

Electronic Supplementary Information for

Insights into the NHC-catalyzed cascade Michael/aldol/lactamization reaction: mechanism and origin of stereoselectivity

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1. Computational details

All the theoretical calculations were performed by using the Gaussian 09 software by using density functional theory. The geometrical structures were optimized in the DCM solvent ($\epsilon=8.93$) using the integral equation formalism polarizable continuum model (IEF-PCM) at M06-2X/6-31G(d, p) level. Correspondingly, vibrational frequency calculations at the same level of theory were performed to reveal that the reactants, catalyst, intermediates, and products have no imaginary frequencies and the transition states have one and only one imaginary frequency. In addition, IRC calculations were also performed to confirm that the transition states indeed connected the correct reactant and product in each elementary step. Furthermore, we have then refined the energy by carrying out the single-point energy calculations at M06-2X-GD3/6-311++G(2df, 2pd)//IEF-PCM_{DCM} level based on the M06-2X/6-31G(d, p)//IEF-PCM_{DCM} optimized structures. The energies discussed in this work were obtained by the addition of a thermal correction at the M06-2X/6-31G(d, p)//IEF-PCM_{DCM} level to the corresponding single-point energy at the M06-2X-GD3/6-311++G(2df, 2pd)//IEF-PCM_{DCM} level.

Moreover, the atom charge and the discussed 3D-structures were employed and rendered by the natural bond orbital (NBO) and the CYLView software, respectively. The non-covalent interaction (NCI) analysis was plotted using the NCIPLOT software developed by Yang's group to distinguish efficient interactions in the stereoselective transition states. Additionally, the extent of enantioselectivity, in terms of enantiomeric excess (ee %), was also calculated by using the Boltzmann distribution of diastereomeric transition states with the following equation:

$$\frac{[R]}{[S]} = \frac{\exp(-G_{[R]}^\ddagger / RT)}{\exp(-G_{[S]}^\ddagger / RT)} = \exp(\Delta G^\ddagger / RT) \quad (1)$$

$$ee = \frac{[R] - [S]}{[R] + [S]} \times 100\% = \frac{\frac{[R]}{[S]} - 1}{\frac{[R]}{[S]} + 1} \times 100\% \quad (2)$$

where G^\ddagger is the Gibbs free energy barrier of the competing diastereomeric transition state and ΔG^\ddagger is the Gibbs free energy difference between the two diastereomeric transition states.

2. Global reactivity index (GRI) analysis

Based on Domingo's definition, a molecule's global electrophilic character was described using the electrophilicity index $\omega = \mu^2/2\eta$. The μ and η were the electronic chemical potential and chemical hardness, respectively. Both characters can be obtained in terms of the energy of the highest occupied molecular orbital HOMO (E_H) and the lowest unoccupied molecular orbital LUMO (E_L), as $\mu = (E_H + E_L)/2$ and $\eta = (E_L - E_H)$. Also, the nucleophilicity index N was defined to produce a nucleophilicity scale. The nucleophilicity index was obtained by $N = E_{H(SR)} - E_{H(TCNE)}$. For this nucleophilicity scale, tetracyanoethylene was taken as reference.

3. Parr function analysis

Pioneered by Domingo and coworkers, the nucleophilic (P_k^-) and electrophilic (P_k^+) Parr functions which allow for the characterization of the nucleophilic and electrophilic sites of a molecule, can be obtained through the analysis of Mulliken atomic spin density (ASD) of the corresponding radical cations (RC) or anions (RA) of the studied molecules, separately. According to Domingo's definition, the Parr functions can be expressed by the following equations:

$$P^- (r) = \rho_s^{rc} (r) \text{ for the electrophilic attacks} \quad (3)$$

$$P^+ (r) = \rho_s^{ra} (r) \text{ for the nucleophilic attacks} \quad (4)$$

where $\rho_s^{rc}(r)$ is the ASD of the radical cation and $\rho_s^{ra}(r)$ is the ASD of the radical anion. Each ASD condensed at the different atoms of the radical cation and radical anion provides the local nucleophilic P_k^- and electrophilic P_k^+ Parr functions of the neutral system, respectively.

