300	3.44572700	4.39171300
C	-2.71713500	-2.22669900	-2.32663700	H	-4.67880800	2.79987500	3.17601800
C	-2.47992000	-3.54103900	-2.74805000	C	-3.03424600	4.31001400	-2.47464000

H	-4.00007100	4.33008400	-1.96103300
H	-2.60633400	5.31693400	-2.42688500
H	-3.21355800	4.07490900	-3.52912800
C	-1.54935700	1.51870500	4.07565600
H	-1.16804200	2.38233100	4.63092100
H	-1.93500600	0.80043200	4.80716900
H	-0.71229000	1.05289400	3.54973300
H	-3.01971200	1.00905900	2.61274900
Cu	-0.39384800	-0.21394000	0.37190200
H	1.67737700	-0.24616600	-1.74674600
C	-0.74611000	3.22186900	-2.61212300
H	-0.92132500	2.98584200	-3.66741200
H	-0.22829700	4.18521900	-2.56666100
H	-0.07451700	2.46651600	-2.19561800
H	-2.55473800	2.28710200	-1.97426500
Si	1.79078400	-1.18856200	1.96623900
H	0.32452200	-0.53401000	1.94284700
O	1.45347700	-2.84618600	1.80084800
O	3.47928100	-0.92929000	1.79543600
C	4.44401000	-0.97281000	2.83392000
C	5.84377400	-0.81015600	2.25339700
H	4.39259900	-1.92370500	3.38512300
H	4.26236600	-0.17512100	3.56902000
H	6.59259200	-0.85686700	3.05239700
H	6.06010100	-1.60313000	1.53079200
H	5.94505700	0.15132900	1.74177800
C	2.02507600	-3.83835600	2.64301400
C	1.54707600	-5.21743000	2.20674900
H	1.74725700	-3.66444400	3.69284700
H	3.12357700	-3.79961600	2.58941100
H	1.97829600	-5.99320200	2.84911400
H	0.45660000	-5.28498800	2.26822900
H	1.84346500	-5.42117400	1.17315700
C	1.67471100	-0.86842000	3.87946000
H	1.75698700	0.20759600	4.08594400
H	0.67819100	-1.17919000	4.21553100
H	2.41833700	-1.37428100	4.50562900
94			
C	-9.84516500	-0.43813800	-1.60665300
C	-10.33009700	-1.55457000	-0.66165500
H	-9.30250300	-0.87872200	-2.44836300
H	-10.73119300	0.06063200	-2.02825000
C	-11.29213400	-2.54173600	-1.33478300
H	-9.45901700	-2.09941800	-0.27378900
H	-10.82282800	-1.10513700	0.21203900
C	-11.76265100	-3.65688400	-0.39561700
H	-12.16284200	-1.99209600	-1.71759300
H	-10.80166800	-2.98393800	-2.21263600
H	-12.44635800	-4.34552100	-0.90308500
H	-10.91534800	-4.24366300	-0.02241400
H	-12.28832700	-3.24639800	0.47427900
C	-9.00832000	0.60413100	-0.91227200
C	-7.72396900	0.91686300	-1.15250000
C	-6.91760600	0.16378700	-2.16960900
C	-6.44807200	0.79647000	-3.33266000
C	-6.60419400	-1.19215200	-1.98056600
C	-5.69723300	0.09598300	-4.27802800
H	-6.68436200	1.84278800	-3.50772400
C	-5.85199400	-1.89532700	-2.92440500
H	-6.95159900	-1.69083800	-1.08100400
C	-5.39487200	-1.25309200	-4.07704600
H	-5.35111600	0.60391700	-5.17394100
H	-5.62137100	-2.94384700	-2.75669900
H	-4.80856300	-1.79766500	-4.81156500
H	-9.54606300	1.16282200	-0.15346400
C	-8.72572000	3.85298800	-0.43016500
C	-7.63345200	3.13696700	0.39537200
H	-8.32656100	4.20160100	-1.39012100
H	-9.59056500	3.22129700	-0.64030900
H	-9.08128400	4.73330900	0.11614300
C	-8.21139300	2.60427600	1.72286000
C	-6.55760600	4.19239700	0.74774200
H	-8.96283000	1.82362200	1.59038700
H	-7.41853200	2.20398900	2.35891800
H	-8.68398800	3.42898700	2.26854000
H	-7.01129800	5.00914200	1.31994000
H	-5.75698700	3.75740600	1.34910200
H	-6.11349700	4.62525700	-0.15657000
C	-6.93586400	2.05487900	-0.49142100
O	-5.76523400	1.51345600	0.14091200
C	4.96498300	-0.04902300	-0.00635300
C	6.74727900	-1.43848300	-0.22658900

C	7.16780700	-0.18199800	-0.54093300	H	6.45164600	2.84023700	-4.64923300
N	6.06635600	0.65732600	-0.40125500	H	7.50189100	1.63939600	-3.88168100
N	5.39738400	-1.34134500	0.09761600	C	5.18728800	-1.99992200	2.95025500
Cl	8.72080800	0.34999000	-1.02095600	C	3.99059300	-2.83056200	-2.00105400
Cl	7.63247000	-2.90163700	-0.20432500	C	6.11453900	-2.92156800	3.76609900
C	6.37573600	2.93724300	0.45732600	H	6.67116100	-2.33618800	4.50537700
C	6.07345700	2.08878800	-0.62655400	H	5.54731800	-3.68592500	4.30756500
C	5.77260300	2.57018700	-1.91635000	H	6.83727300	-3.43166700	3.12172800
C	5.76811300	3.95921800	-2.09689500	C	4.54798900	-4.01832100	-2.80968300
C	6.05360200	4.82421600	-1.04395600	H	5.52005400	-4.34198700	-2.42512600
C	6.35518300	4.31678800	0.21708900	H	3.87034700	-4.87789200	-2.77884300
H	5.53533000	4.36708400	-3.07563900	H	4.67432500	-3.73298100	-3.85929600
H	6.04196300	5.89791800	-1.20696200	C	4.20039800	-1.24980400	3.86640700
H	6.57625800	5.00117400	1.03024900	H	3.54437500	-1.94587100	4.39974600
C	4.44900900	-2.76817600	1.85826600	H	4.74669200	-0.66488500	4.61402100
C	3.61352200	-3.83681500	2.20695200	H	3.56883900	-0.56546500	3.29094200
C	2.92296500	-4.55838500	1.23688900	H	5.82053500	-1.24664600	2.47317200
C	3.05485700	-4.22713200	-0.10898300	Cu	3.18060500	0.63668400	0.32766500
C	3.87394300	-3.16706900	-0.51771800	H	-6.52251200	2.63072300	-1.33201200
C	4.55361500	-2.45232800	0.48888200	C	2.64201800	-2.35185500	-2.57347000
H	3.50279600	-4.10572000	3.25272700	H	2.75713600	-2.06911600	-3.62522000
H	2.28066800	-5.38340100	1.53081400	H	1.88341500	-3.13993900	-2.52061200
H	2.51288400	-4.79905700	-0.85567700	H	2.26496000	-1.48331500	-2.02425600
C	6.70743000	2.41940900	1.85343500	H	4.69854500	-2.00424200	-2.11100000
H	6.71455700	1.32631600	1.82128600	Si	-5.33178500	0.47975300	1.33565000
C	5.63000100	2.83782900	2.87311100	H	1.78081800	1.17895700	0.58980400
H	5.86038800	2.42185000	3.85972600	O	-5.03401800	1.43729100	2.66798900
H	5.57768400	3.92715500	2.97312000	O	-6.55267000	-0.58603200	1.70563000
H	4.64035200	2.47948700	2.57217700	C	-6.39090300	-1.96845000	2.03715400
C	8.10976300	2.86878100	2.30790700	C	-7.65548600	-2.47340200	2.71378300
H	8.34312300	2.43836700	3.28733400	H	-5.52955400	-2.11212100	2.70342700
H	8.88020400	2.54548300	1.60116900	H	-6.19318300	-2.54523200	1.12332100
H	8.17343300	3.95796800	2.40060100	H	-7.55913100	-3.53762700	2.95302500
C	5.45623300	1.65554300	-3.09551700	H	-7.84239000	-1.92516900	3.64236200
H	5.52204600	0.61859100	-2.75428800	H	-8.52155300	-2.34233200	2.05835900
C	4.01854500	1.87460400	-3.60584300	C	-4.81002300	0.91236500	3.97913000
H	3.28657000	1.71581000	-2.80767200	C	-4.59423000	2.06300700	4.94935500
H	3.88177700	2.89031500	-3.99168700	H	-3.92905200	0.25408400	3.97813500
H	3.79589400	1.17578700	-4.41911700	H	-5.67345900	0.30906100	4.29104900
C	6.48257000	1.82808100	-4.23254500	H	-4.42061500	1.68095900	5.96071200
H	6.26667700	1.12703400	-5.04560900	H	-3.72703000	2.66028000	4.65160600

H	-5.47114200	2.71737300	4.97223500
C	-3.77541000	-0.39692800	0.79036400
H	-3.97039700	-1.03742700	-0.07542300
H	-3.01597100	0.33697500	0.50247200
H	-3.35221600	-1.01972400	1.58554700
95			
C	-3.04472400	1.36363500	-0.60610500
C	-4.12135600	1.85355300	0.38208200
H	-3.41839300	0.49487100	-1.15617300
H	-2.87398900	2.15836800	-1.34802100
C	-5.43181900	2.25502000	-0.30542800
H	-4.32158300	1.06441300	1.11943500
H	-3.73136400	2.70917300	0.95098900
C	-6.50383000	2.73718900	0.67654300
H	-5.22583500	3.04428200	-1.04111000
H	-5.81647300	1.39963000	-0.87712700
H	-7.42704900	3.01384800	0.15689900
H	-6.75282400	1.95700900	1.40494600
H	-6.16154400	3.61463000	1.23708900
C	-1.73231000	1.05250700	0.05855100
C	-1.08110800	-0.12437400	0.12107000
C	-1.63795100	-1.36983300	-0.49545100
C	-0.97980400	-2.02658900	-1.54996400
C	-2.85489700	-1.90787100	-0.04007400
C	-1.51821600	-3.17975600	-2.12233600
H	-0.04221300	-1.62619200	-1.91523700
C	-3.39297800	-3.06242500	-0.61115800
H	-3.37907500	-1.41926700	0.77599500
C	-2.72520500	-3.70454900	-1.65530200
H	-0.99341600	-3.66802700	-2.93888900
H	-4.33303900	-3.45935700	-0.23834100
H	-3.14159000	-4.60297100	-2.10155400
H	-1.25339100	1.91138900	0.53118900
C	-0.75215000	-0.70913300	3.06200800
C	0.41046800	-1.03384000	2.10452200
H	-0.80446200	0.36390400	3.27905200
H	-1.71729600	-1.01524800	2.64923200
H	-0.61225000	-1.23452200	4.01305300
C	0.42628200	-2.54216900	1.79412600
C	1.73596100	-0.65781900	2.79983400
H	-0.52310400	-2.88618800	1.37864100
H	1.21738000	-2.78533000	1.07991000
H	0.61404200	-3.10663300	2.71456900
H	1.87377700	-1.25712800	3.70630000
H	2.59361800	-0.82887500	2.14478900
H	1.74352700	0.39844000	3.09373800
C	0.27954100	-0.15069600	0.82216700
O	1.29467300	-0.53127000	-0.13080500
H	0.47244800	0.87929900	1.14246900
Si	2.46988500	0.42131300	-0.79766900
O	1.98925700	1.99256800	-0.60183000
O	3.91951300	0.29636800	0.00559600
C	4.78177600	-0.84665500	-0.02263400
C	6.07335700	-0.51547700	0.70637800
H	4.99604300	-1.13177300	-1.06139100
H	4.28206200	-1.69858000	0.45755600
H	6.74628800	-1.37893800	0.69776100
H	6.58295200	0.32495600	0.22535900
H	5.87093400	-0.24544700	1.74709400
C	2.82764900	3.13403900	-0.82505500
C	2.05028200	4.39508500	-0.48763100
H	3.14986500	3.15810600	-1.87520200
H	3.72733100	3.05723800	-0.20294400
H	2.67381800	5.27979200	-0.65188400
H	1.15840000	4.47950300	-1.11577500
H	1.73483900	4.38467800	0.56008200
C	2.65815300	-0.08341500	-2.58489700
H	2.89747800	-1.14772900	-2.67828100
H	1.72832000	0.09831600	-3.13265200
H	3.45711900	0.48208900	-3.07537000
96			
Si	-0.59081400	-0.62931300	0.34057500
O	0.01010100	-2.13817200	0.88864100
O	-0.02673700	-0.22454500	-1.23624400
C	-0.50098500	-0.72423500	-2.47227600
C	0.33214800	-0.13721700	-3.60724600
H	-1.55581000	-0.47328300	-2.62617900
H	-0.43875600	-1.82295400	-2.49760300
H	-0.02109600	-0.51024300	-4.57553200
H	0.25926400	0.95582300	-3.61526000
H	1.38981200	-0.40276700	-3.50491300
C	-0.76034600	-3.12860500	1.54152800

C	-0.00635700	-3.65511400	2.75952000	C	2.87515800	2.68622300	-1.65803500
H	-0.96823700	-3.96000100	0.85387600	H	3.06827300	2.21339800	0.43105600
H	-1.73499400	-2.73492100	1.85725100	H	4.60902900	2.30731700	-0.42915900
H	-0.57669600	-4.44765300	3.25786800	C	2.87566900	4.20618000	-1.47264700
H	0.96475300	-4.06756700	2.46549600	H	3.36955800	2.43206000	-2.60508100
H	0.17264600	-2.85250400	3.48263800	H	1.84452900	2.32166000	-1.73736500
C	-1.36373100	0.49373200	1.68079800	H	2.37139900	4.70431900	-2.30658000
H	-1.26862200	1.54042300	1.36893100	H	2.35695100	4.49187500	-0.55110300
H	-2.41470100	0.31978900	1.90939900	H	3.89670200	4.60048000	-1.41654100
H	-0.77974500	0.39086500	2.60136400	C	8.89751500	1.03165200	-1.06374300
N	4.14247500	-0.49702200	0.28672500	C	7.96027000	-0.08122100	-0.58649700
C	3.88625200	-0.06225100	1.73916800	H	9.92017500	0.66035900	-1.17999400
C	4.80515300	0.97971200	2.37621100	H	8.57545300	1.43277500	-2.03087800
H	3.96756900	-0.98349200	2.32165600	H	8.92274400	1.86238500	-0.35007900
H	2.83886800	0.24330100	1.75216300	C	6.51248300	0.40675700	-0.40689900
C	4.32439900	1.27470100	3.80816400	H	7.97976800	-0.91075400	-1.30517900
H	5.83562100	0.61045600	2.42269400	H	8.32707100	-0.48864600	0.36441800
H	4.81977300	1.91375000	1.81082200	C	5.62208400	-0.76090000	0.01867900
C	5.22212200	2.28255100	4.53128500	H	6.49772000	1.21512200	0.32727500
H	3.29615300	1.65536500	3.77250100	H	6.15991400	0.82295400	-1.35632300
H	4.28656000	0.33918300	4.38113800	H	5.65246500	-1.51449500	-0.76853300
H	4.85524200	2.47937200	5.54323300	H	6.00633500	-1.22757300	0.92953300
H	6.24955000	1.91112100	4.61488900	F	0.95608200	0.07976300	0.84060400
H	5.25581300	3.23834900	3.99689800	C	-3.95231600	2.52137400	-1.18518000
C	3.40524000	-1.85240500	0.17455700	C	-2.74872400	3.47971700	-1.11597900
C	3.25988900	-2.45452200	-1.22218600	H	-4.72295800	2.84978900	-0.47999600
H	2.41430600	-1.67459400	0.59626300	H	-4.40059700	2.61089000	-2.18785000
H	3.96201200	-2.53409300	0.82353800	C	-3.10873600	4.93118700	-1.45420700
C	2.61220700	-3.84586500	-1.10848800	H	-2.31013300	3.43602700	-0.10995600
H	2.61820200	-1.82141500	-1.84132900	H	-1.96579800	3.12971300	-1.80309100
H	4.22366100	-2.54896500	-1.73688900	C	-1.90923700	5.88149600	-1.38723900
C	2.37980500	-4.49739400	-2.47421700	H	-3.55016100	4.96832400	-2.45984200
H	3.24964400	-4.49644900	-0.49499300	H	-3.89118300	5.28072600	-0.76683000
H	1.65978100	-3.74192300	-0.57662000	H	-2.19651900	6.90898900	-1.63453200
H	1.92046700	-5.48482400	-2.36536800	H	-1.46837400	5.89101400	-0.38392400
H	1.71389800	-3.88733500	-3.09433500	H	-1.12397300	5.57693800	-2.08872000
H	3.32085300	-4.62558500	-3.02143700	C	-3.56029800	1.08836400	-0.93660400
C	3.48391600	0.44560500	-0.73283500	C	-4.11279500	0.17980800	-0.11204700
C	3.57736700	1.95313200	-0.50186800	C	-5.32450100	0.48699000	0.70544500
H	2.42680800	0.17751900	-0.71725600	C	-6.48076700	1.03410400	0.11652500
H	3.91407400	0.17587300	-1.69955600	C	-5.35470400	0.25200600	2.09270700

C	-7.60929400	1.34208600	0.87663200	H	-0.25003500	-0.69960000	4.00680900
H	-6.49711800	1.19893600	-0.95639300	H	-1.69845100	-0.15658600	3.13994800
C	-6.48082700	0.56226000	2.85654800	C	-1.31868400	2.05243000	0.60653200
H	-4.48295700	-0.16475000	2.58650100	H	-1.25682000	2.86006700	-0.13252300
C	-7.61519800	1.10871900	2.25338900	H	-2.28312500	1.55964700	0.50886900
H	-8.48693900	1.75937000	0.39050700	H	-1.21455500	2.50660200	1.59816300
H	-6.46927100	0.37806000	3.92733700	N	4.30645700	-0.59910500	0.25107700
H	-8.49270700	1.34691300	2.84745100	C	3.99984100	0.03938500	1.61775500
H	-2.65992600	0.76729700	-1.45415100	C	5.05534000	0.92940400	2.27275400
C	-5.70188300	-2.48299100	-0.28785900	H	3.80597000	-0.80501500	2.28325800
C	-4.24416100	-2.34153400	-0.76919000	H	3.05991700	0.57501300	1.47756000
H	-5.75762400	-2.62113500	0.79792700	C	4.49737600	1.48890300	3.59363600
H	-6.31485300	-1.61655000	-0.54370600	H	5.96351000	0.35637700	2.48891700
H	-6.15969200	-3.36215500	-0.75697500	H	5.34176600	1.76436500	1.62993000
C	-4.23862100	-2.04203300	-2.27831300	C	5.51513700	2.35923100	4.33583500
C	-3.54423900	-3.69344000	-0.53504800	H	3.59360100	2.07392700	3.38351900
H	-4.73534500	-1.09305300	-2.50219100	H	4.18416500	0.65833600	4.23923500
H	-3.21582700	-1.98572200	-2.65820500	H	5.09219600	2.74876000	5.26675100
H	-4.76362500	-2.83463900	-2.82493200	H	6.41507900	1.78871600	4.59082300
H	-4.05723800	-4.48711200	-1.09159900	H	5.82448100	3.21524100	3.72613800
H	-2.50357800	-3.65341000	-0.85914900	C	3.34183600	-1.80578300	0.17536900
H	-3.56003800	-3.96928200	0.52571300	C	3.19840200	-2.50095100	-1.17765800
C	-3.46246300	-1.22111300	0.03595900	H	2.37270600	-1.42355300	0.50449200
O	-2.12049800	-1.25322200	-0.35552200	H	3.70985100	-2.50912900	0.92683100
H	-3.57087100	-1.50494600	1.09915000	C	2.34637300	-3.77365100	-1.02325000
TS36				H	2.71130200	-1.83736500	-1.89735200
Si	0.07235200	0.84925400	0.32106800	H	4.17153500	-2.78102000	-1.59760900
O	0.43164100	-0.32013900	1.43827900	C	2.14444700	-4.50315700	-2.35416200
O	0.51716900	0.44590000	-1.22553900	H	2.82630800	-4.44873800	-0.30298100
C	-0.29719500	0.57847000	-2.40368000	H	1.37003400	-3.50812800	-0.60021900
C	0.39087500	-0.11690800	-3.56662900	H	1.53946900	-5.40450300	-2.21783500
H	-0.42515000	1.64655500	-2.63356300	H	1.63138100	-3.86470000	-3.08124900
H	-1.26974200	0.13051500	-2.18454200	H	3.10258700	-4.80560000	-2.79158700
H	-0.20420900	-0.00178200	-4.47925100	C	3.95426900	0.33355600	-0.91551500
H	1.38535500	0.30290500	-3.75477300	C	4.33340000	1.81079000	-0.81624900
H	0.49977200	-1.18784800	-3.36518800	H	2.86889300	0.27517700	-1.01645000
C	-0.37324700	-1.39083800	1.94950800	H	4.40466400	-0.12186700	-1.79959100
C	-1.00953600	-0.99670600	3.27535100	C	3.92958900	2.52297400	-2.11914500
H	0.29972000	-2.24538600	2.09988300	H	3.79092200	2.27340800	0.01221400
H	-1.12029600	-1.64562400	1.19791000	H	5.40302100	1.95685600	-0.64811900
H	-1.57526100	-1.83800000	3.69095800	C	4.23354200	4.02341500	-2.08208500

H	4.45519200	2.06295400	-2.96635300	C	-7.68118000	-0.93776300	2.66590100
H	2.85819100	2.36795100	-2.29480900	H	-8.96395400	-0.92693200	0.93161000
H	3.93909800	4.50681500	-3.01862000	H	-6.14469700	-0.89666000	4.17847500
H	3.69226500	4.51633500	-1.26735500	H	-8.49255500	-1.08962700	3.37209900
H	5.30313000	4.20847500	-1.93239600	H	-3.52334900	0.79400900	-1.59299000
C	9.39000000	-0.15148800	-0.62605000	C	-4.71963100	-3.38810300	-0.42123000
C	8.19923200	-1.01451700	-0.19954600	C	-3.47136100	-2.62810200	-0.90470100
H	10.32076400	-0.72575800	-0.59591200	H	-4.69703200	-3.54254300	0.66442600
H	9.26162500	0.22420800	-1.64694600	H	-5.64705800	-2.86065900	-0.65944800
H	9.50919600	0.71349600	0.03535600	H	-4.77331900	-4.37812100	-0.89365900
C	6.87213900	-0.23607300	-0.22561000	C	-3.60659000	-2.32456500	-2.40433500
H	8.12344700	-1.88857300	-0.85901900	C	-2.24603500	-3.53610900	-0.69323000
H	8.37140400	-1.40469100	0.81178900	H	-4.47947300	-1.69500600	-2.60686400
C	5.72610500	-1.16294800	0.17864500	H	-2.71932000	-1.79591800	-2.76327900
H	6.95302100	0.62508200	0.44118500	H	-3.71581400	-3.24952900	-2.98570700
H	6.70884400	0.14848500	-1.23774500	H	-2.32898800	-4.45981600	-1.28073700
H	5.68174500	-1.98012000	-0.54178300	H	-1.33837400	-3.00268100	-0.98369400
H	5.91310900	-1.60489800	1.16056700	H	-2.14870800	-3.82239800	0.36229000
F	1.38841100	1.80184000	0.69014200	C	-3.19848900	-1.28167400	-0.07776000
C	-5.43846100	1.81439400	-1.18024800	O	-2.02895300	-0.70093700	-0.45312100
C	-4.81115800	3.22021200	-1.12897900	H	-3.18568600	-1.64978200	0.98335600
H	-6.23790300	1.74711600	-0.43443200	97			
H	-5.92887500	1.69850500	-2.16068800	N	-2.73282100	0.05846800	0.54045200
C	-5.81912600	4.34530000	-1.39275600	C	-2.61913100	-1.46418400	0.72162800
H	-4.34402700	3.37005700	-0.14629000	C	-3.43458200	-2.37733600	-0.19283900
H	-3.99635800	3.28221500	-1.86444300	H	-2.94737100	-1.64311500	1.74942100
C	-5.19607500	5.74335200	-1.33231300	H	-1.53509800	-1.64560500	0.68432700
H	-6.28125700	4.19241700	-2.37793400	C	-3.13141000	-3.84600900	0.15366400
H	-6.63616500	4.27717000	-0.66146200	H	-4.50879000	-2.20293300	-0.05922000
H	-5.93921600	6.52385000	-1.52751700	H	-3.21066800	-2.21125000	-1.24876000
H	-4.75913800	5.93908800	-0.34630700	C	-3.94227300	-4.82968500	-0.69449700
H	-4.39630200	5.85252000	-2.07401800	H	-2.05957100	-4.03511200	0.01648200
C	-4.42683200	0.71444900	-0.98885200	H	-3.34003200	-4.01979000	1.21732300
C	-4.43811900	-0.32110000	-0.12950300	H	-3.70542200	-5.86507600	-0.43082700
C	-5.56310600	-0.54312900	0.82378200	H	-5.01879400	-4.68598700	-0.54877600
C	-6.89909100	-0.65020800	0.39245100	H	-3.73093700	-4.70064200	-1.76178400
C	-5.32059200	-0.64268100	2.20735500	C	-2.19148000	0.61789000	1.87914500
C	-7.94374700	-0.84469000	1.29731200	C	-1.94190800	2.12373800	1.95187000
H	-7.11414200	-0.59492100	-0.67070100	H	-1.25009500	0.08034500	2.03398400
C	-6.36292900	-0.83338000	3.11555900	H	-2.92879700	0.32027600	2.63019400
H	-4.30290400	-0.55155600	2.57430700	C	-1.54954600	2.51499000	3.38725400

H	-1.12928200	2.40725700	1.27641200	C	2.17033100	5.65518400	-1.49981800
H	-2.82320100	2.70694400	1.65865500	H	3.54711600	4.99494800	0.03150300
C	-1.23423000	4.00725700	3.52257400	H	3.87190200	4.32365200	-1.55690900
H	-2.36278800	2.24684900	4.07416000	H	2.74394700	6.55076300	-1.76113900
H	-0.67710800	1.92578500	3.69570100	H	1.69833800	5.28364900	-2.41674900
H	-0.95698800	4.25936200	4.55080300	H	1.36886800	5.96136900	-0.81738400
H	-0.40108500	4.29569200	2.87224100	C	2.41256900	1.00926400	0.57792200
H	-2.09862900	4.62283500	3.24921400	C	2.61884700	-0.28934300	0.29391800
C	-1.78068500	0.56807500	-0.55040700	C	3.76408900	-0.74391600	-0.54377700
C	-1.73433900	-0.15427000	-1.89686500	C	5.09583500	-0.41952800	-0.22107500
H	-0.79007500	0.44582400	-0.08969900	C	3.54830600	-1.51243200	-1.70358700
H	-2.02881700	1.62245200	-0.68997200	C	6.16177200	-0.84060900	-1.01734700
C	-0.76445500	0.59321700	-2.82889000	H	5.29224100	0.15671500	0.67833400
H	-1.35879300	-1.17217300	-1.75447900	C	4.61164100	-1.93313500	-2.50374100
H	-2.70992500	-0.22772300	-2.38390600	H	2.53242600	-1.76976000	-1.98754300
C	-0.58547300	-0.10930100	-4.17762400	C	5.92531200	-1.60141900	-2.16451900
H	-1.13169800	1.61506800	-2.99310500	H	7.17870800	-0.57706700	-0.73862400
H	0.20844600	0.68976900	-2.33095700	H	4.41279300	-2.51902800	-3.39739100
H	0.10588400	0.44333000	-4.82141900	H	6.75331100	-1.93155300	-2.78540400
H	-0.18310200	-1.11988000	-4.04656800	H	1.51018900	1.19823700	1.16032900
H	-1.53924700	-0.19767800	-4.71018000	C	3.40342200	-2.96292300	1.73134500
C	-6.95807700	1.12465500	-2.24910400	C	2.11202500	-2.18493100	2.03978700
C	-6.27287700	1.03112200	-0.88271500	H	3.30035000	-3.56256700	0.81863700
H	-7.99384200	1.46249200	-2.14701100	H	4.26570600	-2.30525000	1.59735000
H	-6.43902100	1.83202000	-2.90510800	H	3.64003300	-3.65252900	2.55270600
H	-6.97217700	0.15203900	-2.75292500	C	2.33887400	-1.26068900	3.24578200
C	-4.81378900	0.55598900	-0.98727700	C	1.01499400	-3.20688200	2.39151000
H	-6.30306300	2.01114100	-0.38884500	H	3.17987100	-0.58023200	3.07455500
H	-6.83408000	0.34351300	-0.23687100	H	1.44519200	-0.65343900	3.41581100
C	-4.17740500	0.52400900	0.40197700	H	2.55067600	-1.83543300	4.15662300
H	-4.79175300	-0.42622300	-1.46529700	H	1.29385800	-3.80390500	3.26950900
H	-4.26326500	1.24608300	-1.63512000	H	0.07399200	-2.69105400	2.59046200
H	-4.20804000	1.53511700	0.80901000	H	0.84775300	-3.90233600	1.55783800
H	-4.75570700	-0.11361400	1.07640900	C	1.56490300	-1.33687000	0.79768700
C	3.19149600	2.22436300	0.14940100	O	0.35359600	-0.78671300	1.07068800
C	2.29775000	3.30935200	-0.48051100	H	1.52211100	-2.09850000	-0.02617800
H	3.98642900	1.95555600	-0.55506300	3b’			
H	3.69729700	2.66809900	1.02247000	H	0.35181300	-2.08957900	-1.90432800
C	3.06037200	4.58329400	-0.86339200	C	-2.12493500	-0.41420400	0.67485800
H	1.80486200	2.89676200	-1.37195300	C	-3.30736100	-1.01210800	-0.11102100
H	1.49067700	3.56631400	0.22115400	H	-2.15106500	0.67770900	0.60547900