4. Gibbs free energy profiles of the direct [1,2]-proton transfer pathways

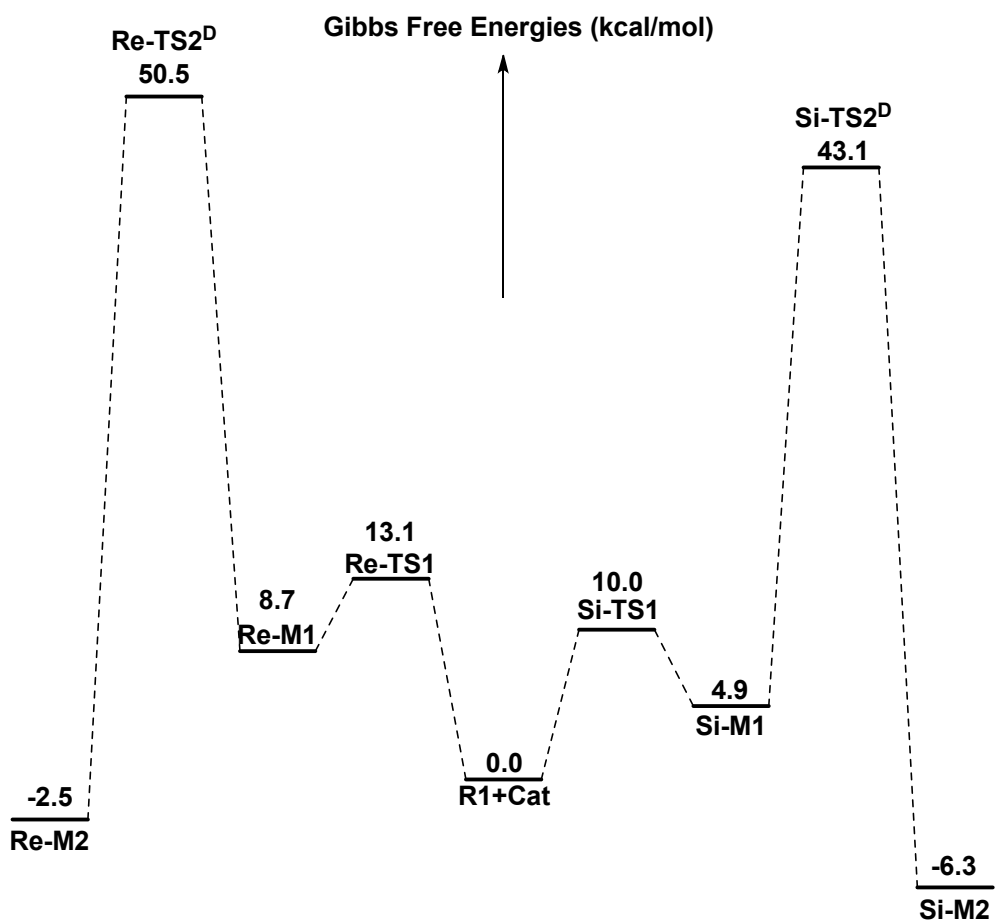


Fig. S1 The energy profiles of the direct [1,2]-proton transfer pathways

5. Gibbs free energy profiles of the other three pathways

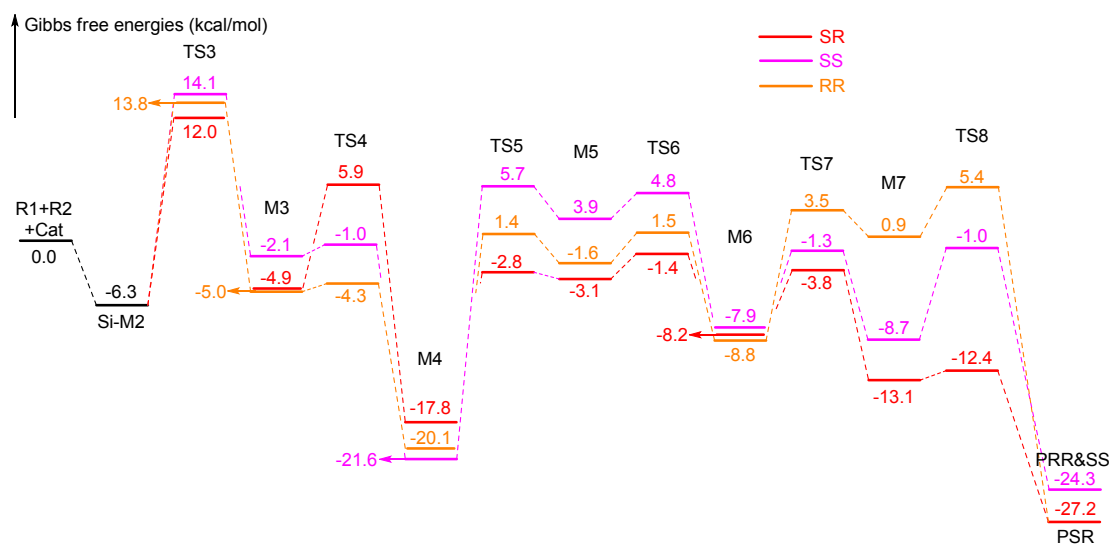
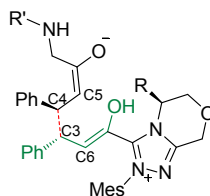


Fig. S2 Gibbs free energy profiles of the other three pathways of the catalytic cycle

6. Different conformations of TS3s

Table S1 Different conformations of the transition states involved in C-C bond formation step



	RR	RS	SR	SS
TS3	0.0	0.0	0.0	0.0
TS3-90	–	–	–	–
TS3-180	10.6	5.2	1.6	4.7
TS3-270	6.9	1.5	6.0	6.1

We have additionally considered and investigated the different conformations of **TS3s** in the C–C bond formation step in the revised manuscript. By rotating dihedral angle $\Phi_1(\text{C6-C3-C4-C5})$ from $0\sim 360^\circ$ at intervals of 90° in the four transition states **TS3RR**, **TS3RS**, **TS3SR**, and **TS3SS**, we have constructed sixteen ($4\times 4=16$) initial structures of **TS3s** and located the twelve conformations after the optimization, which are summarized in **Table S1**. As an important note, the initial structures by rotating the dihedral Φ_1 with 90° would lead to the same conformations of those with $\Phi_1=0/360^\circ$ after the structural optimizations. The relative Gibbs free energies depicted in **Table S1** show that the original conformations of the transition states **TS3RR**, **TS3RS**, **TS3SR**, and **TS3SS** indeed have the lowest energies among their conformers, and thus we only discussed them in the main text.