H	-2.26064200	-0.65961800	1.73964600
C	-4.67284400	-0.52122300	0.38417600
H	-3.19343500	-0.76451000	-1.17527100
H	-3.26980900	-2.10887900	-0.04750000
C	-5.84737900	-1.11457300	-0.39928600
H	-4.78034200	-0.76789000	1.44931900
H	-4.70708000	0.57482600	0.32218200
H	-6.80697200	-0.74604600	-0.02247300
H	-5.78617300	-0.85508200	-1.46228100
H	-5.85985300	-2.20809200	-0.32737900
C	-0.80008800	-0.95231000	0.20784700
C	0.29682000	-0.27372100	-0.18054700
C	0.38522000	1.21572700	-0.14201600
C	0.13244500	1.92925500	1.04237000
C	0.72160500	1.95085000	-1.29203600
C	0.20806500	3.32132300	1.07645800
H	-0.10833100	1.37979100	1.94736500
C	0.79489300	3.34310100	-1.26095900
H	0.90834800	1.43025900	-2.22690300
C	0.54005700	4.03485700	-0.07592300
H	0.01289400	3.84783000	2.00640800
H	1.04832600	3.88813300	-2.16584800
H	0.60112700	5.11883900	-0.05070900
H	-0.74703800	-2.03818000	0.13505400
C	3.19874500	-0.09258300	0.91180900
C	2.64490600	-1.37843600	0.27195300
H	3.51055700	0.63481100	0.15400900
H	2.46666900	0.39582700	1.55953300
H	4.07604800	-0.33246900	1.52247800
C	2.13677600	-2.32786800	1.37081100
C	3.78190200	-2.06684900	-0.51269400
H	1.34301800	-1.86424000	1.96428000
H	1.74499500	-3.25246300	0.93924600
H	2.95570500	-2.58791300	2.05056300
H	4.61090800	-2.31441800	0.15944500
H	3.43358900	-2.98581200	-0.98836700
H	4.17480100	-1.40748600	-1.29588700
C	1.50458500	-1.03664300	-0.74408300
H	1.96818200	-0.39384100	-1.51080200
O	1.11291200	-2.27488400	-1.33844400
99			
C	5.02648600	-0.53152600	-1.54660500
C	4.16709800	-1.73766800	-1.11184400
H	6.06723200	-0.84510300	-1.68207700
H	4.67329200	-0.20343200	-2.53247700
C	4.21443200	-2.88952100	-2.12349700
H	4.50432500	-2.09488300	-0.12951100
H	3.13265100	-1.40581400	-0.97371900
C	3.37834900	-4.09870600	-1.69187300
H	3.85907500	-2.52730900	-3.09744100
H	5.25756100	-3.20032200	-2.27502400
H	3.42252000	-4.90004700	-2.43703700
H	3.73801300	-4.50868200	-0.74073300
H	2.32599000	-3.82446300	-1.55748500
C	4.97680800	0.64648900	-0.59208600
C	5.87821800	0.95384300	0.36376300
C	7.13526600	0.28370800	0.75055000
C	8.14255600	1.07963500	1.33385400
C	7.39197000	-1.09375900	0.60871000
C	9.36440700	0.53560900	1.72344600
H	7.95997800	2.14223500	1.47318100
C	8.61446100	-1.63974000	1.00214000
H	6.62477800	-1.75219100	0.22122600
C	9.60895200	-0.82978400	1.55419200
H	10.12387400	1.17602700	2.16298500
H	8.78442400	-2.70646400	0.88603300
H	10.55824800	-1.25924200	1.86062900
H	5.69094600	1.85826000	0.94005900
C	4.57861900	3.87854400	-0.62016600
C	3.78862300	2.85329000	-1.47029800
H	4.13676900	4.00094200	0.37442100
H	5.62698300	3.59384200	-0.50400200
H	4.55110400	4.85230200	-1.12082600
C	4.50559600	2.67024000	-2.82715600
C	2.36143600	3.37652200	-1.69930800
H	3.95547600	1.98777700	-3.48310100
H	4.57391600	3.63777100	-3.33562100
H	5.52237900	2.28648300	-2.70092700
H	2.40138400	4.32325600	-2.24850800
H	1.76328900	2.66640100	-2.27701800
H	1.84466900	3.55094000	-0.75242000
C	3.72772900	1.49998500	-0.72636000

O	2.67495500	1.06730100	-0.27697700
C	-2.33653100	-0.09923300	-0.08560600
C	-3.70391800	-1.08342300	1.43785700
C	-3.96951100	0.25188400	1.45331800
N	-3.12306400	0.84150800	0.51887100
N	-2.70086300	-1.28257000	0.49399400
Cl	-5.10799300	1.11620600	2.39326800
Cl	-4.41897300	-2.33933600	2.35306900
C	-3.85967100	2.77861800	-0.80147300
C	-3.05482100	2.26029800	0.23272800
C	-2.18240800	3.05837700	1.00082900
C	-2.12206900	4.42234100	0.68824300
C	-2.89455300	4.96278900	-0.33633300
C	-3.75476300	4.14952300	-1.06912800
H	-1.46081100	5.06897200	1.25651200
H	-2.82899300	6.02321500	-0.56196800
H	-4.35530100	4.58427800	-1.86204200
C	-2.63348400	-3.32498800	-0.87246700
C	-2.00901300	-4.54443400	-1.16369100
C	-0.90268600	-4.97919200	-0.43863600
C	-0.39775500	-4.20345700	0.60168600
C	-0.98027000	-2.97522900	0.93947300
C	-2.09166000	-2.55880000	0.17902400
H	-2.39533200	-5.16029600	-1.96973200
H	-0.43455600	-5.92832400	-0.68279200
H	0.46175200	-4.55587100	1.16316000
C	-4.82396200	1.92192400	-1.61581800
H	-4.75549400	0.89158200	-1.25551200
C	-4.44310800	1.90637300	-3.10884300
H	-5.11920300	1.24725600	-3.66380300
H	-4.51469000	2.90565200	-3.55132800
H	-3.41934300	1.54666000	-3.25184400
C	-6.28291400	2.37919000	-1.41935400
H	-6.96278500	1.71593000	-1.96441500
H	-6.56696100	2.36476100	-0.36255200
H	-6.43749800	3.39591300	-1.79603500
C	-1.33970100	2.51010100	2.14905100
H	-1.50374900	1.43065300	2.21127700
C	0.16786300	2.72475400	1.91489400
H	0.51098900	2.24438100	0.99439300
H	0.41497100	3.79051300	1.85684800
H	0.73744100	2.30025800	2.74870900
C	-1.77927300	3.11921300	3.49628500
H	-1.20504700	2.67548700	4.31637800
H	-1.60960500	4.20103800	3.51765400
H	-2.84162600	2.94188300	3.68894700
C	-3.84871800	-2.88632200	-1.68348000
C	-0.41197600	-2.16664900	2.10257800
C	-5.01982200	-3.87567400	-1.52202600
H	-5.89804500	-3.51206900	-2.06580100
H	-4.76738000	-4.86368700	-1.92141800
H	-5.29681500	-3.99844100	-0.47040200
C	-0.55945700	-2.93108300	3.43390800
H	-1.60335400	-3.19297400	3.63173400
H	0.02491300	-3.85742200	3.42922800
H	-0.19903300	-2.31462500	4.26415300
C	-3.49165900	-2.68541200	-3.16902900
H	-3.17169700	-3.62390900	-3.63411100
H	-4.36458100	-2.32051300	-3.72080200
H	-2.68239600	-1.95755900	-3.28554800
H	-4.18628400	-1.91920600	-1.30022100
Cu	-1.08966100	0.14825800	-1.55270500
H	-0.17739400	0.31499100	-2.76240500
C	1.05425500	-1.76106200	1.85925900
H	1.42518800	-1.17687400	2.70822900
H	1.70033300	-2.63915400	1.75469600
H	1.16282600	-1.15109800	0.95814900
H	-0.98940100	-1.24244700	2.19426900

TS37

C	3.53890400	-1.37846300	1.21859300
C	4.94920300	-1.99276600	1.32540200
H	2.84318700	-1.96902600	1.81754000
H	3.54430100	-0.39221600	1.69983900
C	5.42821600	-2.11545400	2.77758100
H	4.95411500	-2.98507600	0.85605900
H	5.66571600	-1.38934900	0.75776000
C	6.82496500	-2.73323400	2.90105400
H	5.42523600	-1.12016200	3.24333800
H	4.70868300	-2.71872200	3.34814500
H	7.14083900	-2.80296600	3.94736800
H	6.84927100	-3.74414800	2.47812400
H	7.57124800	-2.13413400	2.36669100

C	2.98320600	-1.24093100	-0.18773900	C	-4.14831900	-3.37860600	0.66543900
C	3.53072800	-0.48851900	-1.17251100	H	-4.04713400	-3.49513400	-2.72459800
C	4.70868500	0.39530100	-1.21098100	H	-4.61153200	-4.90410500	-0.77842700
C	5.30470400	0.62308900	-2.46954400	H	-4.40830400	-4.00681300	1.51159600
C	5.25209100	1.07902200	-0.10417800	C	0.11860300	2.73760600	1.76240100
C	6.40880500	1.46048900	-2.61453600	C	1.29380800	3.48540100	1.90844000
H	4.89023200	0.12545700	-3.34273800	C	1.96202900	4.00159800	0.80118900
C	6.34920700	1.92785200	-0.25028700	C	1.46387700	3.78527600	-0.48074200
H	4.80373900	0.96836000	0.87542800	C	0.29304300	3.04520700	-0.68903000
C	6.94035800	2.11743000	-1.50192700	C	-0.35326200	2.52590200	0.45092100
H	6.85007700	1.60546700	-3.59675600	H	1.68904400	3.66499400	2.90352700
H	6.74245800	2.44603500	0.62010600	H	2.87302600	4.57701200	0.93780100
H	7.79834100	2.77466100	-1.60972900	H	1.99246600	4.19493200	-1.33573300
H	3.01397100	-0.54890200	-2.12720500	C	-3.60997200	-1.54394000	2.32254200
C	2.57989700	-4.04128000	-1.66612800	H	-3.25328500	-0.51100300	2.28536000
C	1.64047500	-3.54933600	-0.53630500	C	-2.58990000	-2.34379200	3.15555500
H	2.27614800	-3.62510200	-2.63105800	H	-2.51398500	-1.92222400	4.16363900
H	3.61870000	-3.75057400	-1.48014100	H	-2.88818500	-3.39296800	3.25508500
H	2.54139800	-5.13391500	-1.73519000	H	-1.59801700	-2.31205000	2.69531000
C	2.07094100	-4.20186000	0.78823500	C	-4.99193300	-1.52668800	3.00584700
C	0.20365900	-4.00523800	-0.84726100	H	-4.91174800	-1.09035900	4.00708200
H	1.46603000	-3.83949400	1.62510700	H	-5.71376200	-0.93593100	2.43373300
H	1.92478500	-5.28572400	0.71509100	H	-5.39673800	-2.53828800	3.11574700
H	3.12435600	-4.03736700	1.02159400	C	-3.16764500	-0.92848200	-2.78445100
H	0.15301000	-5.09971600	-0.85576300	H	-2.84818400	0.06020900	-2.44340600
H	-0.49004200	-3.63977100	-0.08106400	C	-2.00031800	-1.52712300	-3.59361600
H	-0.13302500	-3.63170400	-1.81511200	H	-1.10016000	-1.62576700	-2.97996800
C	1.69846900	-1.97998600	-0.59829600	H	-2.25805900	-2.51523100	-3.99098600
O	1.03734200	-1.46213400	-1.58109100	H	-1.76645000	-0.87995400	-4.44624700
C	-1.56274100	0.37914000	0.10449300	C	-4.41333200	-0.72472200	-3.66978100
C	-2.85066000	2.24837800	0.22869200	H	-4.17403300	-0.06454800	-4.51015300
C	-3.68505600	1.19167200	0.03881400	H	-4.76942800	-1.67380200	-4.08446300
N	-2.88544100	0.05293400	-0.03440900	H	-5.23623000	-0.27390400	-3.10637600
N	-1.55418700	1.73863400	0.26685800	C	-0.59530300	2.20540500	3.00155300
Cl	-5.39063900	1.16805700	-0.09573100	C	-0.22819300	2.84274900	-2.10858200
Cl	-3.22895300	3.90848100	0.39924000	C	-1.10895000	3.35759700	3.88786600
C	-3.70352700	-2.07004900	0.89314300	H	-1.66266500	2.95745800	4.74383600
C	-3.37240100	-1.29516700	-0.23718500	H	-0.28162700	3.95971200	4.27823000
C	-3.49270500	-1.77476700	-1.55735600	H	-1.77607100	4.02295300	3.33124500
C	-3.94465800	-3.09031900	-1.72259200	C	-0.58804600	4.18824900	-2.76984500
C	-4.26477600	-3.88612400	-0.62596400	H	-1.31844500	4.74464600	-2.17419000

H	0.29647300	4.82154600	-2.89576800	H	-2.65573800	-1.72289700	1.43362600
H	-1.01726400	4.01658400	-3.76261800	C	-3.19174900	-4.17840700	-0.39782100
C	0.30223100	1.24484100	3.80550300	C	-2.80313600	-3.28383700	-1.58676700
H	1.19621000	1.75262300	4.18283000	H	-2.35864500	-4.26180100	0.30509000
H	-0.24605600	0.85133200	4.66810600	H	-4.05342700	-3.77266100	0.14151300
H	0.62400600	0.39990100	3.18926800	H	-3.45315600	-5.18586200	-0.74352200
H	-1.46681000	1.63141300	2.67508000	C	-3.99514500	-3.17541400	-2.55504800
Cu	-0.06356700	-0.80113100	0.11152400	C	-1.63550600	-3.94053000	-2.35072600
H	0.87369900	-1.73415800	0.98278600	H	-3.77102500	-2.51564100	-3.40188700
C	0.77169700	2.04737100	-2.97064100	H	-4.23505300	-4.16341800	-2.96620800
H	0.36297500	1.89987100	-3.97640800	H	-4.89714800	-2.80397900	-2.06298800
H	1.72208400	2.58239700	-3.07352700	H	-1.93686500	-4.91766300	-2.74796200
H	0.97738800	1.06549400	-2.53515900	H	-1.32309300	-3.31916000	-3.19978800
H	-1.14743000	2.25263000	-2.05465500	H	-0.77207000	-4.07958600	-1.69762100
100				C	-2.30857700	-1.86567700	-1.08214000
C	-4.30242700	-0.18356700	-1.23128700	O	-1.15722200	-2.04851900	-0.31023800
C	-5.82141300	-0.35542100	-1.03377800	C	1.72372000	0.26235700	-0.07129600
H	-4.06840500	-0.39913800	-2.28002700	C	3.11567400	2.05209600	-0.18407600
H	-4.05062000	0.87952600	-1.10363700	C	3.84609700	0.99503600	0.26500700
C	-6.64266500	0.51316700	-1.99584600	N	2.98231500	-0.09476000	0.32878900
H	-6.09313700	-1.40841500	-1.17848200	N	1.81730000	1.59067700	-0.38447800
H	-6.09992200	-0.11266000	-0.00350800	Cl	5.50011600	0.92717700	0.69357000
C	-8.15500900	0.33699300	-1.82416500	Cl	3.61315000	3.66149000	-0.47924400
H	-6.37828000	1.56923900	-1.84538700	C	3.81232400	-2.34304700	-0.21274700
H	-6.36172500	0.27564100	-3.03128400	C	3.35086300	-1.42915400	0.75590100
H	-8.71437800	0.97113600	-2.52025800	C	3.22817600	-1.75604500	2.12137600
H	-8.45529500	-0.70154100	-2.00557100	C	3.57378300	-3.05885300	2.50217400
H	-8.47127200	0.59818300	-0.80767800	C	4.02481100	-3.98736400	1.56791800
C	-3.38562900	-1.02310600	-0.35132800	C	4.14397600	-3.63064300	0.22745900
C	-3.38255300	-1.03934600	0.99906800	H	3.48781000	-3.34911200	3.54459000
C	-4.16102700	-0.29637800	2.00676000	H	4.28614100	-4.99238400	1.88607400
C	-4.33755900	-0.89013400	3.27447600	H	4.49839100	-4.36317400	-0.49106600
C	-4.68517700	1.00000300	1.82451400	C	0.45349500	2.45918200	-2.23442600
C	-5.03173800	-0.24373400	4.29556800	C	-0.63462400	3.23575000	-2.65243800
H	-3.92336800	-1.88007600	3.44999900	C	-1.42371800	3.92445600	-1.73484300
C	-5.37224500	1.65269800	2.84877100	C	-1.13868800	3.85363300	-0.37385700
H	-4.53561300	1.51415000	0.88193600	C	-0.06491500	3.09155700	0.10365300
C	-5.55793300	1.03396300	4.08768700	C	0.70855300	2.39879000	-0.84950200
H	-5.15766900	-0.73581600	5.25635400	H	-0.86561100	3.30234000	-3.71093300
H	-5.76046800	2.65349200	2.67813700	H	-2.26204400	4.52122800	-2.08231200
H	-6.09663800	1.54346100	4.88146000	H	-1.75870800	4.39759300	0.33187400

C	3.95783400	-1.99221300	-1.69011700	H	1.08491500	2.39904500	1.76759800
H	3.66443300	-0.94765600	-1.82607000	101			
C	3.01829600	-2.84511700	-2.56497700	C	4.88860200	-0.58670100	-1.51629700
H	3.10381300	-2.54399000	-3.61455000	C	5.57221800	-1.21154800	-0.28071700
H	3.27016200	-3.90907600	-2.50177500	H	5.49909800	0.24305900	-1.88843600
H	1.97464800	-2.72659100	-2.25776100	H	4.89306100	-1.34624400	-2.30592100
C	5.42084200	-2.11992100	-2.15866200	C	6.97513300	-1.74955100	-0.59022000
H	5.50954600	-1.81211700	-3.20584200	H	5.63233100	-0.47035800	0.52569700
H	6.08793600	-1.49125100	-1.56098800	H	4.94408800	-2.02168800	0.10855800
H	5.77623200	-3.15303300	-2.08476400	C	7.65801100	-2.38385400	0.62605600
C	2.73988100	-0.76611600	3.17425300	H	6.90777800	-2.49049500	-1.39886000
H	2.55687900	0.19402400	2.68382700	H	7.60147200	-0.93440000	-0.97850500
C	1.40399100	-1.22112700	3.79408400	H	8.65456900	-2.76265800	0.37499000
H	0.63591000	-1.35387300	3.02573900	H	7.77322100	-1.65812300	1.43950300
H	1.51511200	-2.17055700	4.32863300	H	7.07044700	-3.22379000	1.01445900
H	1.04620000	-0.47425600	4.51073200	C	3.46153800	-0.13154600	-1.27790400
C	3.80473400	-0.52657300	4.26246600	C	3.09133000	1.14705300	-1.06062800
H	3.45368600	0.22912000	4.97297200	C	3.89068100	2.38620000	-1.00898600
H	4.01398700	-1.44108500	4.82713300	C	3.26311900	3.58951700	-1.39577600
H	4.74647100	-0.17572400	3.82917900	C	5.22884300	2.47086100	-0.57277200
C	1.29750500	1.72196900	-3.26957900	C	3.94291500	4.80560500	-1.38735300
C	0.21651300	3.04277800	1.60222000	H	2.22395700	3.55932700	-1.71195800
C	1.92530500	2.69361100	-4.28770300	C	5.91007000	3.68939400	-0.55995700
H	2.57539200	2.14630700	-4.97828200	H	5.73612200	1.58523800	-0.21065700
H	1.16027200	3.20066900	-4.88495300	C	5.27687700	4.86281400	-0.97392600
H	2.52688700	3.46032400	-3.78976500	H	3.43052400	5.71123500	-1.70138800
C	0.57025700	4.43823400	2.15361500	H	6.93982900	3.72055900	-0.21389900
H	1.42959400	4.86880100	1.63060500	H	5.80990000	5.80918600	-0.96280200
H	-0.26985500	5.13318800	2.05037500	H	2.02536900	1.31996500	-0.92249000
H	0.81719800	4.37107500	3.21832600	C	0.77495700	-2.66467800	-2.63309700
C	0.47907900	0.62565200	-3.97958200	C	1.71852400	-1.44740400	-2.71435200
H	-0.35867400	1.05387500	-4.54030900	H	1.31441200	-3.55601900	-2.29631500
H	1.11168200	0.07988900	-4.68767600	H	-0.04867700	-2.49448600	-1.93438800
H	0.07300500	-0.09234100	-3.25979200	H	0.34514100	-2.87884700	-3.61869100
H	2.12031900	1.22405500	-2.74895200	C	0.92541300	-0.20893600	-3.16176700
Cu	0.21675100	-0.85593500	-0.19776000	C	2.77695000	-1.74654900	-3.79695700
H	-2.08626400	-1.30167200	-2.01081200	H	1.57588800	0.66225200	-3.27661400
C	-0.96264500	2.42316500	2.37650000	H	0.44215700	-0.39808800	-4.12681100
H	-0.71546800	2.34466800	3.44053100	H	0.13658000	0.04761200	-2.44420300
H	-1.86570800	3.03603100	2.28949900	H	2.27994700	-1.96569200	-4.74895300
H	-1.20191900	1.42244500	2.00526800	H	3.44427400	-0.89624300	-3.96557700

H	3.38750400	-2.61870300	-3.53699000	H	-1.75357100	-1.23442100	-3.75235900
C	2.41250700	-1.25589100	-1.31076900	H	-3.06679700	-1.94793100	-4.69973400
O	1.45081100	-1.17243700	-0.25489300	H	-2.77736600	-0.20849500	-4.77189800
C	-2.10660100	0.27051200	0.06818200	C	-5.18191600	-0.64295000	-3.45670900
C	-3.80686900	1.66416900	0.64958400	H	-5.21427000	0.19039600	-4.16651100
C	-4.36016900	0.47423300	0.29622900	H	-5.53310000	-1.54047400	-3.97726300
N	-3.31243500	-0.37183400	-0.05888300	H	-5.88393200	-0.42855900	-2.64653700
N	-2.42961000	1.53042300	0.50114900	C	-1.24748900	1.76898500	3.18513800
Cl	-6.01222400	0.03222700	0.26671400	C	-1.88656700	3.44504200	-1.66098300
Cl	-4.58372600	3.08921400	1.18877100	C	-2.10316600	2.49525800	4.24453000
C	-3.53333700	-2.77390800	0.43816600	H	-2.37670300	1.80305400	5.04790200
C	-3.49762100	-1.73619700	-0.51726200	H	-1.54912000	3.32706300	4.69305100
C	-3.68858100	-1.96062100	-1.89766100	H	-3.02426400	2.89885000	3.81398000
C	-3.88020800	-3.28483400	-2.31178500	C	-2.80593700	4.66228100	-1.89139900
C	-3.89467200	-4.33297600	-1.39612500	H	-3.56426800	4.74821000	-1.10835500
C	-3.72883200	-4.07683400	-0.03833700	H	-2.23079600	5.59418400	-1.90716000
H	-4.02825300	-3.49571500	-3.36595400	H	-3.31859400	4.57027700	-2.85472300
H	-4.04613500	-5.35170300	-1.74086500	C	0.00693100	1.15351600	3.83181700
H	-3.76093600	-4.90051700	0.66731300	H	0.61644000	1.91498600	4.32989300
C	-0.90299800	2.70630500	2.03135500	H	-0.28893800	0.42310100	4.59239800
C	-0.00412000	3.76029400	2.24121000	H	0.63368600	0.64642200	3.09433600
C	0.29544000	4.66631300	1.22825600	H	-1.84555200	0.94332200	2.78929300
C	-0.30818400	4.54492200	-0.02041100	Cu	-0.35155500	-0.46104400	-0.10304500
C	-1.21516400	3.51290500	-0.29144500	H	2.95386100	-2.19187900	-1.13884300
C	-1.48171900	2.59898400	0.74999800	C	-0.85985800	3.32122500	-2.80232200
H	0.46301900	3.87439900	3.21399900	H	-1.37645600	3.20937300	-3.76150900
H	0.99752800	5.47366200	1.41385200	H	-0.22836200	4.21324200	-2.87155900
H	-0.07660300	5.26722300	-0.79696500	H	-0.20903200	2.45428500	-2.66319800
C	-3.42156700	-2.53646300	1.94181700	H	-2.51461700	2.55005700	-1.69313100
H	-3.13757500	-1.49267400	2.10508100	Si	1.68744300	-1.98704000	1.52089700
C	-2.33303800	-3.41047500	2.59058000	H	0.20614600	-1.61266100	1.51910200
H	-2.23534500	-3.15558800	3.65108100	O	2.27398600	-3.34590600	0.67371000
H	-2.58068100	-4.47552000	2.53102000	O	2.78142000	-0.73561000	1.86010500
H	-1.36242700	-3.25496600	2.11487600	C	3.62065500	-0.62317700	2.99881600
C	-4.78042100	-2.76638200	2.63667900	C	4.10558500	0.81577700	3.13637000
H	-4.69694500	-2.55139600	3.70728700	H	4.48582300	-1.29634800	2.89675700
H	-5.56333500	-2.12663800	2.22053600	H	3.09541200	-0.91655500	3.91629100
H	-5.10373900	-3.80740900	2.52836200	H	4.76860700	0.91444000	4.00355200
C	-3.74393800	-0.83865800	-2.93202300	H	4.65268500	1.13627800	2.24489200
H	-3.43903400	0.09257400	-2.44576100	H	3.25754300	1.49466700	3.27074600
C	-2.77506400	-1.07651000	-4.10416100	C	2.93484800	-4.46135400	1.25178100

C	3.40421500	-5.39700000	0.14428200	H	0.12862900	-2.65655800	-1.80465400
H	2.26516600	-5.00477200	1.93237300	H	0.43958600	-2.99661400	-3.51715800
H	3.79925000	-4.13539400	1.84894300	C	0.86870800	-0.28644400	-3.03532700
H	3.91467600	-6.26875800	0.56850900	C	2.77314500	-1.68764900	-3.82659500
H	2.55386600	-5.75146000	-0.44778600	H	1.45827700	0.62721200	-3.15129800
H	4.09911600	-4.88565500	-0.52966500	H	0.34910200	-0.47199900	-3.98165900
C	1.50646800	-2.79462000	3.28386000	H	0.10802100	-0.10712700	-2.26789500
H	1.08324700	-2.06009600	3.98186800	H	2.23392700	-1.91818600	-4.75238500
H	0.78644900	-3.62193400	3.22969400	H	3.37335600	-0.79195100	-4.01200000
H	2.41908800	-3.19458800	3.74265100	H	3.45303100	-2.52314600	-3.62506900
TS38				C	2.52606800	-1.27320500	-1.31753500
C	4.94115800	-0.43741200	-1.63882900	O	1.57858100	-1.22884400	-0.23014800
C	5.75445300	-0.99910500	-0.45215100	C	-2.16783100	0.20749700	0.04515500
H	5.45434300	0.43807800	-2.05219300	C	-3.92187700	1.60879900	0.43546900
H	4.94950700	-1.19729800	-2.42762300	C	-4.43826000	0.39408800	0.11678400
C	7.18102500	-1.40047000	-0.84838700	N	-3.36068100	-0.45503200	-0.12620900
H	5.79320700	-0.25627300	0.35549800	N	-2.53566200	1.48837800	0.37877900
H	5.22434300	-1.86309100	-0.03489800	Cl	-6.08056700	-0.08154700	0.04222300
C	8.00092900	-1.94791200	0.32455000	Cl	-4.74817100	3.04589700	0.85916700
H	7.13516100	-2.15420900	-1.64660500	C	-3.61385000	-2.80245700	0.55556500
H	7.69746700	-0.53254300	-1.28171100	C	-3.49988800	-1.85357700	-0.48173400
H	9.01163300	-2.22990700	0.01053900	C	-3.56328100	-2.20382000	-1.84843000
H	8.09637700	-1.20285100	1.12294800	C	-3.69332200	-3.56412300	-2.15513700
H	7.52717600	-2.83617200	0.75840800	C	-3.76975900	-4.52776900	-1.15286500
C	3.50546100	-0.09089500	-1.29359300	C	-3.73834100	-4.14819800	0.18537200
C	3.07336600	1.14686400	-0.97485700	H	-3.74245300	-3.87252800	-3.19406900
C	3.79306200	2.43346900	-0.90471600	H	-3.86753700	-5.57677600	-1.41682000
C	3.05013400	3.60915500	-1.14363400	H	-3.82073500	-4.90617300	0.95786200
C	5.15902900	2.58946800	-0.59201800	C	-1.10483600	2.74696300	1.93574900
C	3.64246800	4.86967000	-1.11200700	C	-0.25126100	3.83655800	2.15352100
H	1.98939100	3.52243100	-1.35974500	C	0.05533200	4.72940500	1.13106600
C	5.75270500	3.85238200	-0.55489000	C	-0.49161800	4.55591500	-0.13738200
H	5.76019400	1.72443300	-0.34372600	C	-1.34601300	3.48274000	-0.41922000
C	5.00337700	4.99964100	-0.82207700	C	-1.62574900	2.58664400	0.63444200
H	3.04056500	5.75263000	-1.31039700	H	0.17139500	3.99159700	3.14078700
H	6.80696500	3.93794300	-0.30523900	H	0.71849500	5.56718300	1.32488500
H	5.46923500	5.98044400	-0.79226300	H	-0.25541200	5.26802300	-0.92211400
H	2.01064900	1.23979600	-0.75954200	C	-3.65235800	-2.42855600	2.03519500
C	0.91412900	-2.76215500	-2.55744100	H	-3.49953200	-1.34912200	2.12288400
C	1.76584000	-1.48136500	-2.67627200	C	-2.52528100	-3.11077400	2.82982600
H	1.53560900	-3.61976800	-2.27484200	H	-2.55713700	-2.79047200	3.87678100

H	-2.62471900	-4.20150700	2.81490600
H	-1.54522700	-2.85102000	2.42483100
C	-5.02880600	-2.75181900	2.65280300
H	-5.05622300	-2.42681100	3.69823700
H	-5.83949400	-2.24895000	2.11810300
H	-5.22848900	-3.82850100	2.63348400
C	-3.56214200	-1.17290100	-2.97522400
H	-3.20475900	-0.22234100	-2.56788200
C	-2.62324900	-1.55559200	-4.13333400
H	-1.61321900	-1.76863700	-3.77846400
H	-2.98619600	-2.43521500	-4.67505300
H	-2.56792300	-0.73181400	-4.85241300
C	-4.99199200	-0.94884000	-3.51319600
H	-4.98443100	-0.18441800	-4.29754600
H	-5.38941600	-1.87272300	-3.94769000
H	-5.67991700	-0.62471900	-2.72849600
C	-1.47361200	1.83342200	3.10151400
C	-1.94384800	3.34912100	-1.81822600
C	-2.42398900	2.55522100	4.08029700
H	-2.71946100	1.87741900	4.88829600
H	-1.93526700	3.42420800	4.53436100
H	-3.33192900	2.90486200	3.57987500
C	-2.86125700	4.54262600	-2.15504100
H	-3.66133700	4.65752000	-1.41879100
H	-2.29578900	5.47999700	-2.18775400
H	-3.32095700	4.39748600	-3.13839000
C	-0.23518900	1.29602800	3.84214500
H	0.31761600	2.10018400	4.33944400
H	-0.54766500	0.58795200	4.61738200
H	0.44864000	0.77999500	3.16341900
H	-2.00939200	0.96810500	2.70146500
Cu	-0.41213000	-0.56036400	0.23218100
H	3.11982100	-2.17809200	-1.17183600
C	-0.85243800	3.18865200	-2.89302500
H	-1.31131100	3.03059000	-3.87479200
H	-0.22498100	4.08347700	-2.96277600
H	-0.20419600	2.33564300	-2.67856400
H	-2.55919200	2.44516700	-1.84578000
Si	1.85634600	-1.87065400	1.43838100
H	0.32274100	-1.29204700	1.54825000
O	2.98366300	-3.00530500	0.78785900
O	2.71172600	-0.58061000	2.12293000
C	3.74802200	-0.75446300	3.07830600
C	4.22477000	0.60808900	3.56463900
H	4.59066400	-1.30244100	2.63091700
H	3.39579400	-1.34838000	3.93531100
H	5.02929000	0.49449800	4.29981600
H	4.60066800	1.20712400	2.72948000
H	3.40329700	1.15846000	4.03438800
C	3.50466500	-4.17911100	1.37915700
C	4.32303800	-4.95276600	0.35037800
H	2.69867600	-4.82512100	1.75358900
H	4.14130700	-3.93427000	2.24395200
H	4.72346500	-5.87235200	0.79182600
H	3.70134300	-5.22622800	-0.50883100
H	5.16336400	-4.35386500	-0.01493500
C	1.28823600	-2.95875200	2.93489100
H	0.69561400	-2.33391500	3.61235300
H	0.63606400	-3.77456600	2.59708500
H	2.09998100	-3.41508100	3.51312100

102

C	-9.93726200	0.92211000	1.55553700
C	-11.02489400	0.68506900	0.48341200
H	-9.93793500	1.97588600	1.85321500
H	-10.22102900	0.35180300	2.44712100
C	-12.43161500	1.05701500	0.96929700
H	-10.78424400	1.26125500	-0.42003500
H	-11.00835800	-0.36923000	0.17830100
C	-13.51409000	0.82306800	-0.08938700
H	-12.66778800	0.47500800	1.87044500
H	-12.44206600	2.11142600	1.27773400
H	-14.50605500	1.09559500	0.28595200
H	-13.32334400	1.41862000	-0.98957600
H	-13.55048200	-0.23001900	-0.39173300
C	-8.55428000	0.49694700	1.10990500
C	-7.61358300	1.30931800	0.58204600
C	-7.60398200	2.76416300	0.33913100
C	-6.34741800	3.40628200	0.31751700
C	-8.74148000	3.56015900	0.09580700
C	-6.23142900	4.77747900	0.10160900
H	-5.45203500	2.81201100	0.48139500
C	-8.62561200	4.93330400	-0.12558900

H	-9.72284600	3.10578900	0.04607900
C	-7.37390100	5.55199100	-0.11734400
H	-5.24875800	5.24094800	0.09926100
H	-9.52034600	5.51981300	-0.31573700
H	-7.28843200	6.62071000	-0.29104000
H	-6.67556900	0.82776300	0.31404000
C	-7.44006200	-2.93867400	2.65320100
C	-7.50353100	-1.39858500	2.59180200
H	-8.44322500	-3.37992300	2.61707500
H	-6.85880300	-3.34381500	1.82112400
H	-6.96605400	-3.26259400	3.58626700
C	-6.07099200	-0.83614100	2.62690800
C	-8.27477800	-0.89123200	3.82518600
H	-6.06697400	0.25709800	2.65875400
H	-5.55169800	-1.19793700	3.52129800
H	-5.50054500	-1.15728900	1.75116100
H	-7.77502100	-1.23171800	4.73864300
H	-8.31644800	0.20164400	3.86036800
H	-9.30084600	-1.27617700	3.85054000
C	-8.25122800	-0.99655800	1.27019500
O	-7.47842200	-1.48755000	0.16520200
C	6.17328300	-0.06993200	-0.05204000
C	7.99945900	1.27544900	0.05163600
C	8.43034300	-0.00906000	0.18841900
N	7.30181900	-0.82086900	0.12285600
N	6.61626500	1.22218000	-0.09464900
Cl	10.02145500	-0.59973200	0.39974400
Cl	8.90570600	2.72575000	0.04663200
C	7.45181300	-3.02549600	-0.95067400
C	7.30783200	-2.26604900	0.22768000
C	7.16777700	-2.84773800	1.50363000
C	7.16153200	-4.24656400	1.57250000
C	7.29450400	-5.02529100	0.42593600
C	7.43941200	-4.41988700	-0.81947900
H	7.04980800	-4.73139400	2.53725400
H	7.28630100	-6.10855900	0.50350600
H	7.54355600	-5.03854100	-1.70534700
C	5.48066800	2.81440400	-1.58134900
C	4.62723800	3.91604700	-1.72158700
C	4.07668600	4.54754800	-0.60963400
C	4.37095400	4.09106800	0.67237100
C	5.21801300	2.99420700	0.87489200
C	5.75201800	2.37199300	-0.27117500
H	4.38921500	4.28118100	-2.71570900
H	3.41581900	5.39910100	-0.74263600
H	3.93431100	4.59163300	1.53085700
C	7.60751300	-2.39797700	-2.33225000
H	7.63314600	-1.31092000	-2.21539700
C	6.40177200	-2.72893400	-3.23357200
H	6.50687300	-2.23227400	-4.20399500
H	6.32371500	-3.80605200	-3.41571600
H	5.46434600	-2.39515400	-2.77734300
C	8.93302900	-2.81422400	-2.99943400
H	9.04637700	-2.30383500	-3.96157500
H	9.79275100	-2.55629300	-2.37331300
H	8.96629200	-3.89198500	-3.19014000
C	7.01532700	-2.02721100	2.78059800
H	7.09588200	-0.96799100	2.52020100
C	5.62522100	-2.23543700	3.41299700
H	4.82801700	-1.97977900	2.70766000
H	5.48059500	-3.27573300	3.72335900
H	5.51454400	-1.60271100	4.30005200
C	8.13792000	-2.33260100	3.79129400
H	8.03582500	-1.68952300	4.67164400
H	8.09921200	-3.37182800	4.13401100
H	9.12619200	-2.15839600	3.35472600
C	6.06116500	2.14629500	-2.82380000
C	5.51167700	2.51864900	2.29443900
C	6.91256800	3.12832800	-3.65199000
H	7.36774000	2.60776500	-4.50103200
H	6.30660800	3.94781500	-4.05225400
H	7.71540600	3.56531100	-3.05020600
C	6.15977800	3.62862500	3.14468500
H	7.07371400	4.00771100	2.67719100
H	5.47909800	4.47398500	3.28946200
H	6.41951300	3.23992900	4.13490100
C	4.95184900	1.50905300	-3.68367000
H	4.25501900	2.26578800	-4.05941700
H	5.38921200	0.99807100	-4.54803100
H	4.37589400	0.77717800	-3.10838400
H	6.72404900	1.33857000	-2.50128400
Cu	4.34532600	-0.70286300	-0.21011100

H	-9.21221400	-1.52562900	1.28541100	H	1.36631700	3.66828700	-2.87327800
C	4.24007900	1.97049900	2.97166800	C	-0.69469900	-0.68714400	-0.74690200
H	4.47604600	1.59601400	3.97344500	C	-1.62657000	-0.83674000	0.21786100
H	3.47735800	2.74950900	3.07621700	C	-3.00634300	-0.32534000	0.32317200
H	3.80575400	1.14950000	2.39229200	C	-3.92571300	-1.08702600	1.07466500
H	6.22890900	1.69483500	2.23956100	C	-3.47049600	0.88050100	-0.23844000
Si	-7.98740400	-2.33490500	-1.16162100	C	-5.25153600	-0.68843500	1.22588700
H	2.91157700	-1.20393400	-0.34030500	H	-3.58774900	-2.01099100	1.53693500
O	-9.56624000	-2.75439700	-0.84270400	C	-4.79766200	1.28263200	-0.08370000
O	-7.87357100	-1.44574200	-2.55556600	H	-2.78688300	1.52841700	-0.77246500
C	-8.57489200	-0.22643900	-2.83265300	C	-5.69761700	0.49954300	0.64125100
C	-8.19691800	0.25779700	-4.22315300	H	-5.93604700	-1.30304500	1.80365000
H	-8.31560500	0.52583500	-2.07820900	H	-5.12540100	2.21999200	-0.52435700
H	-9.65800700	-0.39844400	-2.76980800	H	-6.72941900	0.81656800	0.75993100
H	-8.72083400	1.19071100	-4.45573200	H	-1.34139000	-1.47043200	1.05480700
H	-7.12011800	0.44175300	-4.28744400	C	2.20714300	-3.32556300	-0.96989000
H	-8.46475900	-0.48675200	-4.97940000	C	0.73556200	-2.87019100	-1.05009900
C	-10.37336300	-3.52717400	-1.73957500	H	2.85436000	-2.68529600	-1.58029000
C	-11.71152900	-3.82199100	-1.08193200	H	2.57468500	-3.29651400	0.05874800
H	-9.86156100	-4.46665100	-1.98928400	H	2.30783600	-4.35230100	-1.33836800
H	-10.52187400	-2.97385200	-2.67637100	C	-0.12114100	-3.78226700	-0.15420600
H	-12.34105300	-4.41611700	-1.75228300	C	0.25919700	-3.00362100	-2.50903500
H	-11.56939600	-4.38284200	-0.15312800	H	-1.18595200	-3.54730900	-0.23714700
H	-12.23969300	-2.89277900	-0.84630800	H	0.01339700	-4.82756700	-0.45335100
C	-6.86784600	-3.80076300	-1.42460000	H	0.17164300	-3.69132000	0.89531200
H	-5.82890800	-3.47390900	-1.53323000	H	0.37096300	-4.04141300	-2.84097200
H	-6.91873200	-4.48637800	-0.57329300	H	-0.79520200	-2.73371000	-2.62186100
H	-7.13870300	-4.35634200	-2.32768200	H	0.84942700	-2.37722000	-3.18757100
103				C	0.66740300	-1.37095600	-0.59118200
C	-0.85699600	0.13685000	-2.00655900	O	1.13251300	-1.31095100	0.76851100
C	-0.21532400	1.53832000	-1.90640000	H	1.38144300	-0.82837700	-1.22432700
H	-1.91582200	0.23532300	-2.26666500	Si	2.06008100	-0.10429200	1.41911400
H	-0.38270500	-0.38777000	-2.84406000	O	3.16831000	0.31426300	0.26105800
C	-0.33846000	2.34784000	-3.20316400	O	1.22950600	1.29622600	1.74001500
H	-0.67409500	2.09540200	-1.07904300	C	0.16118200	1.43063300	2.68423000
H	0.84476400	1.43397200	-1.64073200	C	-0.12420400	2.90633200	2.90889200
C	0.29750600	3.73773500	-3.10544900	H	0.43064400	0.94999900	3.63477600
H	0.12846600	1.78748300	-4.02442700	H	-0.73005900	0.92401700	2.29468100
H	-1.39966600	2.44810600	-3.46905700	H	-0.95006300	3.02960200	3.61692300
H	0.19590000	4.29031700	-4.04522100	H	0.75657200	3.41516900	3.31250200
H	-0.17333700	4.33404100	-2.31564000	H	-0.40132000	3.39170800	1.96817700

C	3.99091000	1.48703500	0.30850800	C	4.53800900	-3.08504700	-3.39537800
C	4.78620900	1.59016800	-0.98207900	H	2.76883100	-2.23611500	-2.48296800
H	4.67265200	1.42646700	1.16816400	H	3.65510700	-1.11369600	-3.49953700
H	3.36173900	2.37440400	0.44569800	H	4.01065700	-3.46289000	-4.27658400
H	5.42721800	2.47746000	-0.96242800	H	5.54267100	-2.78259700	-3.71160500
H	5.42042900	0.70888100	-1.11771400	H	4.64727300	-3.91615400	-2.68990100
H	4.11571100	1.66774200	-1.84348000	C	3.48923600	1.90902200	0.24182300
C	2.82563000	-0.81279200	2.96574400	C	3.60067700	2.79711500	1.48024600
H	2.06147800	-1.10760500	3.69214700	H	2.44491100	1.65644600	0.04732800
H	3.41910400	-1.70044200	2.72716200	H	3.90505400	2.42248800	-0.62926400
H	3.48271000	-0.08333700	3.44994600	C	2.95506700	4.16589200	1.20064400
104				H	3.08984000	2.33590400	2.33076400
Si	-0.47495700	0.18987100	-0.36907200	H	4.64308700	2.95676600	1.78037700
O	-0.07380100	-1.43570400	-0.72357700	C	2.98821000	5.08746300	2.42289100
O	0.34604400	1.33303400	-1.34834000	H	3.47233500	4.64862400	0.36147500
C	-0.20774300	2.52555400	-1.86167700	H	1.91650200	4.01726700	0.87993600
C	0.59843900	2.99490300	-3.06774300	H	2.52719300	6.05416300	2.19840600
H	-0.19330200	3.31359400	-1.08877400	H	2.44545300	4.64624900	3.26587800
H	-1.25158400	2.38673400	-2.15556000	H	4.01688700	5.27570900	2.75017700
H	0.20481600	3.94083000	-3.45678800	C	3.81846900	-0.13257000	1.60426200
H	1.64893400	3.14745900	-2.79750500	C	3.92955100	-1.65316300	1.71341400
H	0.55990100	2.24983500	-3.86921400	H	2.76784800	0.12681900	1.72698100
C	-0.67685800	-2.34522400	-1.61784800	H	4.40933300	0.35380700	2.38299500
C	-0.02498700	-3.71468300	-1.44591900	C	3.50835500	-2.09015200	3.12763700
H	-0.55982900	-2.00744000	-2.65839200	H	3.25807400	-2.12678900	0.99107800
H	-1.75462200	-2.42917900	-1.44037900	H	4.94110800	-2.01640200	1.51658800
H	-0.47694100	-4.44607400	-2.12578800	C	3.54628800	-3.61068800	3.30454000
H	1.04920600	-3.67201200	-1.65562600	H	4.16730000	-1.61762000	3.86798900
H	-0.15208100	-4.07492100	-0.41934400	H	2.49580100	-1.72129100	3.33216700
C	-1.33789900	0.86116400	1.19145700	H	3.24644700	-3.89625400	4.31750800
H	-2.21111900	1.47775200	0.97758400	H	2.86718000	-4.10665600	2.60283500
H	-1.68790300	0.02382900	1.80707100	H	4.55355800	-4.00546900	3.13020000
H	-0.63445400	1.43946200	1.79699100	C	9.19820700	-0.71117700	0.96151600
N	4.22345500	0.54674700	0.28936400	C	8.15121600	0.27901900	0.44372800
C	3.67858300	-0.20194200	-0.94163000	H	10.21169900	-0.34021300	0.78150000
C	4.49401900	-1.35789900	-1.51758200	H	9.08897700	-0.87602700	2.03898300
H	3.58567900	0.56667200	-1.71243900	H	9.10481000	-1.68287900	0.46448600
H	2.66578500	-0.49600300	-0.65827800	C	6.71248900	-0.21298400	0.67622800
C	3.77981700	-1.91596800	-2.76094300	H	8.28952700	1.25037600	0.93610400
H	5.49325400	-1.02027800	-1.81408000	H	8.30772500	0.45193400	-0.62876000
H	4.62576100	-2.16437700	-0.79256200	C	5.71877200	0.83769900	0.18097900

H	6.57662200	-1.17016200	0.16797800
H	6.56958000	-0.39044400	1.74741500
H	5.88627400	1.75337200	0.74890100
H	5.89471200	1.07300600	-0.87172400
F	1.01329000	0.10353000	0.60249800
C	-5.26610000	1.19619500	0.06238500
C	-4.86091000	2.15470700	1.20398600
H	-6.17665000	0.65983600	0.35469100
H	-5.54469400	1.82161000	-0.78922400
C	-6.01014000	3.07595800	1.63292600
H	-4.50362800	1.58471200	2.07057600
H	-4.01157800	2.76865800	0.87799200
C	-5.61777600	4.05211500	2.74608200
H	-6.36721900	3.63925400	0.75994200
H	-6.86004100	2.46405000	1.96552100
H	-6.45956800	4.69094900	3.03325300
H	-5.28489300	3.51677700	3.64263300
H	-4.79700500	4.70557000	2.42882200
C	-4.19825200	0.20339200	-0.35904000
C	-4.06908900	-1.04027900	0.14920400
C	-4.86547900	-1.79665700	1.13085800
C	-4.78163200	-3.20559500	1.07514700
C	-5.68476700	-1.24498500	2.13785300
C	-5.49735100	-4.02011200	1.94837000
H	-4.14304600	-3.66006800	0.32200700
C	-6.39959400	-2.06045100	3.01634000
H	-5.74648300	-0.17210800	2.26271200
C	-6.31783200	-3.45083500	2.92583600
H	-5.41170600	-5.10041100	1.86902100
H	-7.01759500	-1.60183600	3.78357700
H	-6.87522000	-4.08095300	3.61268700
H	-3.24177600	-1.61294800	-0.26169700
C	-2.79283600	1.05390400	-3.93498800
C	-3.77700500	0.43082200	-2.92583800
H	-2.74016900	2.14286100	-3.81806100
H	-1.78943600	0.64564400	-3.80340600
H	-3.12217900	0.85058900	-4.96107000
C	-3.90342000	-1.07238600	-3.22889900
C	-5.15228400	1.08725500	-3.15329600
H	-4.60526200	-1.56114800	-2.54674000
H	-4.27162400	-1.21972900	-4.25132200
H	-2.93685500	-1.57029900	-3.13851400
H	-5.43546400	0.98486500	-4.20749800
H	-5.94182200	0.61725700	-2.56021100
H	-5.13882300	2.15939700	-2.92495400
C	-3.20906400	0.66637600	-1.45421700
O	-1.95240200	0.05425900	-1.38475700
H	-3.13059900	1.76585800	-1.34311600

TS39

Si	-0.10921000	0.12862900	0.03274500
O	-0.03770100	-1.26341100	-0.85258300
O	0.35043100	1.49617700	-0.78187600
C	-0.46699400	2.63184500	-1.10703100
C	0.21820700	3.44097200	-2.19593200
H	-0.59313800	3.24934800	-0.20554000
H	-1.44095000	2.25570100	-1.42836900
H	-0.38377800	4.32098500	-2.44721500
H	1.20835100	3.78596100	-1.87828700
H	0.34035700	2.84098800	-3.10341900
C	-0.43631100	-1.46406300	-2.21968600
C	-0.77919200	-2.93123700	-2.42138400
H	0.40491700	-1.18348700	-2.86946800
H	-1.29490200	-0.82232700	-2.43093400
H	-1.04347100	-3.11802900	-3.46821700
H	0.06530100	-3.57908000	-2.16112200
H	-1.63235800	-3.21621200	-1.79702600
C	-1.33200700	0.24865600	1.42900100
H	-1.38362500	1.28369100	1.78560900
H	-2.32330700	-0.04998100	1.09494000
H	-1.00299600	-0.37778000	2.26519900
N	4.61876900	0.37713100	0.08808500
C	3.91068200	-0.51963900	-0.94268000
C	4.60424400	-1.79503000	-1.41924100
H	3.75206600	0.12635200	-1.80901300
H	2.93332800	-0.73195700	-0.50809100
C	3.68802200	-2.52521000	-2.41778500
H	5.54979800	-1.55818300	-1.91888200
H	4.83225900	-2.46996400	-0.59138900
C	4.31855000	-3.81326100	-2.95366600
H	2.73282400	-2.75387200	-1.92954000
H	3.45382800	-1.85476900	-3.25461800
H	3.64777500	-4.31300300	-3.65888500

H	5.25949100	-3.60755800	-3.47588000	F	1.30607200	-0.09945000	0.88778200
H	4.53414800	-4.51700900	-2.14226200	C	-5.57406300	1.21604700	0.57771300
C	3.93313700	1.75423800	-0.08273700	C	-4.92516400	1.75037800	1.87319300
C	4.23207800	2.81788600	0.97316500	H	-6.50264400	0.68830200	0.82910900
H	2.86215200	1.54367000	-0.11070300	H	-5.86567600	2.08677700	-0.01754700
H	4.24381800	2.10498200	-1.07011500	C	-5.85536900	2.66830500	2.67603000
C	3.55131200	4.14249600	0.58461400	H	-4.60333800	0.91203800	2.50484100
H	3.85881600	2.50714500	1.95343600	H	-4.00950900	2.29681700	1.61249600
H	5.30820100	2.99543400	1.08033300	C	-5.21055900	3.21451100	3.95363800
C	3.78325900	5.24236900	1.62432900	H	-6.17389100	3.50538200	2.03966300
H	3.92744200	4.47380600	-0.39175400	H	-6.77194400	2.11995600	2.93443500
H	2.47475700	3.97282200	0.46148900	H	-5.89811200	3.86621400	4.50324300
H	3.29365900	6.17371400	1.32451400	H	-4.91365900	2.40164700	4.62637800
H	3.38256900	4.95398600	2.60215500	H	-4.31095900	3.79747700	3.72479500
H	4.85151000	5.45119600	1.74935200	C	-4.65162700	0.33665700	-0.23991500
C	4.35788500	-0.07570000	1.53033200	C	-4.56401000	-1.00725000	-0.12840700
C	4.41293500	-1.56795900	1.85629000	C	-5.32124100	-1.99173100	0.66034200
H	3.35026600	0.27385700	1.75136300	C	-5.33885400	-3.32422100	0.18900100
H	5.06494200	0.47999000	2.14895700	C	-6.01809600	-1.73475400	1.86095100
C	4.13977100	-1.77143100	3.35720300	C	-6.03299600	-4.33251600	0.85232200
H	3.64596900	-2.10255700	1.28802400	H	-4.79792200	-3.55888800	-0.72443600
H	5.38006200	-2.01094700	1.60765700	C	-6.71180300	-2.74503900	2.52848800
C	4.13457200	-3.25056900	3.75315100	H	-5.99916600	-0.74461500	2.29729400
H	4.89853100	-1.23603300	3.94258700	C	-6.73151300	-4.04857600	2.02922500
H	3.17341300	-1.31960300	3.61365500	H	-6.02677700	-5.34300300	0.45210600
H	3.93765000	-3.36870900	4.82294800	H	-7.23376900	-2.51022100	3.45257800
H	3.36143400	-3.80268000	3.20818900	H	-7.27246400	-4.83159900	2.55262800
H	5.09875500	-3.72359800	3.53659000	H	-3.80917500	-1.44811300	-0.77788600
C	9.59312200	-1.03028800	0.34329900	C	-3.50411700	2.14132400	-3.52380200
C	8.52476600	-0.06770400	-0.18275100	C	-4.42919900	1.24748500	-2.67896500
H	10.58845400	-0.73835800	-0.00461600	H	-3.40090900	3.13658000	-3.07194400
H	9.61165300	-1.04164600	1.43853700	H	-2.51024000	1.69410500	-3.58391600
H	9.40675000	-2.05434600	0.00209100	H	-3.89840700	2.27691500	-4.53930900
C	7.10960400	-0.45135800	0.28413200	C	-4.59232600	-0.10685600	-3.38645700
H	8.75443400	0.95311900	0.14865600	C	-5.80579200	1.93061900	-2.59359300
H	8.55316200	-0.05008900	-1.27969800	H	-5.29244100	-0.75531200	-2.84962400
C	6.10036800	0.56998200	-0.23940500	H	-4.97499400	0.02841300	-4.40654600
H	6.88217500	-1.46156500	-0.06318900	H	-3.62995200	-0.62170100	-3.44142500
H	7.09380500	-0.47117700	1.37881400	H	-6.19992900	2.12084900	-3.60071300
H	6.36760000	1.54736100	0.16233500	H	-6.54330700	1.31351800	-2.06992800
H	6.14896600	0.64158300	-1.32889500	H	-5.74722600	2.89980000	-2.08296300