7. Single-point energies of all the stationary points

Table S2 Single-point energies of all the stationary points involved in the reaction calculated at M06-2X-GD3/6-311++G(2df, 2pd)/IEF-PCM_{DCM} level

R1	-422.934873	Re-M2	-1475.202087
R2	-785.553891	Si-M2	-1475.207245
Cat	-1052.237228	TS3RR	-2260.756876
tBuOH	-233.650877	TS3RS	-2260.76907
DBU	-462.042257	TS3SR	-2260.761416
DBU·H⁺	-462.511059	TS3SS	-2260.759062
Re-TS1	-1475.172096	M3RR	-2260.788876
Si-TS1	-1475.177971	M3RS	-2260.787149
Re-M1	-1475.183951	M3SR	-2260.774042
Si-M1	-1475.190816	M3SS	-2260.782288
Re-M02-tBuOH	-1708.857042	TS4RR	-2260.788467
Re-M02-DBU	-1937.270285	TS4RS	-2260.785979
Re-M02-DBUH	-1937.738276	TS4SR	-2260.781934
Re-TS2-tBuOH	-1708.825059	TS4SS	-2260.779943
Re-TS2-DBU	-1937.214813	M4RR	-2260.818201
Re-TS2-DBUH	-1937.709082	M4RS	-2260.818583
Si-M02-tBuOH	-1708.864333	M4SR	-2260.813841
Si-M02-DBU	-1937.274865	M4SS	-2260.817916
Si-M02-DBUH	-1937.740265	TS5RR	-2260.780465
Si-TS2-tBuOH	-1708.83203	TS5RS	-2260.794649
Si-TS2-DBU	-1937.22162	TS5SR	-2260.786187
Si-TS2-DBUH	-1937.715076	TS5SS	-2260.77361
Re-TS2^D	-1475.117878	M5RR	-2260.787839
Si-TS2^D	-1475.12396	M5RS	-2260.791596

Continued

M5SR	-2260.788849	M7RR	-2260.77977
M5SS	-2260.77659	M7RS	-2260.818115
TS6RR	-2260.776578	M7SR	-2260.805155
TS6RS	-2260.784623	M7SS	-2260.78847
TS6SR	-2260.778562	TS8RR	-2260.776704
TS6SS	-2260.774024	TS8RS	-2260.807383
M6RR	-2260.79746	TS8SR	-2260.801935
M6RS	-2260.809846	TS8SS	-2260.769001
M6SR	-2260.795473	PRR	-1208.559692
M6SS	-2260.799509	PRS	-1208.559886
TS7RR	-2260.783058	PSR	-1208.559886
TS7RS	-2260.803085	PSS	-1208.559692
TS7SR	-2260.78607	TS6RS'	-2260.768209
TS7SS	-2260.784378	M6RS'	-2260.781161

8. Cartesian coordinates of all the stationary points involved in the reaction

R1

C	-3.40868200	0.38467900	-0.00002100
O	-3.84922700	-0.74897600	0.00001800
H	-4.09882800	1.24931300	0.00004800
C	-1.97271400	0.71939000	-0.00000900
C	-1.05272300	-0.25948400	-0.00000400
H	-1.71185800	1.77329500	-0.00001300
H	-1.42980200	-1.28220100	-0.00000900
C	0.40445300	-0.11249400	-0.00000300
C	1.19488900	-1.26994600	-0.00000500
C	1.04080300	1.13825700	0.00000300
C	2.58320700	-1.18499600	0.00000000
H	0.70997200	-2.24230900	-0.00000800
C	2.42610900	1.22321300	0.00000400
H	0.45077600	2.04914100	0.00000600
C	3.20171500	0.06230300	0.00000300
H	3.18064400	-2.09057900	0.00000200
H	2.90602800	2.19642100	0.00001100
H	4.28453900	0.13319200	0.00000600

R2

C	3.62993600	0.50242200	0.00003400
C	3.20525200	-0.85335300	-0.00006000
C	4.17507200	-1.87538800	-0.00006600
C	5.51000100	-1.52593200	0.00001600
C	5.90988700	-0.16904300	0.00011000

C	4.98709400	0.85831500	0.00012100
C	1.39214100	0.48238500	-0.00004600
C	1.77738700	-0.84075700	-0.00013600
H	3.87162800	-2.91777600	-0.00014000
H	6.27037000	-2.29996200	0.00001000
H	6.96870700	0.06903400	0.00017400
H	5.29490400	1.89854600	0.00019400
H	1.12632800	-1.70270900	-0.00022300
N	2.51025300	1.28378500	0.00002700
H	2.45535000	2.29210300	0.00008500
C	0.07520100	1.13836400	-0.00004300
O	0.01763200	2.36447900	-0.00010300
C	-1.12298900	0.27531200	-0.00002200
C	-2.34122500	0.83815300	-0.00001600
H	-0.97749800	-0.79969900	-0.00001400
H	-2.37225700	1.92730500	-0.00002500
C	-3.63842500	0.15756600	0.00000500
C	-4.80190400	0.93881300	0.00000900
C	-3.76514400	-1.23995400	0.00002600
C	-6.05962700	0.34488100	0.00003300
H	-4.71185000	2.02158800	-0.00000700
C	-5.02019800	-1.83287900	0.00004900
H	-2.87905700	-1.86673200	0.00002200
C	-6.17137100	-1.04279600	0.00005300
H	-6.95038600	0.96425500	0.00003600
H	-5.10488500	-2.91461600	0.00006500
H	-7.15071900	-1.51032500	0.00007100