C	-3.70595000	1.04908900	-1.25362600	H	-0.67251100	-3.17248400	3.38832400
O	-2.49059100	0.45817300	-1.40338200	H	-0.44284300	-3.50600800	1.66882200
H	-3.63665000	2.10350400	-0.86210400	H	0.91545800	-3.67719300	2.79327200
105				C	6.63795100	-1.78331700	2.51239400
N	2.75447700	0.49135600	-0.04440400	C	6.13240000	-0.62915800	1.64217600
C	2.56137600	-0.22720500	-1.39034700	H	7.69859600	-1.65975200	2.75139400
C	3.18414700	-1.60922200	-1.58396000	H	6.08644700	-1.83782100	3.45733000
H	3.00749000	0.44609500	-2.12725900	H	6.52044500	-2.74557600	2.00210200
H	1.47704500	-0.21238400	-1.54838700	C	4.64274200	-0.76948200	1.28577800
C	2.84372100	-2.13049800	-2.99151800	H	6.29471900	0.32271900	2.16447600
H	4.27473100	-1.56112700	-1.48590700	H	6.72411400	-0.57851600	0.71896700
H	2.82532400	-2.33013500	-0.84608800	C	4.19499300	0.42863000	0.44823900
C	3.46775000	-3.49901800	-3.27859300	H	4.49006300	-1.71293600	0.75620700
H	1.75376700	-2.19183300	-3.10074000	H	4.06049600	-0.81795000	2.21180700
H	3.18709200	-1.40620600	-3.74166600	H	4.34740700	1.32980200	1.04282100
H	3.20966200	-3.84580700	-4.28397100	H	4.81464600	0.52554500	-0.44771300
H	4.56063000	-3.45940900	-3.20941200	C	-3.72067400	1.22669000	0.13071100
H	3.11633300	-4.25293200	-2.56544000	C	-3.37999400	1.62630100	1.58363200
C	2.44152800	1.97070300	-0.38163900	H	-4.63474800	0.61999600	0.12394000
C	2.31702800	2.94031600	0.79222200	H	-3.95716600	2.14704500	-0.41307500
H	1.48161500	1.91307800	-0.91685000	C	-4.51247100	2.38671000	2.28453000
H	3.24805400	2.28608200	-1.04969100	H	-3.12580000	0.72984300	2.16460200
C	2.16066400	4.37587700	0.26024800	H	-2.47410400	2.24696000	1.57594700
H	1.43890200	2.69363600	1.39652600	C	-4.17182600	2.78453100	3.72412400
H	3.18624500	2.90905200	1.46085500	H	-4.75678900	3.28649500	1.70352700
C	1.97318600	5.40044900	1.38253400	H	-5.42115100	1.76883700	2.28113100
H	3.04274500	4.64138700	-0.33695800	H	-4.99710600	3.32771400	4.19660200
H	1.30248800	4.41606300	-0.42184600	H	-3.95943200	1.90215300	4.33879100
H	1.86720000	6.41210600	0.97872000	H	-3.28646200	3.42989000	3.75733600
H	1.07668800	5.18082500	1.97252000	C	-2.57961000	0.51327600	-0.55954700
H	2.82957100	5.40178800	2.06629800	C	-2.36994400	-0.82155600	-0.54274700
C	1.69817100	0.05874800	0.98191900	C	-3.14588700	-1.95289400	-0.01297700
C	1.42296700	-1.43163200	1.18229000	C	-2.85892300	-3.23374100	-0.53969200
H	0.77771600	0.51444200	0.59114600	C	-4.14093400	-1.88874900	0.98733400
H	1.99644600	0.52220500	1.92495100	C	-3.53641800	-4.37518000	-0.11868100
C	0.40507800	-1.60723200	2.32298400	H	-2.09132300	-3.31945500	-1.30496800
H	0.99437800	-1.85253800	0.26769100	C	-4.81959200	-3.03219100	1.41061600
H	2.32181700	-2.00589000	1.42055100	H	-4.37534300	-0.94455800	1.46108600
C	0.03154900	-3.07389200	2.55616900	C	-4.52917400	-4.28210000	0.86056700
H	0.81846900	-1.18169800	3.24727300	H	-3.28919600	-5.33935900	-0.55513000
H	-0.49932400	-1.03224700	2.09020100	H	-5.57738700	-2.94371500	2.18481800

H	-5.06003100	-5.16872100	1.19469800
H	-1.45617900	-1.11703600	-1.05639400
C	-0.91336700	2.72540300	-3.33439300
C	-1.92302300	1.69279200	-2.80194900
H	-0.98696800	3.66936100	-2.77817300
H	0.10273200	2.34248500	-3.21676300
H	-1.09131500	2.94878500	-4.39421000
C	-1.80283600	0.40913500	-3.63789100
C	-3.33965000	2.26962400	-2.96641900
H	-2.55182600	-0.33283400	-3.34237100
H	-1.94241300	0.62096800	-4.70583100
H	-0.81373800	-0.03437800	-3.49666500
H	-3.52762000	2.53376200	-4.01546800
H	-4.11322200	1.55388800	-2.66902700
H	-3.47506100	3.18281100	-2.37367500
C	-1.52044400	1.40251700	-1.27585600
O	-0.25141200	0.92212900	-1.18037400
H	-1.64342700	2.41033100	-0.79078400

4b

H	-1.41231300	-0.38859100	-2.45414100
C	-0.26832000	1.25724500	0.62371400
C	-0.15061100	2.50826500	-0.27518700
H	0.63277400	1.16334100	1.23819900
H	-1.09873300	1.42476300	1.31878100
C	0.07199300	3.79841700	0.52355200
H	0.67002900	2.37386300	-0.99234700
H	-1.06218700	2.61027600	-0.87942600
C	0.16773600	5.04448600	-0.36179100
H	-0.74748700	3.92214000	1.24436000
H	0.98898800	3.70052300	1.12026000
H	0.32742100	5.94745000	0.23641400
H	0.99913000	4.96399400	-1.07132400
H	-0.75000700	5.18831100	-0.94331100
C	-0.51461700	-0.01944600	-0.15125200
C	0.43292300	-0.91296600	-0.50975000
C	1.87986900	-0.95855100	-0.22868100
C	2.48868200	-2.22928800	-0.16542000
C	2.70791100	0.16692800	-0.04996500
C	3.84753300	-2.37384300	0.10334200
H	1.87560200	-3.11327600	-0.32102700
C	4.07055600	0.02314800	0.21347300
H	2.29708000	1.16391200	-0.14794500
C	4.64722700	-1.24514300	0.29981300
H	4.28364900	-3.36738400	0.15522900
H	4.68527800	0.90955800	0.34219900
H	5.70809300	-1.35274900	0.50521300
H	0.07582700	-1.77829200	-1.06482600
C	-2.35018400	-2.59625800	0.39160800
C	-2.84681300	-1.13958100	0.35654100
H	-2.33568500	-3.03199100	-0.61053600
H	-1.34293400	-2.66757400	0.81188500
H	-3.01638700	-3.20079000	1.01686800
C	-2.84659100	-0.57233500	1.78739100
C	-4.29140600	-1.10903800	-0.18586000
H	-3.18819400	0.46872000	1.81237100
H	-3.52819100	-1.15543600	2.41613300
H	-1.85370500	-0.61986900	2.24510200
H	-4.95011300	-1.70934100	0.45124700
H	-4.68448500	-0.08551800	-0.20147000
H	-4.34023700	-1.50612900	-1.20231000
C	-1.96326200	-0.25693800	-0.59059000
O	-2.03449400	-0.86271700	-1.88567900
H	-2.45301700	0.73122000	-0.62579400

107

C	-5.47025700	-0.75577300	-0.46136200
C	-4.91867400	-0.63231000	-1.89628800
H	-6.12167400	-1.63095900	-0.39010000
H	-4.62630500	-0.92492100	0.21458800
C	-4.12343000	-1.86838800	-2.33525500
H	-5.74543700	-0.45890800	-2.59917600
H	-4.27448100	0.25368400	-1.95815600
C	-3.57665800	-1.75558500	-3.76197500
H	-3.29152700	-2.02529500	-1.63611800
H	-4.76273400	-2.75854000	-2.25586400
H	-3.01283200	-2.65047900	-4.04500900
H	-4.38736800	-1.62826700	-4.48890600
H	-2.90516100	-0.89507900	-3.86058600
C	-6.20511800	0.47507600	0.02655900
C	-7.55034500	0.55135200	0.18252800
C	-8.59687700	-0.44096700	-0.11169500
C	-9.74307100	-0.44645700	0.70962000
C	-8.55173400	-1.34893600	-1.18779300

C	-10.77943800	-1.35226900	0.49700800
H	-9.80874300	0.26305800	1.53048900
C	-9.59619400	-2.24629700	-1.40845900
H	-7.71664100	-1.32978200	-1.87780000
C	-10.70813600	-2.26014600	-0.56313400
H	-11.64544900	-1.34498600	1.15239500
H	-9.54406500	-2.93116900	-2.24982200
H	-11.51818900	-2.96215700	-0.73725400
H	-7.94916100	1.44636500	0.64535800
C	-4.49824800	3.96869800	0.66516500
C	-5.76053700	3.08243600	0.61767300
H	-3.85214300	3.70233300	1.50379800
H	-3.91080900	3.87296800	-0.25262600
H	-4.79622700	5.01644200	0.77461400
C	-6.62948000	3.55837800	-0.56921200
C	-6.50653400	3.26342900	1.96551900
H	-7.59471200	3.05454600	-0.63178600
H	-6.81999100	4.63203900	-0.46753400
H	-6.11005800	3.40303600	-1.52100200
H	-6.70312100	4.32876200	2.12707500
H	-7.46566800	2.74339500	2.00882500
H	-5.89255500	2.90646500	2.79878600
C	-5.30099800	1.60300100	0.45312000
O	-4.11658200	1.33779400	0.65693300
C	3.14580900	-0.29754800	-0.20810200
C	4.32258800	0.57106100	1.52870300
C	3.13266100	0.12891100	2.02140200
N	2.42299300	-0.39901700	0.94701400
N	4.31650100	0.30274700	0.16310800
Cl	2.54604100	0.17112100	3.62741100
Cl	5.62186900	1.32090200	2.35024800
C	0.97703100	-2.36023900	1.25965500
C	1.09529100	-0.97445900	1.03067100
C	-0.01737600	-0.12205200	0.88510800
C	-1.29007600	-0.70419000	0.96466200
C	-1.43721700	-2.07193900	1.18413800
C	-0.31807300	-2.88799400	1.32938200
H	-2.17199600	-0.08042200	0.85466500
H	-2.43174000	-2.50478500	1.24507700
H	-0.45011400	-3.95203900	1.49964100
C	6.40738100	-0.35027900	-0.94766000
C	7.43363700	-0.02744100	-1.84450300
C	7.45340700	1.19678400	-2.50734800
C	6.44376300	2.12954500	-2.28590200
C	5.39161600	1.86270800	-1.40066600
C	5.39714700	0.61218000	-0.75066700
H	8.22669200	-0.74601100	-2.02644000
H	8.25923300	1.42500400	-3.19882300
H	6.47051000	3.08037900	-2.80889800
C	2.17884900	-3.28498500	1.42635400
H	3.08925400	-2.68246000	1.36003700
C	2.24318700	-4.32818100	0.29366100
H	3.14021900	-4.94761200	0.39974700
H	1.37349700	-4.99364800	0.31353200
H	2.27484200	-3.84426800	-0.68778300
C	2.18285500	-3.96436400	2.80979900
H	3.08156100	-4.57932000	2.92565700
H	2.16962400	-3.22525300	3.61683000
H	1.31407500	-4.61845800	2.93837200
C	0.11084500	1.37855600	0.64364800
H	1.17246700	1.64194300	0.66502900
C	-0.42958800	1.76743000	-0.74681200
H	0.07627300	1.20804100	-1.54036800
H	-1.50374800	1.56987300	-0.82009500
H	-0.27205500	2.83636400	-0.92744200
C	-0.58660500	2.19198500	1.75203500
H	-0.40792700	3.26195300	1.59975100
H	-1.66857400	2.02929100	1.74019700
H	-0.20736300	1.92241500	2.74289500
C	6.42096200	-1.70221400	-0.24074000
C	4.30118000	2.90785800	-1.18728900
C	7.68331500	-1.87396500	0.62683300
H	7.64287300	-2.82600300	1.16630300
H	8.59218400	-1.87692200	0.01605400
H	7.77478400	-1.06886000	1.36232400
C	4.87968700	4.23192000	-0.65134500
H	5.43956400	4.07625800	0.27600200
H	5.55305200	4.69972800	-1.37718000
H	4.07047000	4.94037200	-0.44569600
C	6.27682500	-2.86060900	-1.24721500
H	7.12244200	-2.89201900	-1.94237900
H	6.24310200	-3.81908500	-0.71837800

H	5.35922900	-2.76139400	-1.83574300	H	-0.15240000	-5.10018200	-0.85630600
H	5.55852200	-1.74915600	0.43034100	C	-2.07035400	-4.20263700	0.78759400
Cu	2.63868900	-0.89478900	-1.98374300	C	-2.57949500	-4.04175500	-1.66671600
H	2.25480600	-1.37631700	-3.37877800	H	-3.12375500	-4.03818800	1.02105300
C	3.48955900	3.13647400	-2.47750500	H	-1.92418200	-5.28648900	0.71430500
H	2.68002200	3.85104000	-2.29419400	H	-1.46538800	-3.84036000	1.62446500
H	4.11856300	3.54111300	-3.27767300	H	-2.54070700	-5.13435700	-1.73614900
H	3.04673600	2.20200500	-2.83659000	H	-3.61834700	-3.75139800	-1.48045400
H	3.60612200	2.53054900	-0.43204300	H	-2.27602300	-3.62517600	-2.63156000
TS40				C	-1.69806800	-1.98058400	-0.59867600
C	-3.53848800	-1.37932900	1.21832800	O	-1.03696900	-1.46257300	-1.58139500
C	-4.94886500	-1.99346700	1.32502100	C	1.56266200	0.37919000	0.10445200
H	-3.54374500	-0.39317200	1.69976500	C	3.68467600	1.19252900	0.03906300
H	-2.84283700	-1.97008700	1.81715600	C	2.84985600	2.24892100	0.22883600
C	-5.42817300	-2.11574600	2.77713700	N	1.55357600	1.73868200	0.26683900
H	-5.66521200	-1.39012800	0.75708100	N	2.88550400	0.05348900	-0.03427000
H	-4.95376800	-2.98589900	0.85593400	Cl	3.22748000	3.90917200	0.39942000
C	-6.82489400	-2.73360800	2.90051700	Cl	5.39029100	1.16954500	-0.09519200
H	-4.70870600	-2.71877400	3.34803700	C	-0.11972400	2.73709200	1.76217700
H	-5.42537200	-1.12030800	3.24258400	C	0.35231400	2.52547400	0.45074500
H	-7.14112200	-2.80270900	3.94676500	C	-0.29414700	3.04440100	-0.68929000
H	-7.57105900	-2.13492800	2.36551500	C	-1.46532000	3.78397500	-0.48113900
H	-6.84894300	-3.74479300	2.47822100	C	-1.96362300	4.00022700	0.80074500
C	-2.98280100	-1.24158700	-0.18798200	C	-1.29523700	3.48442600	1.90808300
C	-3.53024900	-0.48889900	-1.17258700	H	-1.99404500	4.19330400	-1.33620200
C	-4.70806000	0.39511200	-1.21087900	H	-2.87487300	4.57526400	0.93725100
C	-5.30357100	0.62380800	-2.46952500	H	-1.69060000	3.66394900	2.90313300
C	-5.25180900	1.07818900	-0.10384300	C	3.70404400	-2.06912700	0.89365100
C	-6.40747600	1.46148300	-2.61440900	C	4.14923900	-3.37759000	0.66619500
H	-4.88884100	0.12667300	-3.34288100	C	4.26620600	-3.88518600	-0.62513200
C	-6.34872800	1.92729300	-0.24983400	C	3.94621800	-3.08955100	-1.72192200
H	-4.80391600	0.96677700	0.87588400	C	3.49385300	-1.77411000	-1.55693200
C	-6.93935200	2.11779500	-1.50158300	C	3.37300500	-1.29444600	-0.23684000
H	-6.84834400	1.60716400	-3.59670600	H	4.40915700	-4.00565000	1.51248300
H	-6.74224900	2.44495500	0.62074700	H	4.61327500	-4.90308800	-0.77740900
H	-7.79718600	2.77523600	-1.60929100	H	4.04911000	-3.49442200	-2.72386200
H	-3.01346400	-0.54908700	-2.12727600	C	0.59426100	2.20517500	3.00140400
C	-0.20319500	-4.00571000	-0.84803900	H	1.46608500	1.63160700	2.67502900
C	-1.64001000	-3.54992800	-0.53689500	C	-0.30295600	1.24414700	3.80515600
H	0.13323400	-3.63234200	-1.81604300	H	0.24538200	0.85082000	4.66781000
H	0.49062400	-3.63997100	-0.08207600	H	-1.19721500	1.75150900	4.18238800

H	-0.62426900	0.39911100	3.18881000	H	2.71887600	0.84880400	-1.15417000
C	1.10724500	3.35754200	3.88787100	C	5.05591200	2.06052400	-2.06096300
H	1.66117800	2.95759800	4.74379000	H	5.63868700	0.03128300	-1.59090200
H	1.77399900	4.02334300	3.33134300	H	4.40735700	0.15119200	-2.83153400
H	0.27958300	3.95913800	4.27831800	C	6.12254500	2.30860000	-3.13260300
C	0.22729100	2.84208800	-2.10878500	H	4.13731900	2.60308200	-2.32308600
H	1.14672900	2.25229300	-2.05474500	H	5.39311800	2.48175900	-1.10388200
C	-0.77222000	2.04633500	-2.97093100	H	6.33764300	3.37663800	-3.24489800
H	-0.97763200	1.06441700	-2.53541500	H	7.06264700	1.80494100	-2.87928400
H	-1.72277500	2.58103400	-3.07398200	H	5.79858000	1.92958800	-4.10880400
H	-0.36330600	1.89891000	-3.97663200	C	3.25473300	-1.10010600	-0.51670300
C	0.58675500	4.18770800	-2.77001500	C	3.56107500	-1.72990700	0.63904400
H	1.01593100	4.01620100	-3.76283500	C	4.38830100	-1.28718100	1.77746300
H	-0.29792400	4.82080300	-2.89582500	C	4.04682900	-1.74004900	3.06922800
H	1.31707300	4.74424600	-2.17439100	C	5.53783900	-0.48086900	1.65717100
C	3.60999300	-1.54288500	2.32296900	C	4.78775200	-1.37148300	4.19053800
C	3.16887000	-0.92802100	-2.78417800	H	3.17974000	-2.38561800	3.18623600
C	4.99175000	-1.52542300	3.00668200	C	6.28231300	-0.11269800	2.77897100
H	4.91117900	-1.08924100	4.00794900	H	5.87169600	-0.16553700	0.67503200
H	5.39675000	-2.53694500	3.11657000	C	5.90925700	-0.54850300	4.05230900
H	5.71361300	-0.93443100	2.43485200	H	4.49299400	-1.73068500	5.17293800
C	4.41462800	-0.72425900	-3.66940600	H	7.16633600	0.50704200	2.65413300
H	5.23747300	-0.27343500	-3.10592900	H	6.49235100	-0.26333900	4.92328500
H	4.77076800	-1.67333100	-4.08406800	H	3.08228900	-2.69149700	0.80662300
H	4.17539400	-0.06408300	-4.50979500	C	1.82455600	-3.40652400	-3.37442600
C	2.58973100	-2.34272700	3.15575300	C	2.84849200	-3.04447700	-2.27818300
H	2.88817600	-3.39182400	3.25567000	H	0.85700300	-3.65484600	-2.93261300
H	2.51331800	-1.92091700	4.16369800	H	1.67622600	-2.56829300	-4.06678900
H	1.59803400	-2.31125600	2.69508700	H	2.17132700	-4.26590100	-3.96103100
H	3.25323000	-0.50998300	2.28558000	C	4.20030900	-2.75158400	-2.95245200
Cu	0.06376800	-0.80145400	0.11139700	C	3.00452500	-4.25854300	-1.34370400
H	-0.87334800	-1.73487800	0.98240100	H	4.96693600	-2.47628600	-2.22129200
C	2.00169300	-1.52689800	-3.59338200	H	4.55648100	-3.63763500	-3.49180100
H	1.76788200	-0.87992600	-4.44617700	H	4.11832400	-1.93704100	-3.68127800
H	2.25956900	-2.51507100	-3.99050400	H	3.18930700	-5.16504200	-1.93295300
H	1.10146600	-1.62550900	-2.97983200	H	3.84656100	-4.14029800	-0.65597200
H	2.84929800	0.06069300	-2.44330100	H	2.09480900	-4.41309300	-0.75692900
108				C	2.29852800	-1.76464200	-1.53552800
C	3.63176300	0.33959000	-0.81032600	O	1.05300500	-2.06320000	-0.95627500
C	4.72551500	0.57422300	-1.87143800	C	-1.62387800	0.28034400	0.05372100
H	3.92997000	0.84248200	0.11543000	C	-3.68613600	1.00139500	0.67396200

C	-2.87015800	2.08944600	0.62747700	H	0.80561800	3.82773400	3.74406100
N	-1.61023200	1.63453500	0.24595200	H	-0.91830300	3.85501500	3.34119600
N	-2.91124400	-0.09933600	0.32062700	C	-3.99064500	-1.01812200	-2.24894900
Cl	-3.23468000	3.72785400	0.95461400	C	-2.78261000	-1.79966100	2.70798400
Cl	-5.34585800	0.90935400	1.07518400	C	-5.44557000	-0.85938200	-2.73259100
C	-0.21945200	3.04289500	-1.20730200	H	-5.48590200	-0.17365900	-3.58544900
C	-0.44804500	2.48001500	0.06451500	H	-5.86807900	-1.81637300	-3.05625800
C	0.39294100	2.71712500	1.17053300	H	-6.08759300	-0.45795000	-1.94247300
C	1.50129700	3.54869100	0.96633700	C	-3.83967500	-1.90871000	3.82429800
C	1.75599300	4.11809800	-0.27842800	H	-4.75067300	-1.35976400	3.56659700
C	0.90505700	3.86549500	-1.35151500	H	-4.11671000	-2.95077000	4.01527800
H	2.17282600	3.75087200	1.79470300	H	-3.44488400	-1.49465200	4.75796900
H	2.62074900	4.76117200	-0.41293300	C	-3.08346100	-1.54301500	-3.37894900
H	1.11315600	4.31635000	-2.31677000	H	-3.39989300	-2.53588500	-3.71567900
C	-3.90527600	-1.90656900	-1.01157300	H	-3.12548500	-0.86866000	-4.24099300
C	-4.34741000	-3.23359600	-1.08124000	H	-2.04234600	-1.61399000	-3.04909200
C	-4.28772200	-4.07250600	0.02835900	H	-3.62884600	-0.02077000	-1.98328400
C	-3.78625600	-3.59960300	1.23813000	Cu	-0.20926400	-0.84687900	-0.46442400
C	-3.32846800	-2.28234300	1.36784200	H	2.18085500	-1.02107600	-2.34772300
C	-3.39385400	-1.46161800	0.22421600	C	-1.49207900	-2.55162400	3.08819300
H	-4.74256900	-3.61403800	-2.01797100	H	-1.09092000	-2.16271400	4.03022000
H	-4.63546800	-5.09846500	-0.04938400	H	-1.67994600	-3.62238600	3.22098400
H	-3.74719900	-4.26359300	2.09592800	H	-0.72537400	-2.43679000	2.31561600
C	-1.12948800	2.79310800	-2.40616100	H	-2.52362300	-0.74157900	2.61107100
H	-1.95612600	2.15398300	-2.08338000	109			
C	-0.38425800	2.04041400	-3.52594900	C	-1.01467400	3.81193300	0.04500200
H	-1.06387400	1.83251600	-4.35914200	C	-1.05320900	5.14974600	0.81084200
H	0.45146900	2.63133600	-3.91538900	H	-1.31292000	3.99683800	-0.99256200
H	0.01458500	1.08767800	-3.16384100	H	0.03466000	3.48220500	0.00704700
C	-1.74481300	4.10422200	-2.93359800	C	-0.22001800	6.24177000	0.12679300
H	-2.43627600	3.89149400	-3.75558800	H	-2.09233700	5.49249000	0.91102300
H	-2.29856000	4.62913500	-2.14923300	H	-0.68406400	5.00402200	1.83293200
H	-0.97517200	4.78350500	-3.31481300	C	-0.23722300	7.57563500	0.88046100
C	0.14831400	2.11088600	2.54867300	H	0.81586000	5.89035500	0.02424200
H	-0.76111400	1.50535200	2.50056500	H	-0.59162100	6.39444500	-0.89593300
C	1.29920300	1.17149000	2.95859900	H	0.36407300	8.33403700	0.36769400
H	1.45358400	0.38067900	2.21853400	H	-1.25762000	7.96579800	0.97094200
H	2.24184200	1.71820100	3.06659800	H	0.16324000	7.46294000	1.89464000
H	1.07631900	0.70062400	3.92195000	C	-1.82317700	2.66195300	0.61463800
C	-0.08338300	3.20178800	3.61290300	C	-2.95172700	2.18378000	0.04526200
H	-0.31103300	2.74172500	4.58020800	C	-3.73115300	2.67709900	-1.10469300

C	-4.44689800	1.73489500	-1.87443100	H	4.44094700	3.66083200	2.16332200
C	-3.85678800	4.03502400	-1.46125600	C	1.53824600	-3.81283300	0.74821100
C	-5.20829000	2.12426400	-2.97510400	C	0.61845900	-4.86667400	0.81890300
H	-4.40304700	0.68451300	-1.59706400	C	-0.23145300	-5.15399400	-0.24598500
C	-4.62242700	4.42533600	-2.56119300	C	-0.18194500	-4.38931900	-1.40861400
H	-3.38043600	4.79661200	-0.85436000	C	0.71543400	-3.32144200	-1.53628400
C	-5.29529200	3.47368800	-3.33043800	C	1.55957400	-3.05471400	-0.43955900
H	-5.73873200	1.37286000	-3.55391600	H	0.56932000	-5.47065400	1.71960500
H	-4.70295100	5.48046100	-2.80930200	H	-0.93421700	-5.97882400	-0.17037700
H	-5.89173600	3.78003000	-4.18514700	H	-0.84967500	-4.62494000	-2.23139400
H	-3.32722200	1.24392000	0.44155800	C	4.32156900	0.94908100	2.16765500
C	-1.04214900	1.26737900	4.21747200	H	4.18583300	-0.07782000	1.81676400
C	-1.96191000	1.89837000	3.15135900	C	3.37403100	1.14796300	3.36678200
H	-0.82159700	0.22626100	3.97100200	H	3.62042100	0.43878100	4.16419800
H	-0.09055500	1.80912100	4.28846400	H	3.46030100	2.15849000	3.78017100
H	-1.51710200	1.29700600	5.20570700	H	2.33063300	0.98717500	3.07752200
C	-2.29596800	3.33639300	3.58556700	C	5.79603200	1.09212800	2.59390800
C	-3.26166200	1.07457500	3.08986300	H	6.03496900	0.36031900	3.37263700
H	-2.93343200	3.84114200	2.85286800	H	6.47288400	0.92519400	1.75031400
H	-2.82741900	3.33202600	4.54503100	H	6.00281400	2.08800900	2.99967100
H	-1.38927400	3.93818600	3.71799600	C	2.77614300	1.84634500	-2.67485600
H	-3.66727800	0.93872800	4.10019000	H	2.77034500	0.75281800	-2.67180900
H	-4.03386800	1.56823300	2.49359000	C	1.33540800	2.30702300	-2.97038400
H	-3.07187200	0.08669500	2.66096300	H	0.64057100	1.95469900	-2.20220200
C	-1.16807500	1.89369600	1.78669400	H	1.26720500	3.39933000	-3.01180300
O	-0.87418900	0.56963500	1.41564300	H	1.00368100	1.91470100	-3.93759100
C	2.22278300	-0.66544900	-0.17984900	C	3.74104200	2.29249700	-3.79084000
C	3.79685200	-2.06283400	-1.03303200	H	3.41856200	1.88053400	-4.75276100
C	4.34506700	-0.81877900	-0.97520900	H	3.76523800	3.38281800	-3.88909300
N	3.37054200	0.02780300	-0.45379800	H	4.76175600	1.94847200	-3.59803600
N	2.49783400	-1.95586100	-0.54247100	C	2.45552900	-3.53013000	1.93388500
Cl	5.91199200	-0.30442000	-1.42736200	C	0.73961400	-2.50389200	-2.82358100
Cl	4.49122900	-3.52607200	-1.58185200	C	3.35496900	-4.73933600	2.25731900
C	3.97776700	1.89633900	1.02210500	H	4.04367900	-4.48825700	3.07077400
C	3.53302400	1.45075100	-0.23896300	H	2.76527600	-5.60475800	2.57746800
C	3.24181800	2.32715100	-1.30371300	H	3.94898500	-5.03918400	1.38851300
C	3.39166100	3.69914400	-1.06402200	C	1.07269000	-3.37991000	-4.04683000
C	3.81563800	4.17205000	0.17539500	H	2.02323400	-3.90599700	-3.91431300
C	4.10610300	3.27932300	1.20387900	H	0.29535200	-4.12951000	-4.22828500
H	3.17346800	4.40465200	-1.85960200	H	1.14924600	-2.75829800	-4.94504500
H	3.92509800	5.24024000	0.33858700	C	1.64850500	-3.08987200	3.17098300

H	0.97171800	-3.88213300	3.50850900	C	3.12875600	-3.74069400	4.89900600
H	2.32526900	-2.85282500	3.99888700	H	1.77528100	-3.67337000	3.21338800
H	1.04742000	-2.20151800	2.95373000	H	3.41294800	-4.14426700	2.79299400
H	3.11489400	-2.69924800	1.66779600	H	2.90267000	-4.77996500	5.16025200
Cu	0.64695600	0.01378000	0.58896500	H	4.18482900	-3.56162800	5.13185400
H	-0.24152900	2.45238100	2.01965000	H	2.53282600	-3.09526200	5.55459600
C	-0.58510600	-1.74261300	-3.02586400	C	3.21753500	-0.40613500	0.92806500
H	-0.53074600	-1.12290400	-3.92729800	C	4.25899500	-0.27568600	0.08014800
H	-1.42776100	-2.43197100	-3.14447400	C	5.23020000	-1.29583000	-0.36636300
H	-0.80083100	-1.09063700	-2.17395800	C	5.61789700	-1.30093000	-1.72249900
H	1.53074900	-1.75355700	-2.73883900	C	5.83218800	-2.24090400	0.48591100
Si	-4.55173800	-2.88778400	-0.11920000	C	6.53765600	-2.22699500	-2.21186600
H	-3.21366400	-2.37616100	-0.50362900	H	5.17227100	-0.57546700	-2.39791700
O	-4.79930200	-2.74958200	1.52266200	C	6.75768300	-3.16579400	-0.00150700
O	-5.61636100	-1.85481100	-0.86494400	H	5.59653200	-2.23318100	1.54453000
C	-7.03992200	-1.92159000	-0.71676900	C	7.11173300	-3.16808600	-1.35229400
C	-7.69468100	-1.04536800	-1.77248100	H	6.80867400	-2.21311400	-3.26411300
H	-7.31639800	-1.57956000	0.28853100	H	7.21040700	-3.88083300	0.68024300
H	-7.38530600	-2.95992300	-0.81952700	H	7.83306800	-3.88752600	-1.72916000
H	-8.78353300	-1.06269900	-1.65859900	H	4.34232500	0.67641900	-0.43158800
H	-7.35251400	-0.01049500	-1.67706300	C	1.59431100	2.92619900	2.30856800
H	-7.44647200	-1.39981600	-2.77784600	C	2.77724400	1.97086900	2.04624600
C	-3.98511400	-3.39694200	2.50533100	H	1.23686600	3.37478900	1.38074500
C	-4.44252700	-2.97129800	3.89149900	H	0.75854600	2.39599300	2.78180200
H	-2.93060000	-3.12591100	2.35609700	H	1.90478600	3.72699300	2.99080200
H	-4.06557100	-4.48831700	2.40003000	C	3.24528000	1.41438500	3.40826300
H	-3.83740400	-3.46477500	4.65914400	C	3.94647400	2.76672100	1.44275300
H	-4.34101400	-1.88895300	4.01281800	H	4.09361300	0.73187500	3.30208700
H	-5.49121100	-3.24103500	4.05077100	H	3.56334500	2.24159000	4.05283000
C	-4.78235900	-4.66271100	-0.68239400	H	2.44032000	0.88443400	3.92929900
H	-4.62770400	-4.74544800	-1.76361500	H	4.22332500	3.57651700	2.12917000
H	-4.05922700	-5.32410000	-0.19178400	H	4.82914800	2.13586600	1.30237300
H	-5.78448000	-5.03976100	-0.45249900	H	3.68603300	3.19655700	0.47730100
TS41				C	2.25147300	0.76855200	1.17957100
C	2.81452800	-1.74564300	1.52590600	O	1.52683700	1.13569300	-0.03496100
C	3.14149700	-2.01175000	3.01042500	C	-2.03566500	-0.38083500	-0.11930000
H	3.27217300	-2.54557700	0.93392900	C	-3.92661700	-1.59729000	-0.47000700
H	1.72841300	-1.85613400	1.39814700	C	-4.13327400	-0.83609500	0.63681400
C	2.83200300	-3.45682400	3.42282400	N	-2.96927500	-0.10120200	0.84601900
H	4.20169900	-1.79911000	3.20232500	N	-2.64343100	-1.30892300	-0.92740500
H	2.57680100	-1.32658800	3.65205900	Cl	-5.52334300	-0.73418800	1.62862100

Cl	-4.98427900	-2.71445000	-1.21836700	C	-4.52170400	-0.28386200	-4.31205300
C	-3.07990000	2.21741600	1.65016800	H	-5.19011600	0.58347700	-4.32501700
C	-2.79457000	0.86140900	1.91425800	H	-4.25480100	-0.51337600	-5.34904900
C	-2.38048500	0.39857100	3.17994600	H	-5.07720100	-1.13646000	-3.91061700
C	-2.22279400	1.35361900	4.19239500	C	-1.82268300	-5.09872400	-0.75062200
C	-2.47649300	2.70245900	3.95720200	H	-2.89614800	-4.93331400	-0.88052200
C	-2.90472600	3.12564800	2.70201400	H	-1.48607200	-5.76564300	-1.55176600
H	-1.90108600	1.03542400	5.17914900	H	-1.66997900	-5.61589100	0.20274600
H	-2.34805200	3.42515800	4.75771200	C	-2.52353000	1.25359000	-4.02178300
H	-3.11352000	4.17762200	2.53540300	H	-2.17297800	1.08076300	-5.04491300
C	-2.35745100	-1.19390200	-3.36302700	H	-3.19142000	2.12153900	-4.04186600
C	-1.78457900	-1.72394500	-4.52583600	H	-1.65634200	1.50063600	-3.40416800
C	-0.98227300	-2.86061200	-4.48146100	H	-3.61242800	0.28626100	-2.46139600
C	-0.74314200	-3.50056700	-3.26870300	Cu	-0.34888700	0.46155700	-0.38237000
C	-1.28310200	-3.01357800	-2.07128400	H	1.45416600	0.35115500	1.80809700
C	-2.07243100	-1.84809400	-2.14583200	C	0.46202300	-4.02336000	-0.52363300
H	-1.97557000	-1.24163400	-5.47926700	H	0.60894000	-4.47792300	0.46155700
H	-0.54957200	-3.25465300	-5.39641600	H	0.88602100	-4.70715600	-1.26633300
H	-0.13037400	-4.39589200	-3.25014200	H	1.03331500	-3.09211700	-0.55807200
C	-3.60670600	2.71331300	0.30673700	H	-1.40286400	-3.15784000	0.05764100
H	-3.57651500	1.88104900	-0.40155200	Si	1.58472700	2.21827200	-1.58221100
C	-2.73615800	3.83875100	-0.28264000	H	0.22254100	1.41682900	-1.73339100
H	-3.11529100	4.12102400	-1.27084300	O	1.06510900	3.67895300	-0.89143700
H	-2.75936000	4.73567600	0.34559500	O	3.30134600	2.15805700	-1.55417900
H	-1.69266200	3.53080900	-0.39246100	C	4.16433500	2.70610000	-2.54350800
C	-5.07782400	3.16195500	0.42824600	C	5.60293000	2.73521100	-2.03658000
H	-5.46162500	3.46798700	-0.55076700	H	3.86466100	3.72910300	-2.80903200
H	-5.71463400	2.35679500	0.80738400	H	4.11277700	2.11236200	-3.46732000
H	-5.17548100	4.01578600	1.10742800	H	6.25723000	3.17095300	-2.80013100
C	-2.12118100	-1.07367100	3.48732600	H	5.68562800	3.33953900	-1.12850200
H	-2.30349900	-1.65289800	2.57757300	H	5.96993100	1.72940800	-1.81146300
C	-0.65651200	-1.31807000	3.89384600	C	1.60621900	4.93924700	-1.26532900
H	0.03110400	-0.98348900	3.11232300	C	0.74929800	6.05786300	-0.68779600
H	-0.40255800	-0.78706700	4.81734400	H	1.64858400	5.03631700	-2.36022300
H	-0.48519100	-2.38596500	4.06571600	H	2.63699800	5.03416500	-0.89183300
C	-3.08352500	-1.60231700	4.57018100	H	1.16782000	7.03567400	-0.95061000
H	-2.91577800	-2.67230900	4.73194500	H	-0.27218900	6.00386800	-1.07721000
H	-2.92600400	-1.09300900	5.52675700	H	0.70324100	5.98491000	0.40335800
H	-4.12894400	-1.46128900	4.28132000	C	1.38217800	2.47307900	-3.50050400
C	-3.26965200	0.02599600	-3.46679500	H	1.56059900	1.51408100	-4.00758800
C	-1.03632000	-3.77148500	-0.77055200	H	0.33742100	2.74161600	-3.69623700

H	2.01925000	3.21841000	-3.98890100	H	5.30045300	-2.42109200	-2.52983900
110				C	4.44390300	-0.37593000	-0.83261900
C	5.35132100	1.90326100	0.00690500	O	4.75797500	-1.61349500	-0.16190100
C	4.59272300	3.00217400	-0.76289900	C	-3.86081200	0.05901800	-0.03020700
H	6.29737000	2.32141200	0.36499300	C	-6.06739800	0.54494900	0.19687200
H	4.76958000	1.65242200	0.90487200	C	-5.97712200	-0.71175500	-0.31966200
C	4.42409000	4.28201000	0.06670300	N	-4.62101300	-0.99554200	-0.45233400
H	5.12328200	3.23982700	-1.69529000	N	-4.76449500	1.00376100	0.36788700
H	3.60287200	2.63799700	-1.06145800	Cl	-7.22729900	-1.79667600	-0.74996500
C	3.65981600	5.38353000	-0.67490500	Cl	-7.46042000	1.45606200	0.58970700
H	3.90093400	4.03809700	1.00124600	C	-3.82517400	-3.28640500	-0.06138000
H	5.41418500	4.65629500	0.36116900	C	-4.07603800	-2.23587900	-0.96635300
H	3.55768400	6.28335000	-0.05909200	C	-3.81918300	-2.33593200	-2.34833600
H	4.17500500	5.66943300	-1.59932000	C	-3.27174900	-3.53848600	-2.81280000
H	2.65192800	5.05031500	-0.94777600	C	-3.00269700	-4.59161800	-1.94266600
C	5.62780600	0.59624700	-0.71188300	C	-3.27961100	-4.46584800	-0.58392800
C	6.86134700	0.18427600	-1.07469200	H	-3.05333300	-3.64979900	-3.87018800
C	8.14962600	0.90069300	-1.01923600	H	-2.57751300	-5.51487800	-2.32526300
C	9.31780900	0.16074800	-0.74632800	H	-3.06783000	-5.29539200	0.08341900
C	8.29354100	2.27781600	-1.27650800	C	-4.21326400	2.44494100	2.27988500
C	10.56822800	0.77342000	-0.69146700	C	-3.84727400	3.71134200	2.75309500
H	9.23371100	-0.90809900	-0.56608900	C	-3.68184600	4.78606700	1.88349500
C	9.54578500	2.89183300	-1.22587000	C	-3.88152100	4.61728900	0.51595500
H	7.42437800	2.86590800	-1.55018900	C	-4.24856000	3.37458000	-0.01538700
C	10.68811200	2.14605300	-0.92680400	C	-4.40135400	2.30556100	0.89013300
H	11.45040800	0.17934000	-0.46924000	H	-3.68745600	3.85555500	3.81699600
H	9.62947400	3.95519100	-1.43306700	H	-3.39643000	5.75884200	2.27312600
H	11.66194400	2.62569900	-0.89038300	H	-3.74872500	5.46221600	-0.15244900
H	6.95418500	-0.84855200	-1.40125500	C	-4.11102300	-3.18288200	1.43354600
C	2.65359100	-1.57752400	-2.12395200	H	-4.58474200	-2.21607300	1.62617100
C	3.93582600	-0.73109100	-2.27320100	C	-2.80693600	-3.22331600	2.25396700
H	2.85906800	-2.52237800	-1.61490200	H	-3.02611100	-3.10277700	3.32026300
H	1.88722400	-1.04123600	-1.55211200	H	-2.28577200	-4.17781700	2.12482400
H	2.23421600	-1.80612900	-3.11005700	H	-2.12420300	-2.42289900	1.95172600
C	3.58574200	0.55429900	-3.04395500	C	-5.09656400	-4.27139000	1.90126800
C	4.96759600	-1.53840000	-3.08306300	H	-5.33112800	-4.13506800	2.96212500
H	4.45863900	1.20130000	-3.17187600	H	-6.03339300	-4.23030400	1.33710200
H	3.21003600	0.29806000	-4.04078300	H	-4.67452100	-5.27470800	1.78189800
H	2.80305100	1.12842300	-2.53661500	C	-4.09902900	-1.20327900	-3.33100800
H	4.51270000	-1.87865800	-4.02007800	H	-4.59167600	-0.39149200	-2.78836600
H	5.84373000	-0.93826500	-3.34271400	C	-2.78814400	-0.63583200	-3.91040800

H	-2.12428100	-0.28339000	-3.11434200
H	-2.24914200	-1.39433400	-4.48805500
H	-3.00083600	0.20608200	-4.57778200
C	-5.05831300	-1.64592000	-4.45289600
H	-5.29316300	-0.79685800	-5.10331800
H	-4.61411800	-2.42787100	-5.07756300
H	-5.99732500	-2.03282700	-4.04505300
C	-4.37934500	1.29053700	3.26316100
C	-4.45369300	3.22932500	-1.52008600
C	-5.47222300	1.58657400	4.30869300
H	-5.61169700	0.71936800	4.96255200
H	-5.20345400	2.43888100	4.94149900
H	-6.43109300	1.81069600	3.83138900
C	-5.57046800	4.15935500	-2.03299800
H	-6.51355100	3.97710900	-1.50863800
H	-5.30871300	5.21413500	-1.89853200
H	-5.73719000	3.99285000	-3.10236700
C	-3.04057700	0.93959200	3.94188000
H	-2.66601600	1.77609400	4.54151200
H	-3.16829100	0.08038500	4.60890000
H	-2.27575800	0.68685100	3.20053500
H	-4.69839300	0.40616200	2.70446700
Cu	-1.92416100	0.19225400	0.00566500
H	3.58979100	0.09703000	-0.32702400
C	-3.13752600	3.46403200	-2.28736600
H	-3.29298900	3.31151600	-3.36071500
H	-2.76906600	4.48549200	-2.14459300
H	-2.35658200	2.77385100	-1.95271700
H	-4.76787600	2.20251900	-1.72716200
Si	4.37171600	-2.00051700	1.40077300
H	-0.40602300	0.30811200	0.04135500
O	5.14611100	-3.42508200	1.74136900
O	4.93420200	-0.75226200	2.34654200
C	4.72605800	-0.67639500	3.76212300
C	5.41822700	0.56355300	4.30486400
H	5.12709400	-1.57630000	4.24802800
H	3.65010400	-0.63482600	3.97968000
H	5.27140100	0.63651900	5.38748400
H	6.49293700	0.52547000	4.10277700
H	5.01237400	1.46692600	3.83939200
C	6.56273400	-3.60973400	1.61466300
C	6.92969300	-5.00014900	2.10709100
H	7.09159500	-2.84501600	2.19854400
H	6.85463600	-3.48433600	0.56445500
H	8.00773600	-5.16517400	2.00969400
H	6.65545900	-5.12367700	3.15941300
H	6.40905400	-5.76586900	1.52377700
C	2.55157900	-2.30781300	1.66300800
H	2.21237100	-3.14833800	1.05011000
H	2.33338000	-2.54491600	2.70941900
H	1.95827300	-1.42989400	1.38701700

111

C	1.01334600	0.42116500	1.87333700
C	0.24971100	-0.88335000	2.19337500
H	0.67343500	1.20176100	2.56512000
H	2.07154000	0.25804700	2.08547400
C	0.39623900	-1.31138700	3.65905400
H	-0.81524100	-0.76640400	1.95603500
H	0.62165400	-1.68066200	1.53752700
C	-0.35024200	-2.60942900	3.98116700
H	1.46171800	-1.43231800	3.89711900
H	0.02864100	-0.50590400	4.30939700
H	-0.23027700	-2.88972700	5.03287700
H	-1.42351100	-2.50764500	3.78350900
H	0.01985500	-3.44063900	3.37037700
C	0.81236100	0.87186900	0.43915100
C	1.70658100	0.69882200	-0.55455000
C	3.09366700	0.18579100	-0.49155700
C	3.53851900	-0.70779700	-1.48424300
C	4.02513100	0.60391400	0.47684300
C	4.84215400	-1.20162200	-1.48279100
H	2.84708500	-1.01952300	-2.26289600
C	5.33144700	0.11383400	0.47795500
H	3.73265000	1.34277800	1.21571500
C	5.74465400	-0.79742800	-0.49598300
H	5.15512500	-1.89849700	-2.25516300
H	6.03143300	0.45551400	1.23522900
H	6.76202400	-1.17725400	-0.49480700
H	1.36238100	0.92963700	-1.56112400
C	-2.08322500	3.46938400	-0.06065000
C	-0.60920800	3.03921900	0.08281200
H	-2.51197000	3.10386700	-0.99694400

H	-2.69147000	3.08384200	0.76553600
H	-2.16303700	4.56199300	-0.05379500
C	-0.05249400	3.62288400	1.39527500
C	0.19534400	3.59808700	-1.10372600
H	1.00766600	3.38754700	1.52898700
H	-0.15053300	4.71372300	1.38770700
H	-0.59970200	3.24965500	2.26857600
H	0.08914000	4.68779800	-1.14392700
H	1.26096000	3.36952000	-1.01388000
H	-0.16492000	3.18810500	-2.05120000
C	-0.56293800	1.47178900	0.13126200
O	-1.08861700	0.97799200	-1.11404200
H	-1.24616700	1.17525000	0.93602100
Si	-2.13881800	-0.28785400	-1.29614700
O	-1.42848600	-1.78485700	-1.18978800
O	-3.18409300	-0.22270800	-0.01303100
C	-4.08173400	-1.27497700	0.36219300
C	-4.77935800	-0.89574300	1.65762700
H	-3.52362200	-2.21061000	0.48447000
H	-4.82246100	-1.43094900	-0.43435500
H	-5.47448300	-1.68599000	1.95902500
H	-4.04993200	-0.75258900	2.46082400
H	-5.34446000	0.03331900	1.53590500
C	-0.48401200	-2.32659100	-2.11804500
C	-0.28899400	-3.80540700	-1.82691700
H	0.46863000	-1.79104900	-2.02072500
H	-0.84038100	-2.18801100	-3.14797200
H	0.44315300	-4.23551300	-2.51794000
H	0.07337100	-3.95111200	-0.80481600
H	-1.23182600	-4.34942300	-1.93913000
C	-2.96568100	-0.04673100	-2.95142000
H	-3.49429600	0.91080300	-2.97937200
H	-2.23603600	-0.04806400	-3.76758500
H	-3.69071700	-0.84250600	-3.14986600
112			
Si	-0.45766600	-0.83205000	0.42365900
O	0.12482900	-2.35003700	0.96152400
O	0.12501700	-0.30606200	-1.10960100
C	-0.36866300	-0.54968000	-2.40992200
C	0.23614300	-1.80681600	-3.03174800
H	-0.10013600	0.32007200	-3.02948100
H	-1.45656400	-0.63683600	-2.40934500
H	-0.12057800	-1.94245400	-4.05999800
H	1.32960600	-1.74354600	-3.05782800
H	-0.04096200	-2.69271400	-2.45239900
C	-0.63677800	-3.50236300	1.25597200
C	0.02209300	-4.27131900	2.39785400
H	-0.70763500	-4.15255600	0.37189900
H	-1.66492100	-3.24539600	1.53603400
H	-0.54144900	-5.18298900	2.62792700
H	1.04559000	-4.56015700	2.13604100
H	0.06691500	-3.65674400	3.30315000
C	-1.28232700	0.24682100	1.76460400
H	-1.60168700	1.20995800	1.35139400
H	-2.16967300	-0.22184200	2.19682900
H	-0.57299900	0.44823500	2.57081000
N	4.32502600	-0.18675800	0.42454300
C	3.98188800	0.43905800	1.78683500
C	4.71559400	1.70615900	2.22482500
H	4.20216700	-0.34621800	2.51447100
H	2.89881300	0.56960100	1.76524500
C	4.19016200	2.14763100	3.60222100
H	5.79239800	1.52115600	2.30489300
H	4.57875300	2.52491500	1.51539300
C	4.90414700	3.39587300	4.12825400
H	3.11243200	2.34029600	3.53332200
H	4.31099000	1.32546000	4.31941100
H	4.51137500	3.68977600	5.10636100
H	5.98012700	3.22105600	4.23910700
H	4.77281100	4.24403700	3.44741000
C	3.81157600	-1.64179800	0.54565300
C	3.83731500	-2.49385700	-0.72212300
H	2.78478600	-1.54260700	0.90363500
H	4.43173700	-2.10022400	1.32077400
C	3.37132200	-3.92249600	-0.39049900
H	3.16668600	-2.07577500	-1.47805300
H	4.83824500	-2.54270500	-1.16638400
C	3.34986400	-4.83099600	-1.62276300
H	4.03195100	-4.35445400	0.37281900
H	2.36995600	-3.87013900	0.05095800
H	3.01492200	-5.83948500	-1.36093000
H	2.66922900	-4.44223700	-2.38788900

H	4.34532200	-4.91636000	-2.07319700
C	3.53709600	0.45678300	-0.72776200
C	3.39577300	1.97796900	-0.76161500
H	2.53268400	0.03735100	-0.64819200
H	4.01121200	0.09665700	-1.64306800
C	2.58980400	2.37892400	-2.00993700
H	2.85066200	2.31822700	0.12399300
H	4.36039800	2.49238400	-0.77642900
C	2.36701800	3.89114700	-2.10045000
H	3.11518200	2.03136400	-2.90962300
H	1.62549100	1.85877200	-1.98790800
H	1.79474600	4.15167600	-2.99630900
H	1.81219700	4.26146000	-1.23152700
H	3.31896700	4.43257200	-2.14367100
C	8.78724100	1.80952100	-1.27148000
C	8.03519900	0.66186800	-0.59163400
H	9.85468600	1.58412500	-1.35489900
H	8.40385100	1.99059400	-2.28158000
H	8.68562300	2.74128300	-0.70449600
C	6.52971500	0.94683100	-0.45405500
H	8.18090400	-0.26274500	-1.16505500
H	8.46364200	0.47903000	0.40215200
C	5.83259300	-0.25178100	0.18954000
H	6.39207200	1.85891500	0.13091300
H	6.11461600	1.13334100	-1.44996800
H	5.99871700	-1.11905100	-0.44876500
H	6.27164100	-0.47876700	1.16452000
F	1.09878000	-0.18708000	0.98113500
C	-4.74252700	0.37525200	1.35676700
C	-6.27976000	0.21146200	1.37382700
H	-4.51952700	1.42797400	1.57096700
H	-4.34638300	-0.19191600	2.20826500
C	-6.92449500	0.95172600	2.55361900
H	-6.71505700	0.57494600	0.43362800
H	-6.54432000	-0.84818800	1.43588900
C	-8.44349100	0.76848600	2.62316800
H	-6.46939900	0.60137800	3.49013100
H	-6.68695800	2.02231400	2.48551600
H	-8.87334300	1.31032700	3.47214800
H	-8.92897400	1.13804400	1.71255700
H	-8.71087900	-0.28871200	2.73308000
C	-3.95788900	-0.02067500	0.11324700
C	-3.63788500	0.85335500	-0.86633200
C	-3.94638200	2.28146600	-1.05293900
C	-3.04730700	3.03631500	-1.83843000
C	-5.06916400	2.95823700	-0.53434100
C	-3.23689600	4.39642000	-2.06688500
H	-2.18038500	2.53727700	-2.26352300
C	-5.26214800	4.32109000	-0.76575900
H	-5.81723000	2.41610400	0.02829700
C	-4.34743800	5.05061200	-1.52652400
H	-2.51930800	4.94653800	-2.66936600
H	-6.14042500	4.81173600	-0.35512700
H	-4.50252700	6.11058200	-1.70527100
H	-2.94525600	0.47652700	-1.61304000
C	-3.48929200	-3.85725700	-0.71230000
C	-4.11511400	-2.45848300	-0.86362900
H	-2.44394400	-3.85174900	-1.02326500
H	-3.53424100	-4.20429900	0.32647500
H	-4.03259000	-4.58378500	-1.32830400
C	-5.59184600	-2.55409800	-0.44414200
C	-4.05683800	-2.06337400	-2.34940500
H	-6.13065800	-1.62268500	-0.63338600
H	-6.09215800	-3.34459500	-1.01551100
H	-5.69573100	-2.80239000	0.61858100
H	-4.59636000	-2.80313200	-2.95309200
H	-4.51841000	-1.08836700	-2.52855300
H	-3.02488300	-2.02787800	-2.70534100
C	-3.32683100	-1.44167000	0.06221600
O	-1.97575900	-1.43894800	-0.32890500
H	-3.43497600	-1.85032100	1.08485500

TS42

Si	-0.20527300	-0.72934700	-1.37779000
O	-0.99021900	-1.73767600	-0.31787900
O	-0.32794000	0.86907700	-0.95538700
C	0.77931800	1.78720100	-0.92162600
C	0.26889500	3.17316700	-0.56673000
H	1.25681800	1.81867800	-1.91155200
H	1.49869900	1.40212800	-0.19533100
H	1.09688600	3.89037300	-0.57275100
H	-0.48385000	3.51713900	-1.28441300
H	-0.17850400	3.18273100	0.43235900

C	-0.38276900	-2.77960300	0.46206600	H	-3.93831000	2.10902400	-0.13403800
C	-0.44945600	-4.11764600	-0.26162400	C	-3.75452200	1.91745200	-2.83719400
H	-0.94598900	-2.83620700	1.40212000	H	-3.99235400	-0.12919100	-2.23194600
H	0.63562900	-2.46986700	0.70336200	H	-5.38915200	0.89337100	-1.86183000
H	-0.02918300	-4.90875000	0.36966900	C	-4.26631600	1.71413800	-4.26583900
H	-1.48290200	-4.38749400	-0.50438500	H	-4.03768400	2.91750600	-2.48304500
H	0.12234100	-4.09103800	-1.19502400	H	-2.65949400	1.87718800	-2.82915600
C	1.32389800	-1.36100200	-2.22997800	H	-3.86975900	2.48188900	-4.93730500
H	2.00619000	-0.53586000	-2.44961000	H	-3.96068800	0.73821400	-4.65806800
H	1.85612900	-2.06259500	-1.58733100	H	-5.36013200	1.76499600	-4.30953200
H	1.06088900	-1.85380500	-3.17210100	C	-8.89085000	2.15673900	0.77782100
N	-4.11710300	0.16857300	0.67485600	C	-7.69270300	1.57867800	1.53606500
C	-4.22315800	-1.30376800	0.24192900	H	-9.69255800	2.43741700	1.46736100
C	-5.51476200	-1.80506700	-0.40242300	H	-8.60747600	3.05117200	0.21241400
H	-4.06272900	-1.87189300	1.16130700	H	-9.29976500	1.42945500	0.06797000
H	-3.35507800	-1.48114600	-0.39563900	C	-6.54476900	1.17372300	0.59536200
C	-5.36365200	-3.29761700	-0.74869000	H	-7.32728700	2.31631000	2.26203300
H	-6.35861800	-1.69129000	0.28609400	H	-8.01201000	0.70470800	2.11800700
H	-5.75971700	-1.25565400	-1.31367500	C	-5.36792400	0.64252700	1.41422500
C	-6.63299500	-3.88219300	-1.37451800	H	-6.91321200	0.43117100	-0.11562100
H	-4.52004400	-3.42662900	-1.43810700	H	-6.23752900	2.05179700	0.01786200
H	-5.10959900	-3.85931200	0.15949300	H	-5.03254400	1.43672400	2.08134800
H	-6.50008700	-4.94190500	-1.61216000	H	-5.67616500	-0.20008300	2.03890700
H	-7.48710400	-3.79687300	-0.69366600	F	-1.35456700	-0.74096400	-2.56660500
H	-6.89272900	-3.36187400	-2.30281200	C	4.79151200	-1.09875200	-0.79768200
C	-2.94751700	0.16811200	1.68930400	C	5.96323100	-1.96840800	-0.29841700
C	-2.45193500	1.51807100	2.20280700	H	5.16775500	-0.42874100	-1.58030900
H	-2.13789600	-0.35587400	1.17682400	H	4.07417400	-1.76955200	-1.28795000
H	-3.29096400	-0.44644800	2.52508800	C	6.70030900	-2.67909400	-1.44111600
C	-1.19096400	1.29877900	3.05990800	H	6.67571000	-1.35097700	0.26560800
H	-2.19798800	2.18549900	1.37500700	H	5.59111800	-2.71797800	0.40896500
H	-3.21380100	2.02286200	2.80785400	C	7.85739200	-3.55888400	-0.95761100
C	-0.68056000	2.59766600	3.68968500	H	5.98429000	-3.29278500	-2.00493400
H	-1.41077900	0.57262300	3.85374500	H	7.08061900	-1.93073600	-2.15002400
H	-0.40659800	0.85323700	2.43604500	H	8.36214500	-4.05441500	-1.79376700
H	0.22395200	2.41555300	4.27770100	H	8.60713800	-2.96658000	-0.42047500
H	-0.43286400	3.34084300	2.92362400	H	7.50255600	-4.33850500	-0.27365700
H	-1.43018200	3.04161900	4.35449400	C	4.02838900	-0.30300000	0.24518500
C	-3.70643900	1.09883400	-0.47673300	C	4.18578000	1.03054000	0.41050600
C	-4.29659200	0.85518400	-1.86496600	C	5.10227800	1.99123400	-0.22962200
H	-2.62083200	1.01447500	-0.54989400	C	4.68526900	3.33685700	-0.33099400