Cat

C	-3.78315900	0.57348400	-0.37315100
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C	-2.93275300	0.62429600	0.73392500
C	-2.74379600	1.80356900	1.44450800
C	-3.43242000	2.94467800	1.03620500
C	-4.29135100	2.89655400	-0.06400000
C	-4.47240600	1.71213100	-0.77712700
C	-3.78730300	-0.80545000	-0.98394000
C	-3.22858600	-1.67038600	0.16725300
C	-2.30593000	-0.72646700	0.98128800
H	-2.06951200	1.83115800	2.29430000
H	-3.30419100	3.87611200	1.57796200
H	-4.82589200	3.79178700	-0.36581200
H	-5.14087400	1.68050900	-1.63231700
H	-3.12846200	-0.82931200	-1.86003200
H	-4.05742100	-1.95361200	0.82067700
H	-4.77448600	-1.14303600	-1.30692200
H	-2.26773000	-0.99922700	2.03854700
N	-0.94311500	-0.80531700	0.44599700
O	-2.61582000	-2.88974800	-0.19796800
C	0.10052300	0.00658200	0.81300800
C	-0.53606500	-1.74167000	-0.46833800
N	1.07813100	-0.51827100	0.04685100
N	0.72268200	-1.59150800	-0.74724300
C	-1.48404400	-2.75306500	-1.03491400
H	-1.77156800	-2.46892700	-2.05540300
H	-1.00129400	-3.73066100	-1.08190900
C	2.43007600	-0.05145600	-0.00273900
C	2.69982800	1.16298200	-0.64004300
C	3.43283800	-0.82892300	0.58244100
C	4.02449900	1.59739500	-0.67585400
C	4.74378100	-0.35790100	0.51658500

C	5.05772600	0.84895000	-0.10991400
H	4.25465300	2.54170400	-1.16376400
H	5.53740200	-0.94558900	0.97225700
C	3.09558200	-2.12388200	1.27205100
H	2.75659900	-2.87412400	0.55209000
H	2.28358300	-1.97929200	1.99142200
H	3.96550000	-2.51678500	1.80121200
C	6.48636000	1.32153500	-0.19808800
H	6.95558100	0.96293600	-1.12017800
H	7.07915500	0.94846100	0.64029100
H	6.54264900	2.41255800	-0.20314400
C	1.59116300	1.96882900	-1.26348500
H	0.87720200	2.30157600	-0.50505200
H	1.03109500	1.36443000	-1.98408800
H	1.99331700	2.84225900	-1.77966200

tBuOH

C	0.67343200	1.25812700	-0.52218800
C	-0.00572900	-0.00000300	0.01760500
H	0.19850000	2.14986400	-0.10406500
H	1.73401000	1.26931800	-0.24728800
H	0.60703400	1.30367900	-1.61310800
C	0.67535200	-1.25696700	-0.52244800
C	-1.49027100	-0.00110000	-0.32563100
H	0.20193600	-2.14953100	-0.10437700
H	0.60883900	-1.30247400	-1.61336200
H	1.73601100	-1.26651600	-0.24777800
H	-1.63495300	-0.00062900	-1.40911500
H	-1.97176100	-0.88945700	0.09248700
H	-1.97324800	0.88599200	0.09345700

O	0.04948400	-0.00008300	1.44604100
H	0.98104900	0.00006800	1.70079700
DBU			
C	2.78413000	-0.05200700	0.34619000
C	1.89212800	-1.28076600	0.52457300
C	0.85127500	-1.44033500	-0.59085000
C	2.03933200	1.28290300	0.34443100
C	0.94968400	1.40161900	-0.73528700
C	-0.34015300	0.72000800	-0.33235000
H	3.32227800	-0.15359500	-0.60654000
H	1.37059400	-1.24155000	1.48980400
H	0.53385300	-2.48444100	-0.65079500
H	2.76706200	2.08698100	0.19384300
H	1.32199100	1.01138100	-1.69009900
C	-1.51540400	-1.36420800	0.14705000
H	-1.36606600	-1.57171000	1.21814200
C	-2.53476200	0.85820100	0.52702900
C	-2.76950000	-0.53011600	-0.05652900
H	-3.62822000	-1.01737700	0.41329300
H	-2.97250900	-0.44911300	-1.12987700
H	-2.51803200	0.79783600	1.62475300
H	-1.60367500	-2.32808800	-0.36385100
H	-3.36763600	1.52229500	0.27109100
N	-1.29748800	1.48025800	0.06975800
N	-0.36695200	-0.65738400	-0.40868300
H	1.31042700	-1.20171100	-1.55848400
H	2.52469600	-2.17504600	0.54008300
H	3.54544600	-0.03722500	1.13362600
H	1.57723100	1.45798200	1.32424700