C	6.39325300	1.68599800	-0.70943400	C	2.75945300	1.63598300	-0.87888100
C	5.48810600	4.31354400	-0.91488200	C	2.84600900	2.82567900	0.07581600
H	3.70618800	3.60949100	0.05538600	H	1.77864900	1.62497100	-1.36980300
C	7.19954500	2.66324300	-1.29466000	H	3.56132000	1.68919700	-1.62088500
H	6.78621000	0.68306500	-0.59503500	C	2.85983000	4.13548300	-0.73170300
C	6.75259800	3.98100700	-1.40889700	H	1.98332900	2.83559000	0.74845900
H	5.12848600	5.33693100	-0.98224600	H	3.74442100	2.79299800	0.70420200
H	8.19026100	2.39348300	-1.65104600	C	2.89056200	5.37727900	0.16363900
H	7.38424200	4.73946300	-1.86213400	H	3.73067100	4.14204800	-1.40005800
H	3.47410200	1.51099100	1.07703000	H	1.97380000	4.16987700	-1.37773200
C	2.07582200	-2.16077000	3.12289000	H	2.90248300	6.29372900	-0.43448100
C	3.13113900	-1.18147500	2.57713900	H	2.01149700	5.41585200	0.81608800
H	1.07178600	-1.78039600	2.92584200	H	3.78056200	5.38396800	0.80295900
H	2.16434900	-3.14350500	2.64216200	C	1.86065100	0.17164500	0.89313800
H	2.19247500	-2.30704300	4.20455700	C	1.36479800	-1.19283700	1.37025700
C	4.52451900	-1.74670900	2.89587200	H	0.98834700	0.70177100	0.48979200
C	2.95214400	0.16213700	3.30441200	H	2.31727200	0.72816100	1.71470400
H	5.31976600	-1.09049000	2.52827100	C	0.47079700	-1.00514000	2.60743900
H	4.66120500	-1.86087100	3.97940200	H	0.76692000	-1.64847400	0.57455000
H	4.66776300	-2.73635800	2.44557200	H	2.17429400	-1.88345200	1.61969600
H	2.87959800	0.01057900	4.38951800	C	-0.12460400	-2.32449300	3.10696700
H	3.79298400	0.83891700	3.12678700	H	1.05606600	-0.53969600	3.41196000
H	2.03512000	0.64842200	2.95979000	H	-0.34052200	-0.30766500	2.36689400
C	2.87958900	-1.05530200	1.00018200	H	-0.75257600	-2.16347000	3.98866400
O	1.64176300	-0.55501700	0.70754700	H	-0.74712500	-2.79271500	2.33677000
H	3.00176800	-2.12211300	0.66093200	H	0.66046900	-3.03875100	3.38102700
113				C	6.55635000	-2.08625600	2.55528200
N	2.87826500	0.22437400	-0.25734500	C	6.16664200	-1.05784400	1.48977900
C	2.48043400	-0.70645300	-1.41591600	H	7.63689600	-2.08301900	2.72786900
C	2.87027200	-2.18185700	-1.34758100	H	6.06459400	-1.87257300	3.51060600
H	2.96789800	-0.27313700	-2.29384400	H	6.26963900	-3.09930300	2.25262400
H	1.39873500	-0.53379100	-1.51626100	C	4.65224100	-1.03237800	1.22199400
C	2.35133400	-2.90435900	-2.60344300	H	6.49831100	-0.05981900	1.80471000
H	3.95970800	-2.29654100	-1.30592400	H	6.69806000	-1.27792700	0.55485900
H	2.45977100	-2.67519200	-0.46432300	C	4.32702700	0.03405400	0.17591400
C	2.73295200	-4.38714900	-2.62897800	H	4.33051100	-2.02555500	0.89993500
H	1.26007700	-2.80294600	-2.65337800	H	4.13160800	-0.81100400	2.15948700
H	2.74715100	-2.40877800	-3.49952100	H	4.65233100	0.99893700	0.56669700
H	2.35369000	-4.87565700	-3.53188400	H	4.88748200	-0.14678100	-0.74554600
H	3.82077600	-4.51747200	-2.61061700	C	-2.66329400	-1.24246500	-0.57671500
H	2.31987400	-4.91825100	-1.76423300	C	-3.83335900	-1.59916000	-1.51493800

H	-2.86929700	-1.65374900	0.41800400	4b’			
H	-1.76507900	-1.75815400	-0.94767000	H	-1.41369100	-0.38767400	2.45467900
C	-4.10119500	-3.10745600	-1.59106400	C	-0.26837100	1.25731400	-0.62373100
H	-4.74484300	-1.08409500	-1.18083900	C	-0.15028600	2.50822700	0.27528200
H	-3.62323900	-1.21587300	-2.52127900	H	-1.09888200	1.42505100	-1.31862600
C	-5.27000700	-3.46869200	-2.51288900	H	0.63259800	1.16333600	-1.23839500
H	-3.19137000	-3.61777100	-1.93582700	C	0.07231200	3.79845100	-0.52336000
H	-4.29946900	-3.49211700	-0.58104200	H	-1.06170800	2.61031000	0.87974500
H	-5.43657400	-4.55068700	-2.54456700	H	0.67051000	2.37361200	0.99221400
H	-6.20070400	-2.99879500	-2.17453500	C	0.16854700	5.04438500	0.36211900
H	-5.08458500	-3.13036600	-3.53876400	H	0.98912300	3.70047000	-1.12034200
C	-2.32440600	0.23189100	-0.49118700	H	-0.74735400	3.92241000	-1.24391500
C	-2.61689000	0.99970700	0.58276200	H	0.32816400	5.94740300	-0.23602200
C	-3.34925800	0.68598900	1.82430200	H	-0.74896900	5.18827600	0.94398300
C	-2.98409200	1.37177300	3.00345900	H	1.00018000	4.96366200	1.07134500
C	-4.43042200	-0.21444100	1.91727200	C	-0.51468200	-0.01940700	0.15114300
C	-3.63080900	1.14308800	4.21587400	C	0.43282800	-0.91295600	0.50963900
H	-2.17064700	2.09198900	2.95797700	C	1.87977100	-0.95864600	0.22859100
C	-5.08034800	-0.44425400	3.13067700	C	2.48856000	-2.22942800	0.16581400
H	-4.78947700	-0.71626600	1.02628600	C	2.70784300	0.16673400	0.04939900
C	-4.68268000	0.22575100	4.28938500	C	3.84740500	-2.37412800	-0.10289800
H	-3.31618500	1.68403100	5.10444700	H	1.87546000	-3.11333500	0.32178800
H	-5.91264900	-1.14228700	3.16610900	C	4.07048400	0.02281000	-0.21399600
H	-5.19281400	0.04699500	5.23141400	H	2.29706300	1.16377800	0.14698200
H	-2.19383300	2.00060100	0.59098300	C	4.64712600	-1.24552500	-0.29983500
C	-1.03970300	2.15061500	-3.67794000	H	4.28350300	-3.36769700	-0.15439400
C	-1.91536300	2.04346000	-2.41356800	H	4.68521900	0.90915500	-0.34311400
H	0.01629300	2.19539800	-3.39799500	H	5.70798400	-1.35324500	-0.50522200
H	-1.17856700	1.27488600	-4.32483500	H	0.07569300	-1.77814200	1.06489800
H	-1.28945900	3.04317100	-4.26518200	C	-4.29157600	-1.10874400	0.18590200
C	-3.38553900	1.91004000	-2.84185600	C	-2.84699800	-1.13930500	-0.35655500
C	-1.71912700	3.32753000	-1.58744500	H	-4.34040600	-1.50598500	1.20229300
H	-4.05003200	1.83180900	-1.97554800	H	-4.68457000	-0.08519400	0.20170100
H	-3.70583400	2.77761000	-3.43358700	H	-4.95036000	-1.70886900	-0.45129200
H	-3.53832200	1.01838600	-3.46291500	C	-2.84677200	-0.57184100	-1.78732500
H	-1.74047500	4.21804400	-2.22872800	C	-2.35048200	-2.59600300	-0.39187100
H	-2.50077200	3.45793600	-0.83299500	H	-1.85387500	-0.61927600	-2.24503000
H	-0.74930100	3.28368100	-1.08229100	H	-3.52833800	-1.15487000	-2.41617300
C	-1.40861200	0.74613500	-1.64236800	H	-3.18838600	0.46921200	-1.81216000
O	-0.11525500	0.85204600	-1.20992000	H	-3.01670600	-3.20035100	-1.01728100
H	-1.52342500	-0.04170500	-2.43480900	H	-1.34320300	-2.66732300	-0.81208500

H	-2.33607500	-3.03194700	0.61018800	C	1.19968300	-4.71853600	0.24610400
C	-1.96329800	-0.25690700	0.59064800	C	1.05740700	-4.03227100	-0.95757900
O	-2.03431400	-0.86302900	1.88553900	H	2.08614600	-4.73146600	2.20084100
H	-2.45294900	0.73128300	0.62613300	H	0.70270600	-5.67406700	0.38678200
17’				H	0.44469500	-4.45797300	-1.74624200
C	-8.14929500	2.23438200	0.68873100	C	2.83210900	3.28156600	-1.21868800
C	-6.72720900	2.03420800	0.14935600	C	2.68014900	4.65966500	-1.02045300
H	-8.33695200	1.50847000	1.49278600	C	3.07844800	5.26484500	0.16871200
H	-8.22560300	3.22800500	1.15337400	C	3.64162200	4.50233400	1.18857400
C	-5.63714100	2.16380900	1.22133600	C	3.81685200	3.11989200	1.04786900
H	-6.65315500	1.04322800	-0.31982300	C	3.39749100	2.53697500	-0.16445600
H	-6.53764400	2.76457800	-0.65053300	H	2.24220800	5.26512800	-1.80769500
H	-5.71026500	3.15149900	1.69941100	H	2.95042200	6.33521700	0.30075000
H	-5.82266100	1.42624400	2.01527300	H	3.94924600	4.98638300	2.11030900
C	-4.21786500	1.96633300	0.67391900	C	1.51163100	-2.07742000	-2.50032200
C	-3.11584400	2.08343600	1.74521300	H	2.12511300	-1.17231200	-2.48472600
H	-4.02818900	2.70328300	-0.11974700	C	0.04941300	-1.62948900	-2.69311100
H	-4.14707700	0.98014800	0.19655600	H	-0.05467100	-1.06882000	-3.62810700
H	-3.19925900	3.07630800	2.21596700	H	-0.62792700	-2.48898900	-2.74212000
H	-3.29626900	1.34365200	2.53725000	H	-0.27741600	-0.98612900	-1.87009800
C	-9.23744900	2.09258300	-0.38315900	C	1.99352900	-2.93409800	-3.68717100
C	-10.66073800	2.29305100	0.15288100	H	1.90841000	-2.36612100	-4.61939900
H	-9.16261900	1.09835200	-0.84629000	H	3.03904900	-3.23320700	-3.56442600
H	-9.05023200	2.81666700	-1.18931200	H	1.39328300	-3.84323200	-3.79709000
C	-11.74001600	2.14564500	-0.92468100	C	3.49290800	-2.40926000	2.25214000
H	-10.84794900	1.57062700	0.95897200	H	3.94205800	-1.46855400	1.92136300
H	-10.73665600	3.28757300	0.61337700	C	2.62799800	-2.09029400	3.48720600
H	-12.74322500	2.29464500	-0.51157200	H	1.83095400	-1.38238800	3.23897200
H	-11.59928600	2.87750200	-1.72861200	H	2.16277300	-2.99526200	3.89247000
H	-11.71172000	1.14847900	-1.37878700	H	3.24438800	-1.64905500	4.27750300
C	2.59672000	0.18987800	0.01023500	C	4.64773800	-3.36400700	2.61322800
C	4.67677500	0.47727400	-0.85596800	H	5.27499100	-2.91796000	3.39219500
C	4.42307300	-0.86027400	-0.83981900	H	4.27414200	-4.31986700	2.99527300
N	3.14644900	-1.02059400	-0.30770200	H	5.27988300	-3.57231700	1.74461100
N	3.55069100	1.10666400	-0.33289500	C	2.37561400	2.65119500	-2.53079300
Cl	5.41627800	-2.15676800	-1.34903400	C	4.43434800	2.31671500	2.18855900
Cl	6.07102900	1.30781700	-1.39618900	C	3.09938400	3.26724000	-3.74353800
C	1.69414500	-2.80293500	-1.17091600	H	2.79480100	2.75532100	-4.66228300
C	2.47773100	-2.29107900	-0.11725700	H	2.85847800	4.32894500	-3.86114900
C	2.64354700	-2.96118900	1.11123200	H	4.18587100	3.17698700	-3.64751900
C	1.98278000	-4.18649700	1.26776700	C	5.86215300	2.79879400	2.51139300

H	6.50798600	2.75217200	1.62919500
H	5.86330500	3.83142500	2.87579900
H	6.30489600	2.17088800	3.29169800
C	0.84494500	2.74565400	-2.68744400
H	0.51452300	3.78874500	-2.73539700
H	0.52690100	2.24999000	-3.61081700
H	0.33241200	2.26634400	-1.84716500
H	2.63254900	1.58831100	-2.50919400
Cu	0.85192500	0.54420600	0.76351300
H	-1.43747300	2.63378200	0.43742000
C	3.53857200	2.34766700	3.44255600
H	3.97292900	1.72631800	4.23310200
H	3.43607100	3.36476700	3.83528700
H	2.53592000	1.96894200	3.22043100
H	4.50897800	1.27234900	1.87229300
C	-1.72383800	1.88783500	1.18679600
C	-0.86687800	0.89325500	1.50556900
H	-1.27561100	0.21027000	2.26898300
C	-3.01001300	-3.08253200	0.67412300
C	-2.34798300	-3.04388500	2.05804000
C	-3.22582500	-4.52394300	0.16803500
H	-2.95444600	-3.57127500	2.79995400
H	-1.36973900	-3.52874900	1.99964800
H	-2.20115100	-2.01543600	2.39749900
H	-2.25480400	-5.02309100	0.11217700
H	-3.86256700	-5.08847700	0.85614700
H	-3.68079300	-4.53963000	-0.82436300
C	-4.32786800	-2.33590400	0.71568000
O	-4.95795200	-1.96795600	1.64864300
Br	-5.05640400	-1.94905500	-1.15643100
H	-2.38582700	-2.55259400	-0.05354000

TS6’

C	-9.18759800	0.67577300	0.59688900
C	-7.89340800	0.10787000	0.00024900
H	-9.10463800	0.69363600	1.69322300
H	-9.30104700	1.72394800	0.28461900
C	-6.63546700	0.88835100	0.40300100
H	-7.78226300	-0.94180900	0.30813600
H	-7.97558000	0.09464500	-1.09606900
H	-6.74960500	1.94024700	0.10358600
H	-6.54711800	0.89295000	1.49910500
C	-5.34524400	0.32728000	-0.20823800
C	-4.07956000	1.10170700	0.20790700
H	-5.42916200	0.33621400	-1.30407600
H	-5.22967300	-0.72673100	0.07960300
H	-4.22862100	2.16352700	-0.04449000
H	-3.96051700	1.05400800	1.29870200
C	-10.44350300	-0.10931600	0.19770000
C	-11.73935600	0.46001100	0.78917500
H	-10.33229700	-1.15703900	0.51273000
H	-10.52549100	-0.13023700	-0.89868100
C	-12.98754600	-0.33235200	0.38675600
H	-11.65729600	0.48216800	1.88458100
H	-11.85208600	1.50597000	0.47241000
H	-13.89454100	0.09746300	0.82499300
H	-13.11622800	-0.34189900	-0.70184700
H	-12.91884300	-1.37465400	0.71936300
C	1.85401100	0.29245600	0.22205100
C	3.58016600	1.53245600	1.03992300
C	3.76537500	0.25423100	1.46147000
N	2.70993700	-0.49724200	0.94908500
N	2.40967800	1.54456400	0.28465700
Cl	5.01171800	-0.37218500	2.45409800
Cl	4.55177200	2.90881600	1.34305800
C	3.21718500	-2.83241000	0.34863500
C	2.53230100	-1.91798800	1.17840000
C	1.70322100	-2.32948600	2.24549200
C	1.54157400	-3.70729700	2.44006100
C	2.18156600	-4.63280100	1.62002800
C	3.01339100	-4.19738500	0.59291500
H	0.91324000	-4.05924000	3.25158700
H	2.04164200	-5.69631800	1.79065400
H	3.52262800	-4.92830000	-0.02691500
C	2.20814100	3.07952600	-1.63154100
C	1.65497000	4.24917800	-2.16880300
C	0.78759400	5.04601500	-1.42717000
C	0.45961900	4.69379100	-0.12148300
C	0.98104500	3.53712100	0.47204400
C	1.84288400	2.73994700	-0.31129100
H	1.91283000	4.54267100	-3.18112900
H	0.37206500	5.94850500	-1.86605000
H	-0.20838200	5.32930800	0.45102300

C	4.19270300	-2.41280600	-0.74982400
H	4.15065200	-1.32387500	-0.84962300
C	3.82690200	-3.01181500	-2.12091000
H	4.53430100	-2.65818000	-2.87878000
H	3.88016600	-4.10566600	-2.10924100
H	2.82230700	-2.71629900	-2.43064800
C	5.64020300	-2.79720200	-0.37545000
H	6.33394800	-2.43606300	-1.14198200
H	5.94145100	-2.37145200	0.58487600
H	5.75134900	-3.88513200	-0.31167200
C	1.04193300	-1.35123300	3.21361800
H	1.09187100	-0.35059200	2.77598900
C	-0.44632100	-1.66396400	3.45155400
H	-0.99841200	-1.71336300	2.50988200
H	-0.58497600	-2.61264200	3.98032900
H	-0.89531000	-0.87904700	4.06905900
C	1.80476700	-1.31659800	4.55527800
H	1.35250900	-0.58078100	5.22870400
H	1.76670500	-2.29332800	5.04997800
H	2.85676500	-1.05162300	4.41773500
C	3.20314800	2.27100400	-2.46063700
C	0.62851200	3.22107100	1.92352000
C	4.56158900	2.99892100	-2.54834700
H	5.27867400	2.39358400	-3.11316500
H	4.45561800	3.96040600	-3.06278400
H	4.98504000	3.19326300	-1.55910600
C	1.25819900	4.25165200	2.88374500
H	2.34466800	4.30037900	2.77016600
H	0.85573000	5.25428800	2.70309100
H	1.03496400	3.98469900	3.92227100
C	2.67530700	1.95635200	-3.87249500
H	2.55883700	2.86401600	-4.47399900
H	3.38552500	1.30769000	-4.39614200
H	1.71206900	1.44216400	-3.83347600
H	3.36941600	1.31411200	-1.95715000
Cu	0.05280800	-0.19749300	-0.52635600
H	-2.85313400	0.64890300	-1.55848200
C	-0.89363500	3.13711800	2.14281300
H	-1.10471600	2.83736200	3.17516300
H	-1.37688700	4.10602500	1.97751400
H	-1.34998500	2.40703600	1.47002300
H	1.04517500	2.24088400	2.17251100
C	-2.82436900	0.59303800	-0.46566000
C	-1.74848100	0.06773700	0.14190200
H	-1.81745700	0.01308500	1.23732100
C	-0.85813800	-3.09890600	-1.09079600
C	-1.98791000	-3.44151900	-0.10763400
C	-0.57663400	-4.26075400	-2.06446200
H	-2.89410900	-3.73571800	-0.64492800
H	-1.66950200	-4.27845800	0.52072600
H	-2.22453800	-2.58891100	0.53125800
H	-0.26508600	-5.13415400	-1.48406900
H	-1.47735800	-4.52172700	-2.62788900
H	0.21858000	-4.00829200	-2.76804900
C	-1.26770500	-1.86990700	-1.89198700
O	-2.26870500	-1.60853600	-2.45800500
Br	0.58664700	-1.10467800	-3.00159800
H	0.05648400	-2.85949600	-0.54442400
18’			
C	-7.19301700	3.26822300	0.51353500
C	-6.61948200	2.05589100	-0.23132600
H	-7.87492200	2.91878600	1.30223900
H	-6.37844000	3.79677400	1.02893800
C	-5.87363200	1.07291100	0.67958400
H	-7.43603400	1.52689900	-0.74373100
H	-5.93945800	2.40377500	-1.02195200
H	-5.03981800	1.59105300	1.17325700
H	-6.54681200	0.73879500	1.48202900
C	-5.33151200	-0.15129500	-0.06846100
C	-4.59507400	-1.14140800	0.85919800
H	-4.64508400	0.17834300	-0.85987100
H	-6.15652600	-0.67335700	-0.57114200
H	-3.77210400	-0.60059700	1.34879200
H	-5.27269900	-1.49148700	1.64729600
C	-7.93722200	4.25110800	-0.39882300
C	-8.52730000	5.45564100	0.34565800
H	-8.74470400	3.71962300	-0.92319900
H	-7.25285500	4.60958000	-1.18137500
C	-9.26592800	6.43333800	-0.57410500
H	-9.21360600	5.09743800	1.12529000
H	-7.72138500	5.98566700	0.87154000
H	-9.67731400	7.27909900	-0.01300800

H	-8.59577400	6.83763600	-1.34169300	H	1.84405300	-2.20221000	4.36651600
H	-10.09785200	5.93990300	-1.09008500	H	3.09143300	-0.95126000	4.47500100
C	2.23686400	0.28166200	0.02917800	C	4.18613900	-3.05507300	3.04509300
C	4.28486200	0.29638000	-0.94006100	H	4.91220500	-2.56581900	3.70278000
C	3.94913900	-1.00401000	-0.71123100	H	3.74145800	-3.88596800	3.60278400
N	2.69165000	-0.99702900	-0.11655100	H	4.72772900	-3.47377000	2.19136200
N	3.22517600	1.07314800	-0.48127400	C	2.07689200	2.33196200	-2.87093400
Cl	4.83309700	-2.42630600	-1.05284200	C	4.26120900	2.60441600	1.79938800
Cl	5.70368500	0.93978400	-1.64353000	C	2.85646200	2.66270900	-4.15892500
C	1.04658800	-2.74908800	-0.62476200	H	2.49721900	2.04251900	-4.98674500
C	1.94552400	-2.17047800	0.29342200	H	2.72590600	3.71082600	-4.44785100
C	2.13879700	-2.66510600	1.59891200	H	3.92805900	2.47857300	-4.03498000
C	1.37594200	-3.77588200	1.97969300	C	5.73214700	3.02226900	1.99364700
C	0.46610200	-4.35925500	1.10161000	H	6.33581500	2.77864300	1.11397400
C	0.30383200	-3.85302400	-0.18542500	H	5.82245500	4.09815400	2.17648000
H	1.49198500	-4.18381900	2.97905100	H	6.16058700	2.50148200	2.85632900
H	-0.12171400	-5.21442000	1.42275300	C	0.56387400	2.55212300	-3.06527300
H	-0.42228600	-4.30900700	-0.85045900	H	0.33950700	3.59721300	-3.30339900
C	2.60523300	3.12558800	-1.67977100	H	0.19606500	1.93496200	-3.89173400
C	2.54342300	4.52468000	-1.69733900	H	0.00477100	2.28455100	-2.16316800
C	3.01631400	5.28075600	-0.62813100	H	2.22336300	1.26724400	-2.66817200
C	3.56530900	4.65195100	0.48616600	Cu	0.57940900	0.82970800	0.78215800
C	3.65396900	3.25624100	0.56117400	H	-3.28067500	-2.07650800	-0.65286200
C	3.16160700	2.52006600	-0.53528600	C	3.42704000	2.90774600	3.05959800
H	2.11779700	5.02690100	-2.56029700	H	3.85455200	2.39464200	3.92749300
H	2.95715600	6.36460000	-0.66359000	H	3.41162600	3.98035500	3.27988300
H	3.93042200	5.25286100	1.31313000	H	2.39158800	2.57354400	2.94083300
C	0.85906400	-2.23187700	-2.04772000	H	4.24906800	1.52006100	1.65874700
H	1.52312300	-1.37507800	-2.19391800	C	-4.02390600	-2.30417100	0.11128000
C	-0.58182700	-1.73899100	-2.28533800	C	-4.35588200	-3.59371900	0.28922400
H	-0.67994400	-1.34193200	-3.30167600	H	-5.09415900	-3.87232900	1.03885700
H	-1.30687300	-2.55005700	-2.16561200	C	-4.25478300	-6.10114700	-0.21782600
H	-0.84446400	-0.94147800	-1.58241400	C	-5.65997400	-6.25835700	-0.84230800
C	1.25710900	-3.29979100	-3.08617900	C	-3.29073700	-7.17636700	-0.72329100
H	1.16942400	-2.89203400	-4.09877400	H	-5.60745100	-6.16795900	-1.93264500
H	2.28961700	-3.63304200	-2.94157800	H	-6.06926200	-7.24455700	-0.60255600
H	0.60675000	-4.17827900	-3.02331600	H	-6.36039300	-5.50317100	-0.47304600
C	3.11720700	-2.04251000	2.59001900	H	-3.68449100	-8.17396800	-0.50501000
H	3.64252900	-1.22526600	2.08733700	H	-3.14703800	-7.09042600	-1.80401700
C	2.37829400	-1.43364900	3.79808800	H	-2.30829300	-7.08623200	-0.24970700
H	1.64788100	-0.68309700	3.47980700	C	-3.73911800	-4.68807100	-0.49921900

O	-2.87512200	-4.48332800	-1.35117100
Br	-1.40227000	1.46620300	1.69006900
H	-4.36449900	-6.19171300	0.87212800

19’

C	-4.37166600	0.21876600	0.41303900
C	-3.00332900	0.04686500	-0.25820900
H	-4.34415300	-0.23672500	1.41326700
H	-4.56479900	1.28925600	0.57264500
C	-1.84769900	0.65159500	0.54837600
H	-2.81098400	-1.02313800	-0.42089100
H	-3.02854400	0.50618200	-1.25654500
H	-2.03809100	1.72174600	0.71194100
H	-1.82106900	0.19091600	1.54591300
C	-0.48090600	0.47973500	-0.12489200
C	0.67360800	1.08170800	0.70280900
H	-0.49840700	0.95025600	-1.11706900
H	-0.28334500	-0.58688300	-0.29290300
H	0.45919800	2.14783900	0.87003700
H	0.71363700	0.60645900	1.69008500
C	-5.52881200	-0.39027400	-0.38791000
C	-6.89750700	-0.21660600	0.28200600
H	-5.33722600	-1.46142400	-0.54593700
H	-5.55642100	0.06327600	-1.38912600
C	-8.04719600	-0.83157200	-0.52183900
H	-6.86910500	-0.66740600	1.28342400
H	-7.09042100	0.85375300	0.43678100
H	-9.00945200	-0.68880800	-0.01911800
H	-8.12121700	-0.37820400	-1.51701800
H	-7.90099000	-1.90896300	-0.66076900
H	2.09414100	1.43591700	-0.96021100
C	1.99885700	0.96299100	0.01779000
C	3.07465100	0.31895600	0.49595500
H	3.03763500	-0.17236900	1.46624800
C	5.48704200	-0.54246300	0.38404900
C	5.17727900	-2.05069400	0.25393000
C	6.84882200	-0.19148600	-0.21798200
H	5.15862800	-2.34904200	-0.79969100
H	5.94979200	-2.63823000	0.75937800
H	4.21153100	-2.31199900	0.69687400
H	7.64108500	-0.76791200	0.26950800
H	6.86831500	-0.41469600	-1.28838500
H	7.07512600	0.87199800	-0.09750000
C	4.35409500	0.26015200	-0.25834100
O	4.49437500	0.80972300	-1.34737200
H	5.48669700	-0.29562800	1.45535700

23’