H	0.69326100	2.45147600	-0.88230700
DBU•H ⁺			
C	2.83746700	-0.01137200	0.29230200
C	1.99719700	-1.27214600	0.49249200
C	0.90249500	-1.45898300	-0.55873100
C	2.05100800	1.29735400	0.35130400
C	0.93965800	1.40212400	-0.71112600
C	-0.29884700	0.65238500	-0.31002400
H	3.33918300	-0.07620500	-0.68195100
H	1.53526500	-1.27930400	1.48723900
H	0.57784100	-2.49913300	-0.58151900
H	2.73764200	2.13222000	0.19006600
H	1.29410300	1.02065300	-1.67436700
C	-1.51354300	-1.40956100	0.14257200
H	-1.40715000	-1.66686000	1.20223200
C	-2.61649000	0.78417400	0.52089300
C	-2.76925500	-0.59056500	-0.10678700
H	-3.62936800	-1.10504000	0.32392200
H	-2.93497000	-0.48865900	-1.18284200
H	-2.60590300	0.72125400	1.61337600
H	-1.54316200	-2.33611800	-0.43268600
H	-3.42219600	1.45386400	0.21955400
N	-1.35455200	1.36203700	0.05894400
N	-0.31343200	-0.66866000	-0.28565400
H	1.27285300	-1.21486500	-1.55989700
H	2.65448500	-2.14527800	0.44180000
H	3.62696100	0.01715400	1.04901600
H	1.61155400	1.43734900	1.34573500
H	0.66273000	2.44694200	-0.86533100

H	-1.27211000	2.36793900	0.01525500
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Re-TS1

C	0.59235400	1.08061700	-1.36744200
O	0.86892300	0.32927500	-2.33071600
H	1.34919100	1.79306300	-0.97822400
C	-0.81015800	1.58958400	-1.20073300
C	-1.09821800	2.70624700	-0.52608500
H	-1.57763300	1.00151500	-1.70365200
H	-0.26971800	3.26418500	-0.08505600
C	-2.43546900	3.27780300	-0.30061000
C	-2.54334700	4.57117000	0.22618100
C	-3.61489200	2.57036600	-0.57842200
C	-3.78779200	5.15043900	0.45489100
H	-1.63751100	5.12637900	0.45471700
C	-4.85801800	3.14775600	-0.34982800
H	-3.56098900	1.55761500	-0.96846500
C	-4.95044100	4.44085400	0.16571200
H	-3.84942200	6.15522600	0.86052500
H	-5.75987300	2.58566500	-0.57061800
H	-5.92281700	4.88832000	0.34415100
C	-2.98606000	-2.83987800	-0.00422400
C	-2.01429100	-1.94212600	-0.43854100
C	-1.54165600	-1.94760900	-1.74864700
C	-2.08871800	-2.87382000	-2.63599800
C	-3.07584000	-3.76809800	-2.21395800
C	-3.52940700	-3.76077800	-0.89609100
C	-3.29155000	-2.64814200	1.45982000
C	-2.20051300	-1.68303200	1.97990400
C	-1.56983600	-1.03966800	0.69189000

H	-0.75689900	-1.25992500	-2.06764700
H	-1.74030900	-2.90470200	-3.66326800
H	-3.48648700	-4.48432000	-2.91862700
H	-4.28474300	-4.46867700	-0.56778100
H	-3.26776600	-3.58102000	2.03124000
H	-2.62327800	-0.90592200	2.61744200
H	-4.28400000	-2.20749400	1.59988900
H	-1.92493400	-0.01366000	0.56360600
N	-0.11857900	-0.98314100	0.79427300
O	-1.24867600	-2.33407300	2.81142900
C	0.74786500	-0.08858300	0.26319800
C	0.58145200	-1.98949700	1.40737500
N	1.93285600	-0.61117200	0.59893200
N	1.86051200	-1.78532600	1.31886100
C	-0.21568800	-3.02604300	2.12891100
H	-0.61883500	-3.76840600	1.42639600
H	0.39427700	-3.53562200	2.87448800
C	3.20899500	-0.03508600	0.29039200
C	3.95354600	-0.58448200	-0.75721200
C	3.64432100	1.05728500	1.04225300
C	5.18965300	-0.00614000	-1.03596400
C	4.88673800	1.60563300	0.72170400
C	5.67126900	1.08457400	-0.30695400
H	5.78892200	-0.41106600	-1.84820400
H	5.24766900	2.45862800	1.29102000
C	2.79178100	1.62627400	2.14551400
H	2.47372600	0.84346500	2.84059400
H	1.88427700	2.08717000	1.74065500
H	3.34150300	2.38562000	2.70386300
C	7.02191300	1.67260500	-0.62488900

H	7.82278400	1.01577100	-0.27077900
H	7.15221700	2.64715400	-0.15020000
H	7.15269500	1.79368100	-1.70345900
C	3.40487600	-1.73327600	-1.55881000
H	2.45283000	-1.43304200	-2.00961800
H	3.22137300	-2.60491100	-0.92373800
H	4.10105300	-2.01854200	-2.34941800

Si-TS1

C	0.04176900	1.55712400	-0.78903200
O	0.26464400	2.20455400	0.25755100
H	0.71230700	1.68606100	-1.66290300
C	-1.35652900	1.19048200	-1.19359100
C	-2.40345700	1.63568500	-0.49280100
H	-1.46173300	0.59213800	-2.09734400
H	-2.17836500	2.24827500	0.37971000
C	-3.82751300	1.40773700	-0.78132200
C	-4.78689000	2.16843800	-0.10109400
C	-4.27221500	0.46309200	-1.71836800
C	-6.14583200	2.01730300	-0.36618400
H	-4.45594700	2.89473300	0.63676900
C	-5.62763000	0.30547200	-1.98011600
H	-3.54993000	-0.16754600	-2.22957300
C	-6.57136300	1.08779900	-1.31148100
H	-6.87076500	2.62414900	0.16722500
H	-5.95339600	-0.43238600	-2.70692100
H	-7.62916300	0.96391300	-1.52016100
C	5.36308700	0.64874600	-0.42747400
C	3.99958000	0.92061300	-0.34787000
C	3.50373100	1.96966800	0.42082100

C	4.41903700	2.75532400	1.11951800
C	5.78936400	2.49212000	1.04518100
C	6.27209600	1.43875500	0.27110400
C	5.63250800	-0.53125300	-1.32629900
C	4.24755900	-1.16639500	-1.58516100
C	3.20282400	-0.05797300	-1.18460100
H	2.43206600	2.16409600	0.47589600
H	4.06460700	3.57943500	1.73040700
H	6.48529700	3.11298900	1.60070300
H	7.33720000	1.23299200	0.22037100
H	6.30592700	-1.27139000	-0.88382700
H	4.11833400	-1.44330900	-2.63205400
H	6.08209100	-0.20649700	-2.27065100
H	2.78447500	0.41373900	-2.07767500
N	2.09224500	-0.64303500	-0.44480500
O	4.07635500	-2.38716500	-0.87630700
C	0.77679600	-0.31113000	-0.44260500
C	2.30886400	-1.65891700	0.44826800
N	0.27768900	-1.15897500	0.46643500
N	1.20143100	-2.01456600	1.02505700
C	3.67861100	-2.25157600	0.47920900
H	4.37324600	-1.61779000	1.04649800
H	3.65879800	-3.24695400	0.92249600
C	-1.10821200	-1.25825100	0.82219400
C	-1.56699200	-0.56102400	1.93745100
C	-1.94980100	-1.98970900	-0.01944100
C	-2.93952400	-0.58755800	2.18896100
C	-3.30970600	-1.99362000	0.27612100
C	-3.82267800	-1.27908900	1.36078400
H	-3.32827800	-0.03306000	3.04008500

H	-3.99009900	-2.54086100	-0.37275900
C	-1.40052500	-2.70884000	-1.22255100
H	-0.55600100	-3.34907900	-0.95072400
H	-1.03651800	-1.99357100	-1.96818400
H	-2.17076300	-3.32658900	-1.68746400
C	-5.30963700	-1.20838000	1.58102600
H	-5.78378500	-2.17904300	1.41330400
H	-5.75024300	-0.49541600	0.87429500
H	-5.54873800	-0.87446700	2.59315900
C	-0.61902800	0.24966300	2.77830100
H	-0.24234100	1.09120600	2.18498300
H	0.23891500	-0.34926600	3.09783600
H	-1.12450600	0.63459300	3.66604600

Re-M1

C	0.51001700	0.79686400	-1.12838700
O	0.72497100	0.03024600	-2.19854300
H	1.27151200	1.59667200	-0.93766500
C	-0.85003600	1.48711800	-1.09848700
C	-1.09684400	2.63654700	-0.46355500
H	-1.61805600	0.97404800	-1.67847100
H	-0.26962200	3.11857900	0.06171600
C	-2.38250000	3.35191100	-0.37945200
C	-2.43047200	4.57627800	0.29861000
C	-3.56958400	2.85406400	-0.93759000
C	-3.62147600	5.28678800	0.41637900
H	-1.51849200	4.97275800	0.73719900
C	-4.75880100	3.56350400	-0.82304600
H	-3.56475500	1.90529200	-1.46602500
C	-4.79119000	4.78268000	-0.14530100

H	-3.63491500	6.23348000	0.94710700
H	-5.66722700	3.16296300	-1.26193400
H	-5.72270000	5.33220200	-0.05627400
C	-2.86236800	-3.09273300	0.06296400
C	-1.96299600	-2.16387000	-0.45290200
C	-1.42934000	-2.27848200	-1.73442600
C	-1.83665300	-3.36393900	-2.50857500
C	-2.74685100	-4.29886100	-2.00671200
C	-3.26556900	-4.17196400	-0.71943100
C	-3.26995000	-2.74329400	1.47123100
C	-2.34786800	-1.57244400	1.88981300
C	-1.66516700	-1.07973600	0.55746600
H	-0.70581700	-1.54170200	-2.09699000
H	-1.43930900	-3.48784500	-3.51096300
H	-3.04801900	-5.13896300	-2.62470300
H	-3.96496200	-4.90617500	-0.33086700
H	-3.15457700	-3.57591000	2.17251900
H	-2.91546500	-0.75395500	2.33245700
H	-4.31839900	-2.43203200	1.51264600
H	-2.06894800	-0.10841000	0.26666800
N	-0.22064000	-0.91140500	0.74207500
O	-1.42376400	-1.93987100	2.90287000
C	0.66775300	-0.11000100	0.12100900
C	0.48099000	-1.73638500	1.58209600
N	1.84944900	-0.46807000	0.62653500
N	1.75305600	-1.48010900	1.54414300
C	-0.30533200	-2.67224600	2.43813600
H	-0.60573000	-3.56197800	1.86788000
H	0.28135500	-2.98287000	3.30208800
C	3.13756700	0.06068900	0.27078100