C	-7.81121900	3.22273800	-0.32669000
C	-6.52934300	2.43688600	-0.02245800
H	-7.67156500	4.27399600	-0.03584000
H	-7.98218100	3.22904500	-1.41287100
C	-5.28570200	2.98693000	-0.73312300
H	-6.35498800	2.43415100	1.06331400
H	-6.67349300	1.38507200	-0.30828700
H	-5.46857000	3.00873100	-1.81725600
H	-5.12592200	4.03220800	-0.43128000
C	-4.01465000	2.17446800	-0.45536700
C	-2.76290500	2.70887700	-1.17716300
H	-4.18154100	1.13225100	-0.76015800
H	-3.82109800	2.15097500	0.62650200
H	-2.99818200	2.78022100	-2.25171000
H	-2.54460900	3.73057200	-0.83701300
C	-9.05465500	2.66358200	0.37634900
C	-10.33969800	3.44146700	0.06520300
H	-8.88773800	2.66108300	1.46333200
H	-9.19093000	1.61097400	0.08879200
C	-11.57682900	2.87268300	0.76789800
H	-10.20517600	4.49276200	0.35474900
H	-10.50519600	3.44511600	-1.02092600
H	-12.47659600	3.44818100	0.52554300
H	-11.75682600	1.83281300	0.47127500
H	-11.45530200	2.88814000	1.85729500
C	2.81420400	0.09595200	-0.02788300
C	4.27041800	-1.64581000	0.07238900
C	4.99281000	-0.50124800	0.21778600
N	4.08920500	0.55555800	0.15511600
N	2.93961600	-1.26514600	-0.07629700
Cl	6.67856200	-0.30651000	0.43425800
Cl	4.80805400	-3.26972200	0.05872900
C	4.44854900	2.53289200	1.56541300
C	4.43733200	1.95596500	0.27954600
C	4.74370800	2.68104800	-0.88920600
C	5.05833100	4.03753400	-0.73764200

C	5.07341300	4.63813200	0.51834600	H	3.46591300	-3.79960700	-3.02126800
C	4.77334500	3.89233900	1.65515200	H	1.99242200	-3.87567800	-3.99922500
H	5.29220000	4.63097600	-1.61594500	H	3.31440300	-2.80612200	-4.48174600
H	5.32028000	5.69169500	0.61160400	C	0.47222200	-1.39765700	2.98800600
H	4.78812800	4.37291600	2.62847900	H	-0.45073700	-1.97535800	3.10859100
C	1.17740400	-2.65793100	0.91278000	H	0.79222000	-1.06645900	3.98175800
C	0.10818500	-3.54315700	0.72493300	H	0.24076200	-0.51123900	2.38899900
C	-0.28736200	-3.93466800	-0.55189400	H	2.46845900	-1.61264700	2.25795400
C	0.38009100	-3.44749000	-1.67239800	Cu	1.20622800	1.15099700	-0.22563000
C	1.45721900	-2.56111800	-1.54617700	H	-1.68336200	0.80442900	-1.31692400
C	1.83004800	-2.18093800	-0.24143700	C	1.22282100	-1.18486200	-3.65638400
H	-0.41756000	-3.93323600	1.59109700	H	1.75927700	-0.79241100	-4.52679700
H	-1.11673700	-4.62519400	-0.67442900	H	0.37037400	-1.76648300	-4.02292200
H	0.06148700	-3.76088800	-2.66154700	H	0.83364400	-0.33796000	-3.08271700
C	4.11888700	1.75064100	2.83317200	H	2.99326500	-1.40702800	-2.48311800
H	3.91191000	0.71375900	2.55348600	C	-1.54134400	1.83793800	-0.98294300
C	2.84859500	2.29790000	3.51337100	C	-0.35657300	2.21522000	-0.45442200
H	2.60227700	1.69647300	4.39498800	H	-0.34042000	3.27622500	-0.15510200
H	2.98628800	3.33306800	3.84332300	C	-4.11098900	-3.92965200	1.37738700
H	1.99273700	2.27153600	2.83158800	C	-3.85611000	-2.44914600	1.04928100
C	5.31010800	1.73115200	3.81085500	H	-5.17471500	-4.12047200	1.53815300
H	5.06943000	1.12031300	4.68725400	H	-3.75579600	-4.58778200	0.57924900
H	6.20536300	1.31343200	3.34006100	H	-3.57254200	-4.18404700	2.29494900
H	5.55462800	2.73811000	4.16488800	C	-4.34264200	-1.51159400	2.16709300
C	4.73418100	2.05922200	-2.28237300	H	-3.79857100	-1.74877700	3.08589100
H	4.50834100	0.99395100	-2.18169900	H	-4.15703100	-0.46240600	1.92194100
C	3.62735100	2.67633700	-3.15974300	H	-5.41105900	-1.64408900	2.35379200
H	2.64337600	2.55503900	-2.69563700	C	-4.45364800	-2.06702800	-0.29126300
H	3.79654900	3.74646600	-3.32028200	O	-3.90481100	-1.68793000	-1.27068200
H	3.60638600	2.18958700	-4.14064500	Br	-6.49160500	-2.24963600	-0.35092300
C	6.11213900	2.17014300	-2.96333700	H	-2.78189700	-2.29679000	0.89347600
H	6.09462300	1.66065800	-3.93247500	TS8’			
H	6.38927800	3.21416500	-3.14312300	C	-9.16107700	0.10700100	-0.68587900
H	6.89706400	1.71352900	-2.35251600	C	-7.80188700	-0.54459700	-0.39908900
C	1.57765700	-2.24342000	2.32522900	H	-9.20933200	1.08094900	-0.17782100
C	2.16558100	-2.04934900	-2.79661300	H	-9.23971500	0.32261100	-1.76131500
C	1.94608700	-3.46007500	3.19600900	C	-6.60793900	0.30917000	-0.84516200
H	2.28854300	-3.12717200	4.18132000	H	-7.71871600	-0.75099300	0.67757600
H	1.08627100	-4.12027400	3.35048100	H	-7.75547100	-1.52256200	-0.89952200
H	2.74605500	-4.05026700	2.73853000	H	-6.68785600	0.50630800	-1.92422500
C	2.76935300	-3.20413000	-3.61946000	H	-6.66160900	1.29146200	-0.35374400

C	-5.24469500	-0.32901300	-0.54830000
C	-4.05328500	0.52664000	-1.01763700
H	-5.19255600	-1.31600100	-1.03012500
H	-5.15128700	-0.51152700	0.53111900
H	-4.18040800	0.72291900	-2.09553300
H	-4.08634400	1.50465200	-0.51843300
C	-10.35891800	-0.74817300	-0.25400900
C	-11.71605400	-0.08988400	-0.53483700
H	-10.27975000	-0.96902900	0.82028700
H	-10.31571000	-1.71999200	-0.76677600
C	-12.90806700	-0.95183100	-0.10616600
H	-11.76056800	0.87917500	-0.01917500
H	-11.79353000	0.13392100	-1.60772200
H	-13.86038400	-0.45541200	-0.32097200
H	-12.90888200	-1.91452500	-0.63051200
H	-12.87774400	-1.16259400	0.96915600
C	1.69527900	0.30246600	-0.18952000
C	3.40294600	0.80516600	-1.61353300
C	3.03702800	1.95752500	-0.99827300
N	1.97705700	1.64904600	-0.14962700
N	2.60016800	-0.20998900	-1.09142100
Cl	3.75187700	3.50531700	-1.13844400
Cl	4.56304700	0.59081900	-2.85357900
C	1.42217500	2.74470800	1.98444100
C	1.21893200	2.64274800	0.59045900
C	0.32796800	3.48396600	-0.11506200
C	-0.42423200	4.39214700	0.64193100
C	-0.28401200	4.47892700	2.02289500
C	0.64111000	3.67456800	2.68208100
H	-1.12799700	5.04606000	0.13671900
H	-0.88331600	5.18881400	2.58556900
H	0.76518000	3.77760700	3.75431100
C	3.93546100	-2.27414400	-0.89164800
C	4.05881400	-3.64453700	-1.16205800
C	3.11215100	-4.32128200	-1.92353100
C	2.02719500	-3.63324000	-2.45905600
C	1.84088100	-2.26592600	-2.22077100
C	2.78970200	-1.61649000	-1.39924900
H	4.91853800	-4.18453200	-0.77813200
H	3.22996900	-5.38343400	-2.11720800
H	1.31408000	-4.16742800	-3.07612900
C	2.51166800	1.96582700	2.71962700
H	2.75167300	1.07681100	2.12936800
C	2.08140600	1.48471100	4.11618600
H	2.86848900	0.85771500	4.54801300
H	1.92559200	2.32054700	4.80588400
H	1.16098100	0.89651600	4.07204900
C	3.79575300	2.81810800	2.82014600
H	4.59275400	2.24807400	3.30971400
H	4.15629200	3.13057300	1.83591700
H	3.61422300	3.72178600	3.41231100
C	0.18218600	3.50995000	-1.63865200
H	0.84792100	2.75529100	-2.06690400
C	-1.24387900	3.17363600	-2.11321100
H	-1.54593300	2.17622000	-1.79088800
H	-1.97209500	3.89604200	-1.72826800
H	-1.28558600	3.21645200	-3.20733600
C	0.60266500	4.88425100	-2.20517400
H	0.59675500	4.85312800	-3.29982600
H	-0.09758500	5.66660400	-1.89383800
H	1.60231000	5.17821900	-1.87811700
C	5.07080700	-1.58120700	-0.13147700
C	0.69664100	-1.51950700	-2.90476400
C	6.41400300	-1.75025600	-0.87468300
H	7.18556400	-1.14262000	-0.39070400
H	6.75126300	-2.79166600	-0.85035100
H	6.34380000	-1.44298600	-1.92028800
C	1.16359400	-0.96399900	-4.26808900
H	2.02666000	-0.30012300	-4.16698300
H	1.44695900	-1.77980500	-4.94260800
H	0.35445500	-0.39839800	-4.74224400
C	5.21738700	-2.08058600	1.31720300
H	5.38187200	-3.16266800	1.35609700
H	6.07757700	-1.59721400	1.79214500
H	4.33498100	-1.84709300	1.91343000
H	4.85685300	-0.51087800	-0.07738900
Cu	-0.01458200	-0.42553200	0.57198500
H	-2.58201300	-1.08590100	-1.26590900
C	-0.56947700	-2.37308600	-3.08553300
H	-1.38410700	-1.74106200	-3.45122500
H	-0.42620400	-3.17297200	-3.82014900
H	-0.88678100	-2.82368500	-2.14151600

H	0.41680700	-0.67056200	-2.27573900
C	-2.70442500	-0.11714100	-0.77108900
C	-1.70651400	0.38955100	-0.02265700
H	-1.93739200	1.36853600	0.42389400
C	1.19697000	-4.47465800	2.51155200
C	1.63773600	-3.03936400	2.15258000
H	0.39569200	-4.45506100	3.25612200
H	0.84558900	-5.01555000	1.63019100
H	2.04877800	-5.01293200	2.93720000
C	2.20830500	-2.29824400	3.35792600
H	3.13380200	-2.78905500	3.67251000
H	2.43101800	-1.25493000	3.12571600
H	1.50846700	-2.31651900	4.19502100
C	0.48363200	-2.35911600	1.43232100
O	-0.17559100	-2.78850800	0.52777300
Br	-0.79915200	-1.15588500	2.93296500
H	2.40002000	-3.09926400	1.36408800

24’

C	-8.81744600	-0.00226400	-0.77004800
C	-7.45334500	-0.56195100	-0.34635700
H	-8.91867800	1.02767600	-0.39843400
H	-8.85567200	0.06643600	-1.86688200
C	-6.26570800	0.26938200	-0.84831900
H	-7.41233900	-0.62779100	0.75022100
H	-7.35454800	-1.59295200	-0.71556000
H	-6.31155200	0.34116600	-1.94477300
H	-6.35881400	1.29866400	-0.47281200
C	-4.90187700	-0.29962000	-0.43651500
C	-3.71178900	0.53147500	-0.95095400
H	-4.81036900	-1.32924700	-0.81069000
H	-4.84475300	-0.36689600	0.65823100
H	-3.80273900	0.62433200	-2.04527400
H	-3.77093700	1.54929600	-0.54461000
C	-10.00493800	-0.83740300	-0.27484300
C	-11.36898700	-0.28228000	-0.70447600
H	-9.97068900	-0.90346400	0.82222300
H	-9.90227200	-1.86843900	-0.64330000
C	-12.54889400	-1.12470400	-0.20865900
H	-11.47328600	0.74694900	-0.33436500
H	-11.40244000	-0.21494400	-1.80060300
H	-13.50684700	-0.70288600	-0.53094800
H	-12.49119600	-2.15037400	-0.59126300
H	-12.56187400	-1.18179000	0.88598000
C	1.57186500	0.26293500	-0.21908400
C	3.19019000	0.70000400	-1.75397400
C	2.85760700	1.87779400	-1.17078100
N	1.84046700	1.61125900	-0.25598900
N	2.42438900	-0.29268700	-1.14076900
Cl	3.57690000	3.41012500	-1.40637200
Cl	4.27625900	0.42964100	-3.04622100
C	1.35558000	2.81198700	1.84197800
C	1.12278900	2.65667100	0.45762000
C	0.24880400	3.49906800	-0.26930600
C	-0.46472700	4.45751000	0.46255200
C	-0.30329900	4.59248100	1.83703200
C	0.61076300	3.79006100	2.51292000
H	-1.15595900	5.11236400	-0.05834300
H	-0.87467100	5.33956600	2.38007100
H	0.75493300	3.93225200	3.57768300
C	3.82965800	-2.30123200	-0.88301000
C	3.99169900	-3.67740000	-1.09609000
C	3.04859200	-4.41796400	-1.80028300
C	1.92540200	-3.79186200	-2.33283100
C	1.69546000	-2.42391300	-2.14433300
C	2.64473200	-1.70905100	-1.38231900
H	4.88109700	-4.17055300	-0.71689000
H	3.19868000	-5.48278100	-1.95236300
H	1.21465200	-4.37701100	-2.90474700
C	2.44435700	2.04367900	2.59023600
H	2.61923700	1.09970700	2.06619100
C	2.06337200	1.69428500	4.03872300
H	2.84424900	1.06783200	4.48159300
H	1.97799700	2.58729600	4.66628600
H	1.11893400	1.14521100	4.08215800
C	3.76625500	2.84256900	2.56115900
H	4.56102300	2.27899800	3.06152600
H	4.09289700	3.05677900	1.53944500
H	3.65081700	3.79929700	3.08233800
C	0.07163200	3.47655200	-1.79073400
H	0.72899300	2.71059200	-2.21113000
C	-1.36306200	3.12205700	-2.22342300
H	-1.64322500	2.12730800	-1.87803600

H	-2.08806500	3.84251700	-1.82950700	O	0.17690200	-2.91363900	0.64152900
H	-1.43395600	3.14600900	-3.31636900	Br	-1.01526700	-0.79111200	3.02448000
C	0.47471300	4.83325500	-2.40997500	H	2.69918900	-3.15605200	1.76371500
H	0.45928900	4.76212600	-3.50258800	17”			
H	-0.22963100	5.62045600	-2.12158300	C	7.13284100	-4.40443400	1.35674400
H	1.47426400	5.14793100	-2.10294500	C	5.89968000	-3.72800800	0.74383400
C	4.97193400	-1.53484100	-0.20599100	H	7.23267200	-4.09347800	2.40666200
C	0.49735000	-1.75162300	-2.81214700	H	6.97574800	-5.49255800	1.37691200
C	6.28554700	-1.69522200	-1.00354000	C	4.59483200	-4.04348500	1.48627100
H	7.05438700	-1.03533800	-0.58861800	H	6.05406700	-2.63929700	0.72657700
H	6.66252500	-2.72119300	-0.93958300	H	5.80217000	-4.03673900	-0.30699700
H	6.15765000	-1.44846600	-2.05950000	H	4.44493900	-5.13272700	1.50706000
C	0.87557600	-1.27864800	-4.23307300	H	4.69031300	-3.73116300	2.53624700
H	1.72429500	-0.58894800	-4.22372200	C	3.35794300	-3.37727100	0.87031300
H	1.14509600	-2.13151100	-4.86587100	C	2.04848200	-3.70521200	1.61334200
H	0.02718800	-0.76627100	-4.69906000	H	3.26330100	-3.68894300	-0.17986300
C	5.21044500	-1.95693800	1.25545300	H	3.49656500	-2.28728600	0.85340100
H	5.40500000	-3.03148900	1.33836600	H	1.94975500	-4.80216900	1.65739700
H	6.08426900	-1.43097200	1.65400300	H	2.11808000	-3.35624900	2.65287100
H	4.35936400	-1.71209200	1.89130300	C	8.43772300	-4.09673600	0.61176900
H	4.72436300	-0.47028600	-0.19028300	C	9.67048600	-4.77522000	1.22281500
Cu	0.10564400	-0.51476900	0.89244600	H	8.59725600	-3.00858800	0.59323500
H	-2.22417100	-1.08786900	-0.99727200	H	8.33839100	-4.40609000	-0.43877500
C	-0.75007700	-2.65004500	-2.86701900	C	10.96810600	-4.46475300	0.46953400
H	-1.60133700	-2.07065000	-3.23725300	H	9.77199800	-4.46330700	2.27134200
H	-0.61709300	-3.49637900	-3.54915000	H	9.51077800	-5.86201800	1.24390600
H	-1.00348100	-3.04137400	-1.87816600	H	11.82854400	-4.96178700	0.92997100
H	0.22705100	-0.86715700	-2.22890300	H	10.90970600	-4.79810700	-0.57311400
C	-2.36966100	-0.08048400	-0.60116500	H	11.17199700	-3.38757600	0.45985100
C	-1.42456200	0.48590200	0.16027300	C	-3.18573900	-0.67066100	-0.02664700
H	-1.60208100	1.48814000	0.55807000	C	-4.76950100	0.01207400	-1.50574000
C	1.25652500	-4.25595700	2.92293300	C	-5.15027500	0.44421700	-0.27221300
C	1.83442600	-2.92737500	2.40362500	N	-4.17182900	0.01948900	0.62233400
H	0.36720500	-4.07410900	3.53387900	N	-3.56682500	-0.66897000	-1.33970900
H	0.98116800	-4.91718900	2.09834200	Cl	-6.53638100	1.33770700	0.18184500
H	2.00186400	-4.76203800	3.54405700	Cl	-5.54826000	0.22055100	-3.01437400
C	2.28561700	-2.00168900	3.53157400	C	-3.56866400	1.44554000	2.52863400
H	3.11313400	-2.46263500	4.07987900	C	-4.18134100	0.27059900	2.04883800
H	2.62388000	-1.03669400	3.14714400	C	-4.79890600	-0.67260900	2.89421300
H	1.46535300	-1.81114000	4.22601000	C	-4.77541600	-0.41229800	4.27024700
C	0.87088300	-2.28680500	1.40718500	C	-4.16915200	0.73436000	4.77654300

C	-3.57468000	1.65170600	3.91395600	H	-4.80396100	-4.67186000	-3.73015600
H	-5.23697200	-1.11878400	4.95303200	H	-6.01640300	-4.51305000	-2.45437800
H	-4.16148500	0.91472200	5.84755800	C	-0.09697800	1.06498900	-2.13795900
H	-3.10610200	2.54223100	4.32104800	H	0.66348300	0.78625400	-2.87566000
C	-1.82277000	-0.53783700	-3.06432700	H	0.08461200	2.10299100	-1.84066400
C	-1.09586700	-1.17654600	-4.07701100	H	0.03671500	0.42732700	-1.25805300
C	-1.34585700	-2.50355800	-4.41660300	H	-2.21671900	1.23548400	-1.93776100
C	-2.33446300	-3.22321200	-3.75028900	Cu	-1.59977800	-1.46161700	0.74441900
C	-3.09381800	-2.63733200	-2.72975500	H	0.65765700	-3.44843500	-0.06552600
C	-2.81086900	-1.29565400	-2.40430300	C	-3.53831000	-4.61438800	-1.21421100
H	-0.32301200	-0.62617400	-4.60447800	H	-4.31592900	-5.16669800	-0.67585800
H	-0.76873800	-2.97854400	-5.20464900	H	-3.02063700	-5.32061000	-1.87219400
H	-2.51958700	-4.25696900	-4.02491600	H	-2.81498700	-4.24133300	-0.48228200
C	-2.90157100	2.46770400	1.61396800	H	-4.67517400	-2.80723300	-1.30160200
H	-3.06596700	2.15967200	0.57771500	C	0.81984600	-3.10894900	0.96349600
C	-1.37727500	2.50474500	1.84042600	C	-0.04127600	-2.23124100	1.52336200
H	-0.90825300	3.19883500	1.13563700	H	0.23163200	-1.96959300	2.55912800
H	-1.13563400	2.83738000	2.85581100	C	2.65699300	3.85916800	0.40697200
H	-0.93263400	1.51512800	1.69347700	C	3.94451900	3.73590900	-0.43652000
C	-3.52097100	3.86955400	1.77443100	H	3.67997800	3.42499400	-1.45422600
H	-3.06197700	4.56581100	1.06497100	H	4.41926800	4.71979300	-0.51429100
H	-4.59911100	3.85323400	1.58716300	C	1.66181800	4.81374400	-0.19186900
H	-3.35971200	4.26843900	2.78131200	O	0.63567200	4.58537200	-0.74326000
C	-5.46629300	-1.94302000	2.37632200	Br	2.25067500	6.75233400	-0.00554200
H	-5.42214400	-1.93256000	1.28356900	H	2.90321200	4.20730500	1.41459700
C	-4.71100800	-3.20083000	2.84923300	H	2.15026000	2.89136800	0.47812400
H	-3.66381100	-3.17492000	2.53147000	C	4.92540500	2.72846100	0.17691000
H	-4.73096900	-3.29083600	3.94061900	H	5.17111800	3.04015000	1.20133600
H	-5.17409700	-4.10061600	2.43035500	H	4.43760000	1.74796600	0.26077900
C	-6.95459000	-2.00488900	2.77105900	C	6.21748500	2.58812400	-0.63818400
H	-7.42209000	-2.89517200	2.33753400	H	6.70150700	3.57130800	-0.72205400
H	-7.08071400	-2.06045100	3.85733000	H	5.96787100	2.28182800	-1.66370700
H	-7.49907500	-1.12566600	2.41310000	C	7.20839500	1.58420600	-0.03551200
C	-1.51810300	0.91578500	-2.71601500	H	7.45285700	1.88801000	0.99231600
C	-4.16504700	-3.45774400	-2.01748300	H	6.72396800	0.60054400	0.04522700
C	-1.72897800	1.84598000	-3.92641600	C	8.50445800	1.44572900	-0.84429600
H	-1.56009900	2.88752700	-3.63395600	H	8.99022200	2.42903900	-0.92328700
H	-1.03294000	1.61249400	-4.73894400	H	8.26033900	1.14448800	-1.87316700
H	-2.74656800	1.76316500	-4.32077300	C	9.49583800	0.44002500	-0.24562000
C	-5.23249700	-3.97746300	-2.99995600	H	9.73862300	0.73990600	0.78297200
H	-5.70113300	-3.15622200	-3.55085200	H	9.00988000	-0.54247000	-0.16872600

C	10.78808600	0.30673200	-1.05790000
H	11.31678100	1.26494200	-1.12114600
H	11.47146900	-0.42094500	-0.60729400
H	10.57901700	-0.02291500	-2.08218300
TS6''			
C	-8.10147700	-3.57626100	-0.58023100
C	-6.94665300	-2.90301000	0.17250200
H	-8.14871400	-3.17790100	-1.60401800
H	-7.89003900	-4.65044000	-0.68257000
C	-5.58210300	-3.08095700	-0.50593300
H	-7.16022800	-1.82971100	0.27916400
H	-6.89780900	-3.30488600	1.19470100
H	-5.37015800	-4.15398800	-0.61931800
H	-5.62804200	-2.67155100	-1.52549700
C	-4.42898700	-2.41621500	0.25658700
C	-3.05967100	-2.58053600	-0.43094200
H	-4.37552700	-2.83503800	1.27137300
H	-4.63920700	-1.34498200	0.38042400
H	-2.87943600	-3.65624000	-0.58514100
H	-3.09210200	-2.12368900	-1.42925300
C	-9.46523800	-3.39201700	0.09754300
C	-10.62099000	-4.06956900	-0.64980600
H	-9.67921600	-2.31790300	0.19651600
H	-9.41752400	-3.78663700	1.12279200
C	-11.97844400	-3.87857800	0.03485900
H	-10.66889900	-3.67593900	-1.67440800
H	-10.40830700	-5.14306900	-0.74708600
H	-12.78184300	-4.37328700	-0.52123200
H	-11.97125900	-4.29358800	1.04942800
H	-12.23487900	-2.81583300	0.11550800
C	2.41192100	-0.23194700	-0.22761600
C	4.30590400	-0.76293000	-1.37475100
C	4.15412900	0.58528700	-1.44595100
N	3.00048500	0.90164100	-0.73013800
N	3.23436400	-1.25206800	-0.63173900
Cl	5.12063600	1.72299400	-2.28437800
Cl	5.54642000	-1.73512200	-2.04301600
C	3.02810600	3.06145500	0.45998800
C	2.49494200	2.25175000	-0.56778600
C	1.52226800	2.71977600	-1.47808100
C	1.06916300	4.03600600	-1.31769700
C	1.56553200	4.85236000	-0.30558100
C	2.53468000	4.36848500	0.56796200
H	0.32584500	4.42931900	-2.00353000
H	1.20232600	5.87078300	-0.20269800
H	2.92252400	5.01841000	1.34548200
C	3.47323200	-3.23170600	0.81605900
C	3.23608800	-4.59799300	1.01478400
C	2.56230300	-5.36098500	0.06524000
C	2.11648900	-4.77328000	-1.11461400
C	2.32492000	-3.41232500	-1.37226300
C	2.99532100	-2.66119700	-0.38315900
H	3.58999800	-5.07194900	1.92421700
H	2.39057800	-6.41869200	0.24283900
H	1.60067800	-5.37984000	-1.85234400
C	4.13048700	2.60380300	1.41425900
H	4.26901900	1.52587100	1.28500100
C	3.76610400	2.84426400	2.89156600
H	4.55086900	2.43340600	3.53567400
H	3.68547700	3.91262800	3.11796600
H	2.82330400	2.36089800	3.15428600
C	5.46963900	3.30053000	1.08986900
H	6.25688200	2.92715500	1.75341000
H	5.78468400	3.12999700	0.05798700
H	5.38984600	4.38248100	1.24271600
C	0.99136900	1.88471300	-2.64077700
H	1.31134100	0.84966900	-2.49521500
C	-0.54738000	1.87666900	-2.70037000
H	-0.98086500	1.55711500	-1.74907000
H	-0.95063100	2.86513000	-2.94410000
H	-0.88615500	1.18509500	-3.47883000
C	1.58208400	2.37277100	-3.98035900
H	1.22491400	1.74414200	-4.80300400
H	1.27817800	3.40428200	-4.18921200
H	2.67530700	2.33982500	-3.97592200
C	4.27039100	-2.44604900	1.85460400
C	1.85055100	-2.82603400	-2.70027000
C	5.77667900	-2.76470000	1.74179300
H	6.34445100	-2.16932400	2.46486600
H	5.96712000	-3.82244200	1.95431000
H	6.16578500	-2.54885200	0.74287600
C	2.63042500	-3.42963000	-3.88677000

H	3.70838300	-3.27887300	-3.78237500	H	-5.28184300	7.11585600	-1.60666300
H	2.44740000	-4.50622100	-3.97184000	C	-7.43987100	7.06039400	-1.47624400
H	2.30957400	-2.96255600	-4.82401800	H	-8.22820900	6.79793600	-0.76121100
C	3.77861600	-2.69451600	3.29216200	H	-7.57666000	8.11160100	-1.75114000
H	3.96433500	-3.72451400	3.61429100	H	-7.59841600	6.45699200	-2.37755000
H	4.31542300	-2.03662100	3.98367900	18”			
H	2.71033000	-2.48778700	3.39037000	C	-4.32539500	-6.66158100	0.61432200
H	4.13822100	-1.37967800	1.65005100	C	-3.02483000	-6.01529800	0.12002900
Cu	0.62257600	-0.43803500	0.65678500	H	-4.40146900	-6.53736200	1.70403800
H	-1.80147500	-2.41571100	1.36443700	H	-5.18345400	-6.12341400	0.18648000
C	0.33434100	-3.01060200	-2.90077500	C	-2.90866000	-4.52504600	0.46561500
H	0.01845400	-2.51908900	-3.82751400	H	-2.16725500	-6.55355800	0.54799000
H	0.06857500	-4.06996200	-2.98344900	H	-2.94927800	-6.14066000	-0.96950600
H	-0.22999200	-2.58105600	-2.06960900	H	-3.76534200	-3.98382400	0.03940500
H	2.04647400	-1.74996300	-2.69178800	H	-2.97572700	-4.39670200	1.55503700
C	-1.92029200	-1.98452700	0.36534100	C	-1.60704300	-3.89165900	-0.04147100
C	-1.10838200	-0.98905400	-0.02596300	C	-1.48097000	-2.39457200	0.32293500
H	-1.32491400	-0.58696200	-1.02583600	H	-1.54358500	-4.01157900	-1.13129700
C	-2.59079100	1.89947800	1.49681000	H	-0.74593900	-4.42910800	0.37631400
H	-2.72119100	1.24995200	0.62480500	H	-2.36049000	-1.85925400	-0.05237200
H	-3.34343200	1.59678200	2.23395500	H	-1.48082900	-2.29146700	1.41308200
C	-0.98396500	0.23323000	2.49976800	C	-4.43622900	-8.15112000	0.26513400
O	-1.70479100	-0.55262100	3.00664900	C	-5.73600500	-8.80301900	0.75396000
Br	1.15393100	0.08906200	3.24457900	H	-3.57857100	-8.68933400	0.69388900
C	-1.19066500	1.66947800	2.08206600	H	-4.35737000	-8.27512200	-0.82461200
H	-0.40338800	1.96636100	1.38792700	C	-5.83669400	-10.29005200	0.39866000
H	-1.04949100	2.25708800	2.99973800	H	-5.81438300	-8.68050900	1.84295000
C	-2.80387000	3.36677400	1.10191700	H	-6.59303800	-8.26520300	0.32580000
H	-2.65711700	4.00878700	1.98166400	H	-6.77375600	-10.72637000	0.76039000
H	-2.03575600	3.66298600	0.37405000	H	-5.79609000	-10.44113100	-0.68627900
C	-4.19520000	3.62616600	0.50949200	H	-5.01145500	-10.85942500	0.84186300
H	-4.96074700	3.32284800	1.23742900	C	-1.11507100	1.57863600	-0.18929700
H	-4.33908700	2.98287500	-0.36999000	C	-2.23061400	2.97132400	-1.60269500
C	-4.42542000	5.08963300	0.11171400	C	-2.64305400	3.25786300	-0.34119100
H	-3.65770500	5.39347000	-0.61437500	N	-1.94101100	2.41640900	0.51959800
H	-4.28190000	5.73199500	0.99230300	N	-1.31408300	1.92748100	-1.50149700
C	-5.81537700	5.34903400	-0.48307100	Cl	-3.82645700	4.38993600	0.15363600
H	-6.58334100	5.04478000	0.24264100	Cl	-2.64543300	3.76441400	-3.06080600
H	-5.95913700	4.70630100	-1.36353700	C	-1.31505600	3.58983800	2.59224400
C	-6.04961800	6.81163100	-0.88205600	C	-2.01170500	2.53080600	1.96762400
H	-5.90724000	7.45349500	-0.00186500	C	-2.81093300	1.61476400	2.68511500