C	3.86183100	-0.59779900	-0.72421900
C	3.60651400	1.18692500	0.94997100
C	5.11903200	-0.08246600	-1.03775600
C	4.86621100	1.66544500	0.59674200
C	5.63438300	1.04101400	-0.38931200
H	5.70673900	-0.57000200	-1.81153800
H	5.25756400	2.54422200	1.10328900
C	2.76897900	1.85004700	2.01061800
H	2.47998400	1.13498700	2.78679500
H	1.84564100	2.25834200	1.58477400
H	3.31678000	2.66826800	2.47978900
C	7.00898600	1.55873700	-0.72490200
H	7.75212900	1.15067000	-0.03220800
H	7.05054000	2.64768500	-0.64716400
H	7.30372300	1.27099500	-1.73617600
C	3.27931100	-1.79356800	-1.42466100
H	2.33349900	-1.49388900	-1.89341000
H	3.07534500	-2.60035300	-0.71311800
H	3.96800100	-2.16793400	-2.18391400

Si-M1

C	-0.12417600	-1.02220100	-0.95131400
O	-0.36472100	-1.99358300	-0.07212000
H	-0.64135500	-1.12927700	-1.94202300
C	1.33722800	-0.75499200	-1.30407000
C	2.31290100	-1.47195700	-0.74574500
H	1.53605400	0.02480100	-2.04088400
H	1.99254000	-2.23697100	-0.03881900
C	3.76176900	-1.32679200	-0.96315600
C	4.63165700	-2.26367500	-0.39031100

C	4.32163800	-0.27720000	-1.70790900
C	6.01013000	-2.17467600	-0.57084200
H	4.21406000	-3.07536100	0.19990900
C	5.69622400	-0.18403000	-1.88809200
H	3.67399400	0.48246900	-2.13671100
C	6.54875400	-1.13590600	-1.32532000
H	6.66264800	-2.91705900	-0.12165700
H	6.10805400	0.63664200	-2.46780700
H	7.62196800	-1.06121200	-1.46864700
C	-5.32055900	-0.66483300	-0.38270500
C	-3.96104500	-0.95814700	-0.32463700
C	-3.45997900	-2.00144500	0.44902200
C	-4.37164900	-2.75519500	1.18572000
C	-5.73936300	-2.46941500	1.13896700
C	-6.22503500	-1.42600300	0.35345600
C	-5.59443500	0.49281400	-1.30787600
C	-4.20626800	1.08765600	-1.63882600
C	-3.16535900	-0.01182800	-1.19742800
H	-2.38533600	-2.19941700	0.45156400
H	-4.01815900	-3.57526300	1.80275100
H	-6.43181700	-3.06792300	1.72278400
H	-7.28814900	-1.20710500	0.32055000
H	-6.23323500	1.26322900	-0.86486400
H	-4.09705300	1.29724600	-2.70296400
H	-6.08766300	0.15207900	-2.22397900
H	-2.73677100	-0.51179600	-2.06891600
N	-2.06116100	0.60671800	-0.46134600
O	-3.99706800	2.34561400	-1.01182700
C	-0.75843700	0.27124700	-0.37561100
C	-2.28148800	1.65557300	0.38961400

N	-0.25318000	1.12997700	0.51438200
N	-1.18841100	2.00780500	0.99646700
C	-3.63912900	2.27548500	0.35735800
H	-4.35741400	1.68412600	0.94066000
H	-3.60553600	3.29063200	0.75160000
C	1.11552800	1.19753800	0.94792900
C	1.52754300	0.34135000	1.96719100
C	1.98003400	2.04461200	0.25213900
C	2.89249300	0.30840300	2.24991800
C	3.33201800	1.97915200	0.57651400
C	3.80647500	1.09254600	1.54589800
H	3.25332100	-0.37310200	3.01651400
H	4.03602100	2.60472800	0.03277600
C	1.46619400	2.95336900	-0.83241200
H	0.68249000	3.61646300	-0.45439200
H	1.03196400	2.37704500	-1.65722100
H	2.27431400	3.56565800	-1.23555500
C	5.28561500	0.93363200	1.76972400
H	5.81937900	1.87184300	1.60004800
H	5.67939900	0.19180100	1.06409600
H	5.50235000	0.58500400	2.78209400
C	0.54280500	-0.56081700	2.65662600
H	0.14046700	-1.26964800	1.91981400
H	-0.29193300	0.01313800	3.07222200
H	1.02646100	-1.10609100	3.46917800