C	-2.87381400	1.76885200	4.07563600	C	-3.75571300	0.43743600	-4.13682000
C	-2.18269700	2.78997300	4.72165800	H	-3.76806000	1.52843700	-4.15928800
C	-1.41837400	3.68861600	3.98590100	H	-3.52383000	0.08272800	-5.14689900
H	-3.47668600	1.08369200	4.66102400	H	-4.76288500	0.08979500	-3.88359200
H	-2.24619000	2.88816200	5.80148300	C	2.76633400	2.50207300	-1.75279100
H	-0.89057700	4.48549900	4.49984200	H	3.43131700	2.34116900	-2.60794100
C	0.64213700	1.83046500	-2.98445400	H	3.21138800	3.28604300	-1.13149800
C	1.25620400	1.28950000	-4.12158800	H	2.73471200	1.57885500	-1.16899600
C	0.62122900	0.32359300	-4.89491500	H	0.78341700	3.14144300	-1.29760200
C	-0.65170000	-0.12153300	-4.54927000	Cu	0.18008800	0.23827900	0.50526700
C	-1.31879000	0.37883800	-3.42395700	H	-0.18138900	-1.63887500	-1.32758700
C	-0.64092800	1.34816900	-2.64974500	C	-2.82806200	-1.65358900	-3.10066100
H	2.24452500	1.63604000	-4.40575000	H	-3.82050200	-1.96102700	-2.75519400
H	1.11639600	-0.07997300	-5.77323500	H	-2.68572800	-2.07716500	-4.09987700
H	-1.14060700	-0.86736300	-5.16741600	H	-2.08361500	-2.10282300	-2.44154400
C	-0.49379800	4.64021800	1.84319000	H	-3.01687800	0.24426400	-2.12519600
H	-0.48963400	4.38397200	0.77949800	C	-0.22106700	-1.80092000	-0.25168900
C	0.97462000	4.67334600	2.30963800	C	0.97295600	-1.77489700	0.42801100
H	1.54032900	5.38377400	1.69669200	H	1.01270600	-2.10387700	1.46366400
H	1.05180200	5.00527400	3.35094300	C	3.51798300	-1.93214300	0.53186900
H	1.43919100	3.68867900	2.22992400	C	4.83729200	-1.75030000	-0.21755300
C	-1.11623900	6.04576200	1.98646300	H	4.82988900	-2.36794900	-1.12426700
H	-0.54837700	6.76740900	1.38963800	H	4.91291600	-0.71112900	-0.56063200
H	-2.15659000	6.07339000	1.65509400	C	2.28095400	-1.60556900	-0.28089100
H	-1.08537900	6.38196400	3.02843900	O	2.33607700	-1.24777400	-1.45315500
C	-3.63643200	0.52563600	2.00381500	Br	1.80011800	0.98510000	2.16407100
H	-3.16922600	0.30148400	1.04028800	H	3.47650900	-1.29629000	1.42779600
C	-3.67659000	-0.78542000	2.80917300	H	3.41200100	-2.96387000	0.90019900
H	-2.67389100	-1.11072300	3.10128500	C	6.05934000	-2.10194700	0.63974900
H	-4.27681100	-0.68609100	3.71935700	H	6.05442500	-1.48623400	1.55040000
H	-4.13280600	-1.57768800	2.20766900	H	5.97991500	-3.14514900	0.97828600
C	-5.07236200	1.01933300	1.72541900	C	7.39210100	-1.90828600	-0.09451200
H	-5.64936200	0.24188800	1.21305300	H	7.47199800	-0.86412000	-0.42894700
H	-5.58599800	1.25849500	2.66316400	H	7.39523800	-2.52052000	-1.00781900
H	-5.08279100	1.91679700	1.10126900	C	8.61783600	-2.26253600	0.75700900
C	1.35704800	2.93041800	-2.20358000	H	8.61203400	-1.65243600	1.67169000
C	-2.73376500	-0.11546200	-3.11985700	H	8.53859400	-3.30765500	1.08946600
C	1.41703300	4.23399700	-3.02700000	C	9.95157700	-2.06430900	0.02585000
H	1.89006300	5.02907700	-2.44102800	H	10.03251800	-1.01877800	-0.30495300
H	2.00471900	4.09653500	-3.94103900	H	9.95800200	-2.67283400	-0.89012800
H	0.41834400	4.57354000	-3.31837900	C	11.17768900	-2.42040600	0.87620900

H	11.17162400	-1.81220000	1.79116900
H	11.09726600	-3.46523200	1.20634700
C	12.50538700	-2.21891100	0.13845700
H	12.62979400	-1.17568700	-0.17435800
H	13.35994100	-2.48030300	0.77158100
H	12.55597500	-2.84126400	-0.76256400

19’’

C	7.51611000	0.14121600	-0.38996800
C	6.12749000	0.16370100	0.26081000
H	7.86711500	-0.89832400	-0.45975300
H	7.43710300	0.50442000	-1.42465600
C	5.08386700	-0.66422600	-0.49893600
H	6.20379500	-0.20675500	1.29291000
H	5.77910000	1.20355900	0.33648800
H	5.00651000	-0.29206000	-1.53024300
H	5.42939700	-1.70484700	-0.57578900
C	3.69632600	-0.63932900	0.15299300
C	2.65029700	-1.45541100	-0.63491600
H	3.34807600	0.39799400	0.24066600
H	3.76387800	-1.02941800	1.17737300
H	2.56304200	-1.06290300	-1.65498600
H	3.01193100	-2.49080700	-0.72049700
C	8.55913300	0.97794500	0.36070600
C	9.94796500	0.95483000	-0.28944900
H	8.63853300	0.61673200	1.39616000
H	8.20913200	2.01808600	0.42900900
C	10.98301200	1.79617400	0.46352500
H	10.29872200	-0.08420100	-0.35500000
H	9.86806200	1.31345700	-1.32476300
H	11.96256600	1.75798500	-0.02440300
H	10.67724500	2.84754200	0.51402900
H	11.10958900	1.44010500	1.49239700
H	1.25687300	-1.89642700	1.03125300
C	1.30922100	-1.46882900	0.02943500
C	0.17162100	-0.98624100	-0.49282700
H	0.16243000	-0.54272400	-1.48688200
C	-1.11625400	-1.03148300	0.24746000
O	-1.21270800	-1.52536800	1.36724100
C	-2.31344000	-0.42338800	-0.46691000
C	-3.62894600	-0.51039300	0.30463000
H	-2.39992600	-0.91358300	-1.44814400
H	-2.06195300	0.62269200	-0.69876300
H	-3.85124100	-1.56341100	0.51686600
H	-3.50575100	-0.02793500	1.28187400
C	-4.80412100	0.12734200	-0.44552800
C	-6.13474400	0.02703800	0.31016100
H	-4.91080600	-0.34979400	-1.43036500
H	-4.57887500	1.18488500	-0.64474600
H	-6.36259700	-1.03112600	0.50205400
H	-6.02755400	0.49778000	1.29779700
C	-7.31060200	0.67196400	-0.43365900
C	-8.64561500	0.56087700	0.31245100
H	-7.41046400	0.20741200	-1.42523700
H	-7.08528600	1.73227800	-0.61758300
H	-8.87325900	-0.49952500	0.49339000
H	-8.54706000	1.02274200	1.30545300
C	-9.82027500	1.20896700	-0.43071000
H	-9.91667500	0.74928800	-1.42388100
H	-9.59456900	2.26934400	-0.60841800
C	-11.15101000	1.08923700	0.31819400
H	-11.96824000	1.56006900	-0.23817100
H	-11.42058000	0.03931200	0.48064600
H	-11.09678900	1.57114700	1.30121100

23’’

C	-7.40121900	-4.24205500	0.05885700
C	-6.00717800	-3.83686400	0.55523900
H	-7.76734200	-3.48343000	-0.64766300
H	-7.32553600	-5.17798400	-0.51359200
C	-4.98539700	-3.64932600	-0.57342600
H	-6.08500000	-2.90128300	1.12578500
H	-5.63785600	-4.59670100	1.25942000
H	-4.91584900	-4.57602900	-1.16180800
H	-5.35049100	-2.87547600	-1.26328100
C	-3.58703000	-3.25982600	-0.07693600
C	-2.56694500	-3.05337500	-1.21331900
H	-3.21340500	-4.03512400	0.60759900
H	-3.65427300	-2.33741500	0.51551000
H	-2.53061600	-3.97951900	-1.81004900
H	-2.92452000	-2.26232100	-1.88682700
C	-8.42694400	-4.41962000	1.18542900
C	-9.82215000	-4.82129800	0.68973600
H	-8.50285400	-3.48390900	1.75796400

H	-8.06264100	-5.17850800	1.89317500	H	5.02079600	1.82922200	-4.59923700
C	-10.84018900	-4.99550000	1.82155600	C	4.67341400	-3.55299700	-0.87773100
H	-10.18630000	-4.06258800	-0.01649600	H	4.61572000	-2.96843300	0.04483400
H	-9.74695200	-5.75629300	0.11765000	C	3.53204100	-4.58771900	-0.83058600
H	-11.82483400	-5.28062500	1.43593400	H	2.55536300	-4.09569800	-0.78655600
H	-10.52047700	-5.77290100	2.52527700	H	3.54379800	-5.23553200	-1.71363400
H	-10.96190300	-4.06635400	2.39042400	H	3.63591300	-5.22597300	0.05340200
C	3.03443400	-0.56875700	0.14300100	C	6.05123500	-4.24337100	-0.89370700
C	4.77724100	0.23661700	1.35764500	H	6.16593800	-4.87603800	-0.00730100
C	5.27321100	-0.18342500	0.16133500	H	6.17041100	-4.88229400	-1.77503000
N	4.19585900	-0.67350500	-0.57112100	H	6.86423000	-3.51074900	-0.89657700
N	3.40675800	-0.00589500	1.33215200	C	2.12142100	2.62978000	1.36794800
Cl	6.88485000	-0.15318600	-0.41136200	C	2.93108400	-2.05270600	3.38042100
Cl	5.60015000	0.93856200	2.68285600	C	2.66499300	3.93275300	1.98513700
C	4.13112800	-0.34517800	-3.00458200	H	2.89894300	4.65435700	1.19537000
C	4.28049200	-1.22003000	-1.91008600	H	1.93248400	4.39863400	2.65251400
C	4.50779500	-2.60276100	-2.05942300	H	3.57765100	3.75099400	2.56106700
C	4.57224000	-3.10444500	-3.36547500	C	3.79501600	-2.26405400	4.63946200
C	4.42178800	-2.26723700	-4.46768500	H	4.54589500	-1.47508900	4.74557100
C	4.20472800	-0.90390500	-4.28682200	H	3.18338000	-2.27111600	5.54779200
H	4.73965800	-4.16581800	-3.51961800	H	4.31599600	-3.22552500	4.58235200
H	4.47414300	-2.67878900	-5.47141400	C	0.85190700	2.89438900	0.53478900
H	4.08906700	-0.26136000	-5.15405700	H	0.04393100	3.29624600	1.15564200
C	1.86907000	1.56357000	2.42931100	H	1.06197900	3.62370300	-0.25492500
C	0.97701700	1.82508600	3.47691400	H	0.49131700	1.97360700	0.06535500
C	0.71939800	0.87207100	4.45878600	H	2.88446800	2.25614900	0.67937800
C	1.35252600	-0.36718800	4.41524600	Cu	1.25828600	-1.08935100	-0.41863700
C	2.25434000	-0.68548700	3.39187500	H	-0.73535100	-3.47069000	-0.07673800
C	2.48811400	0.29761900	2.41002700	C	1.90162200	-3.18800400	3.21706600
H	0.47754100	2.78781900	3.52270600	H	2.41193100	-4.15574300	3.16658600
H	0.02357800	1.09644100	5.26197000	H	1.20648100	-3.22103800	4.06260000
H	1.14339500	-1.10096600	5.18738000	H	1.31477800	-3.06168100	2.30185600
C	3.88808300	1.15247500	-2.84674200	H	3.60032600	-2.09813000	2.51657000
H	3.90273400	1.39307700	-1.77985900	C	-1.17891500	-2.70558500	-0.72363700
C	2.49892200	1.55094200	-3.38279800	C	-0.48833400	-1.57837000	-1.00105400
H	2.32166900	2.61916600	-3.21834800	H	-1.04584000	-0.89242200	-1.66059600
H	2.41645000	1.35977500	-4.45805300	C	-4.51881300	3.03904900	-0.27400900
H	1.70620800	0.98915500	-2.87861200	C	-4.00454600	1.59580500	-0.08661600
C	5.00201000	1.98163100	-3.51505100	H	-4.94806300	3.14041000	-1.27631000
H	4.83800000	3.04892100	-3.33310600	H	-5.32748300	3.22865000	0.44209700
H	5.98756400	1.71608600	-3.12037100	C	-5.09475800	0.57108100	-0.23711400

O	-5.63082400	-0.08559800	0.59149000	H	-9.47648200	4.53162800	-0.19485800
Br	-5.69274900	0.37244500	-2.17795800	H	-9.73771400	4.17014100	1.50357600
H	-3.59482900	1.45976400	0.91939400	C	-12.11472200	5.15528600	0.44404600
C	-3.39928500	4.06948400	-0.07789200	H	-11.65751200	3.42365000	-0.76814000
H	-2.59085600	3.86645900	-0.79357700	H	-11.91940700	3.05677000	0.92806100
H	-2.96316300	3.94892100	0.92318300	H	-13.19434600	5.11033100	0.26550500
C	-3.88622800	5.51387300	-0.25161300	H	-11.96117700	5.52664000	1.46389000
H	-4.69768800	5.71079800	0.46302200	H	-11.69414900	5.89798700	-0.24382500
H	-4.32555400	5.63051400	-1.25215700	C	0.78375100	-1.69892700	0.16344800
C	-2.77714600	6.55615900	-0.05931500	C	1.90132200	-3.38284200	1.21371000
H	-1.96697400	6.36027100	-0.77611800	C	1.43314000	-3.87884100	0.04060100
H	-2.33505700	6.43498800	0.93997600	N	0.73517000	-2.84994200	-0.58724700
C	-3.26265500	8.00162100	-0.22610300	N	1.53057400	-2.03944800	1.26695700
H	-3.70533900	8.12341200	-1.22513700	Cl	1.68106100	-5.43471000	-0.62438100
H	-4.07336300	8.19714400	0.49049400	Cl	2.73419800	-4.20811100	2.46026300
C	-2.15627600	9.04667600	-0.03344800	C	0.68814200	-2.41290700	-3.00366400
H	-1.34737400	8.85321500	-0.75128100	C	0.06429900	-2.97835100	-1.86796100
C	-2.65053300	10.48763100	-0.19769800	C	-1.15829000	-3.68250400	-1.93826500
H	-3.06903200	10.65094700	-1.19758200	C	-1.79011500	-3.73776800	-3.18820000
H	-3.43555600	10.72215400	0.53053500	C	-1.22646600	-3.14626400	-4.31371500
H	-1.71269300	8.92321300	0.96405900	C	0.00645800	-2.50551300	-4.22294800
H	-1.83858700	11.20856800	-0.05526200	H	-2.73722300	-4.26003700	-3.27842200
H	-3.22327500	1.37618200	-0.82023000	H	-1.73957200	-3.20065300	-5.26947300
TS8''				H	0.45126700	-2.07937900	-5.11543500
C	-9.27053000	2.43659800	0.29877700	C	3.39865900	-0.72895400	2.19056400
C	-7.75323200	2.46187200	0.52501400	C	3.84800300	0.20807900	3.13138600
H	-9.47960100	2.06673000	-0.71535800	C	3.00001500	0.71522300	4.11119400
H	-9.72884500	1.71109000	0.98637500	C	1.68267600	0.27360400	4.19097000
C	-7.07921000	1.09488900	0.35020300	C	1.16946100	-0.65648300	3.27773400
H	-7.29625400	3.18161600	-0.16919700	C	2.03816300	-1.11376000	2.26356700
H	-7.54363900	2.84147400	1.53546500	H	4.88275500	0.53458000	3.10120900
H	-7.52388200	0.37813800	1.05594600	H	3.37239800	1.44165200	4.82753700
H	-7.30006100	0.70740200	-0.65489700	H	1.04322900	0.65412800	4.97950000
C	-5.55919100	1.13319700	0.55488200	C	2.09446900	-1.81488700	-2.96312700
C	-4.87554600	-0.23810800	0.39666900	H	2.30545800	-1.50831200	-1.93529700
H	-5.33755800	1.53228100	1.55525100	C	2.25992900	-0.56503000	-3.84486500
H	-5.11108300	1.83770900	-0.15935900	H	3.25679000	-0.13836200	-3.68998800
H	-5.34605600	-0.93877600	1.10635300	H	2.17556300	-0.80022600	-4.91093600
H	-5.07445100	-0.63180800	-0.60943800	H	1.51826800	0.19922400	-3.59901300
C	-9.94009000	3.80378700	0.48670300	C	3.13584800	-2.88672900	-3.35343400
C	-11.45570900	3.78580200	0.24933100	H	4.14839300	-2.47414700	-3.28718100

H	3.08288500	-3.76414000	-2.70242800	C	0.71870900	1.55614300	0.14105600
H	2.97575100	-3.22467000	-4.38326500	O	0.00454000	1.80673100	1.06782700
C	-1.79173600	-4.43208900	-0.76452100	Br	-0.33914100	1.74659300	-1.92661600
H	-1.16791300	-4.28085700	0.12155300	H	2.70931200	1.51998900	0.74640200
C	-3.20310200	-3.92185100	-0.41793800	C	3.80680900	3.84642300	-0.36557100
H	-3.18817700	-2.86735000	-0.13900600	H	4.18954900	3.37533900	-1.28130600
H	-3.89033300	-4.04887000	-1.26172700	H	4.40474200	3.44335400	0.46326100
H	-3.60494200	-4.49923300	0.42221000	C	4.01110400	5.36502700	-0.45105700
C	-1.85038400	-5.94919600	-1.05061400	H	3.62188000	5.83538400	0.46276900
H	-2.21189900	-6.48108700	-0.16418200	H	3.41009900	5.76428600	-1.27987500
H	-2.54366300	-6.16504400	-1.87052900	C	5.47786600	5.76993100	-0.64554800
H	-0.87432400	-6.35889200	-1.31898800	H	5.86721500	5.29493300	-1.55737300
C	4.41509000	-1.31606000	1.20476600	H	6.07752600	5.37100600	0.18514500
C	-0.24707200	-1.19897000	3.45403100	C	5.68493800	7.28706900	-0.73682100
C	5.57263200	-2.00464800	1.96115200	H	5.08692200	7.68577600	-1.56884300
H	6.22338500	-2.52490300	1.25080800	H	5.29272000	7.76296000	0.17351500
H	6.18655000	-1.27321200	2.49685300	C	7.15108400	7.69579900	-0.92804500
H	5.20781400	-2.73499800	2.68690200	H	7.54340200	7.21933700	-1.83690800
C	-0.23929500	-2.38496800	4.44319400	C	7.34788100	9.21248500	-1.02072400
H	0.42829500	-3.18625300	4.11364000	H	6.79036600	9.63266800	-1.86583900
H	0.09198400	-2.06018400	5.43586700	H	6.99512400	9.71337500	-0.11168000
H	-1.24744500	-2.80122700	4.54192600	H	7.74828200	7.29909700	-0.09555800
C	4.98926600	-0.27558300	0.22374100	H	8.40300000	9.47277900	-1.15585700
H	5.44476000	0.56869400	0.75196100	H	2.49647300	1.44903200	-1.02088400
H	5.76644300	-0.73937800	-0.39227900	24''			
H	4.22311500	0.11547700	-0.44791500	C	-8.71696100	3.01210700	0.40854500
H	3.91969500	-2.08006600	0.60093400	C	-7.19153700	2.96747700	0.56564000
Cu	-0.47453900	-0.18421300	-0.20452400	H	-8.98799900	2.65334900	-0.59485200
H	-3.10403300	0.14305400	1.63729700	H	-9.17508400	2.30617700	1.11635700
C	-1.25647600	-0.13099600	3.90824200	C	-6.59471600	1.57085400	0.34874200
H	-2.26435100	-0.55699000	3.90261000	H	-6.73298100	3.67164600	-0.14315600
H	-1.05862300	0.21495600	4.92835200	H	-6.91946700	3.32670300	1.56853200
H	-1.24877400	0.73599200	3.24259200	H	-7.05268200	0.86678500	1.05866300
H	-0.59288100	-1.57518100	2.48776600	H	-6.86897300	1.21171700	-0.65363200
C	-3.38029600	-0.19023200	0.63201500	C	-5.06911000	1.52255400	0.50207800
C	-2.42138200	-0.48739900	-0.26580200	C	-4.48005800	0.11673300	0.28043800
H	-2.81607400	-0.81241700	-1.24128500	H	-4.79229000	1.87753100	1.50489400
C	2.33550300	3.45875600	-0.17121800	H	-4.60467800	2.22006300	-0.20794900
C	2.15198000	1.92687400	-0.10422500	H	-4.97403200	-0.57866100	0.97822100
H	1.73194900	3.85040600	-0.99694600	H	-4.72844300	-0.22610100	-0.73212100
H	1.94861300	3.90497000	0.75224800	C	-9.31762100	4.40673300	0.62602800

C	-10.84285100	4.45014800	0.46708100	H	3.95297500	-2.72903700	-3.18592100
H	-8.86015100	5.11373800	-0.08106600	H	2.65778700	-3.88764700	-2.83383800
H	-9.04858100	4.76607400	1.62984100	H	2.75579500	-3.12988000	-4.42932200
C	-11.43493200	5.84614100	0.68738700	C	-2.37484600	-4.02323700	-1.26419000
H	-11.11136400	4.09240700	-0.53636400	H	-1.81020900	-4.08794800	-0.32968700
H	-11.29991600	3.74325700	1.17317200	C	-3.72441100	-3.36215500	-0.92913100
H	-12.52356200	5.84413500	0.56769900	H	-3.58143500	-2.38226300	-0.47566400
H	-11.21139800	6.21579400	1.69488800	H	-4.34497400	-3.24495800	-1.82409500
H	-11.02270100	6.56798700	-0.02720200	H	-4.27757200	-3.99348300	-0.22514300
C	0.50938200	-1.73229300	0.14141700	C	-2.62395800	-5.46227100	-1.76972000
C	1.17688700	-3.66107900	1.13472100	H	-3.10046200	-6.05581100	-0.98248400
C	0.74505000	-3.97700900	-0.11156400	H	-3.29600400	-5.46112500	-2.63429700
N	0.30826300	-2.79422200	-0.70650900	H	-1.70022000	-5.96468200	-2.06376700
N	1.06590800	-2.27693200	1.27005400	C	4.03322600	-2.18433400	1.40036900
Cl	0.80406200	-5.49501900	-0.89356800	C	-0.63080700	-1.22836600	3.43564700
Cl	1.72270600	-4.71028200	2.36947000	C	4.97757100	-3.12606100	2.18058300
C	0.53671500	-2.13975000	-3.06406800	H	5.53840600	-3.75408800	1.48075500
C	-0.25537400	-2.71359500	-2.04371700	H	5.70463700	-2.55919400	2.77102100
C	-1.54954400	-3.23145200	-2.28232300	H	4.42815900	-3.78003400	2.86157300
C	-2.07472200	-3.05950200	-3.57007000	C	-0.94256700	-2.46380600	4.30841500
C	-1.34554800	-2.43569900	-4.57699700	H	-0.45172100	-3.36547300	3.93144200
C	-0.04673900	-2.00173200	-4.32967300	H	-0.60595100	-2.30509200	5.33898300
H	-3.07179400	-3.42931800	-3.78671200	H	-2.02189500	-2.64855000	4.32979700
H	-1.78080000	-2.30999500	-5.56402600	C	4.86371500	-1.25722400	0.49384600
H	0.52827300	-1.55854700	-5.13515200	H	5.43988400	-0.53029000	1.07648300
C	3.10203100	-1.44051500	2.36620600	H	5.57540900	-1.85225800	-0.08787500
C	3.67715000	-0.67336800	3.38849600	H	4.23532800	-0.71237700	-0.21320600
C	2.89640800	-0.07905200	4.37468400	H	3.42851400	-2.80818900	0.73816700
C	1.51620300	-0.25728400	4.37529300	Cu	-0.14255300	0.09471000	-0.28369900
C	0.87650500	-0.99327300	3.37044800	H	-2.65385100	0.35288000	1.48299300
C	1.68990600	-1.54302200	2.35867400	C	-1.41079500	-0.00521700	3.94793500
H	4.75585400	-0.55753500	3.42083800	H	-2.48540200	-0.19318200	3.86127900
H	3.36702900	0.50799200	5.15788400	H	-1.20624200	0.19958700	5.00396400
H	0.92545500	0.18624900	5.16861200	H	-1.17017100	0.89217600	3.37157900
C	2.01129700	-1.78514000	-2.87350500	H	-0.99009700	-1.43797000	2.42414000
H	2.20065600	-1.65139500	-1.80558100	C	-2.97864200	0.06171300	0.48170100
C	2.42398300	-0.47626500	-3.56898800	C	-2.07238300	-0.25995000	-0.45207600
H	3.45798300	-0.23079500	-3.30366500	H	-2.43469800	-0.53501700	-1.44680800
H	2.38688400	-0.56238000	-4.65991400	C	2.93799300	3.14221200	0.05833500
H	1.78117200	0.35546500	-3.26814400	C	2.71421500	1.62338000	-0.06432000
C	2.89514400	-2.95611600	-3.35667500	H	2.19169700	3.65764900	-0.55624300

H	2.76234900	3.44463000	1.09699600
C	1.35650100	1.18763800	0.43636800
O	0.82342900	1.58979800	1.44141800
Br	-0.24641400	1.98139600	-1.79223600
H	3.43491300	1.09279400	0.56898200
C	4.35107000	3.55147600	-0.37497200
H	4.51553700	3.24670200	-1.41790700
H	5.09039000	3.00293800	0.22575000
C	4.60744700	5.05839500	-0.23950400
H	4.44155800	5.36067600	0.80416900
H	3.86691700	5.60761700	-0.83752500
C	6.01973200	5.47481100	-0.67020800
H	6.18064100	5.18145500	-1.71745300
H	6.75835400	4.91294100	-0.08046900
C	6.28970900	6.97702600	-0.51779500
H	5.55198700	7.54103900	-1.10643900
H	6.12963300	7.27021200	0.52982600
C	7.70261600	7.39233200	-0.94766300
H	7.86088800	7.10321900	-1.99561200
C	7.96763600	8.89274900	-0.78592400
H	7.26974400	9.48533500	-1.38872700
H	7.84816600	9.20491700	0.25812100
H	8.43935600	6.82551400	-0.36195400
H	8.98366300	9.15670600	-1.09794300
H	2.84880200	1.27732200	-1.09061100