Re-M02-tBuOH

C	-4.31025000	-2.10142900	0.59332500
C	-3.22961300	-1.28770600	0.25725300
C	-3.32863100	-0.32725500	-0.74510400

C	-4.55495700	-0.16420000	-1.38798000
C	-5.64826200	-0.95928600	-1.03812500
C	-5.53215400	-1.93727500	-0.05136700
C	-3.92850100	-3.09525100	1.66172300
C	-2.38707500	-3.05000400	1.70718400
C	-2.02093000	-1.65118400	1.09788000
H	-2.47215800	0.27885000	-1.03168200
H	-4.65654400	0.58253300	-2.16839700
H	-6.59542500	-0.82367000	-1.54998200
H	-6.37854800	-2.56825800	0.20179400
H	-4.26858900	-4.11289900	1.45209200
H	-2.00325900	-3.13298400	2.72429300
H	-4.34123800	-2.80231900	2.63311400
H	-1.83767300	-0.93544100	1.90355000
N	-0.80890100	-1.74860200	0.29215100
O	-1.79162900	-4.13799600	1.01171300
C	0.22103200	-0.89940300	0.10629100
C	-0.61038000	-2.83401600	-0.51563100
N	0.99577400	-1.50010600	-0.79640000
N	0.48999500	-2.71267400	-1.19312000
C	-1.58207500	-3.96080500	-0.37957000
H	-2.51465100	-3.73956400	-0.91419100
H	-1.15307200	-4.88246000	-0.77116500
C	2.23028200	-1.06426400	-1.40709300
C	3.41976900	-1.63227400	-0.96054300
C	2.15486700	-0.15602600	-2.46263300
C	4.58879900	-1.25437900	-1.62415200
C	3.34683900	0.18743000	-3.09221200
C	4.57084700	-0.35449400	-2.68850200
H	5.53591000	-1.67274700	-1.29278600

H	3.32178300	0.89901200	-3.91418000
C	0.83828500	0.45845400	-2.84524300
H	0.47725800	1.07577200	-2.01460000
H	0.08157100	-0.30582700	-3.05248000
H	0.94377600	1.08746700	-3.73058600
C	5.84132800	0.01955800	-3.40790000
H	5.87779000	1.09369100	-3.60687900
H	5.90676100	-0.49403200	-4.37255700
H	6.72222700	-0.25288400	-2.82312200
C	3.44619800	-2.55763000	0.22577300
H	2.70066700	-3.35193200	0.13116400
H	3.23861300	-1.98885500	1.13944600
H	4.43039700	-3.01851500	0.32707900
C	0.51499000	0.43612500	0.82111800
O	1.68009800	0.94222500	0.41063500
C	-0.69467700	1.35206200	0.63191500
C	-0.55395000	2.55453000	0.06964200
H	-1.66065600	1.01814900	1.00798700
H	0.45694400	2.82293300	-0.23465500
C	-1.61606400	3.54589900	-0.17194000
C	-1.25878300	4.81449900	-0.64586100
C	-2.97715600	3.27362700	0.03469400
C	-2.22344900	5.78585800	-0.89769100
H	-0.20873400	5.03648000	-0.81621900
C	-3.94166600	4.24121200	-0.21886500
H	-3.29003400	2.29445400	0.38619400
C	-3.56981100	5.50285100	-0.68429400
H	-1.92211000	6.76305600	-1.26153900
H	-4.98964200	4.01016900	-0.05489100
H	-4.32550300	6.25669100	-0.88004000

H	2.65975400	0.40273900	1.45243400
C	2.15229800	1.77179800	3.59926000
C	3.46153800	1.17242000	3.07182300
H	1.53827800	2.10320100	2.75495300
H	1.59658400	1.01438600	4.16241700
H	2.33696500	2.62812600	4.25680200
C	4.32131900	0.67546300	4.23013600
C	4.21775100	2.22687600	2.25644000
H	5.24819600	0.23878500	3.84594900
H	4.57582200	1.49100000	4.91426500
H	3.78503700	-0.09672700	4.79049000
H	4.45755900	3.11001600	2.85800000
H	5.15002100	1.80199800	1.87151800
H	3.59965800	2.53391600	1.40689000
O	3.18523500	0.05176000	2.25430500
H	0.50202700	0.12678700	1.89936500

Re-M02-DBU

C	4.08962100	2.65505400	-1.42205000
C	3.22018800	1.97468800	-0.57383500
C	3.43172400	1.93900600	0.80238400
C	4.52341800	2.62808600	1.32635100
C	5.38714600	3.32932500	0.48156100
C	5.18004700	3.34321500	-0.89653900
C	3.68047600	2.50017500	-2.86468500
C	2.55163200	1.44055600	-2.86351200
C	2.11999900	1.28679300	-1.35432800
H	2.76978200	1.36972700	1.45038900
H	4.70783800	2.61391700	2.39539900
H	6.23613400	3.85804500	0.90310100

H	5.86553100	3.87385100	-1.55085700
H	4.50189100	2.16751300	-3.50716500
H	1.69562400	1.77273800	-3.45216100
H	3.31284000	3.44646000	-3.27410000
H	1.15189100	1.77679600	-1.21992600
N	1.96101900	-0.10388500	-0.97897300
O	2.94599000	0.22418200	-3.47744300
C	1.09447300	-0.71596800	-0.08039500
C	2.72374100	-1.08605400	-1.55978200
N	1.37403900	-2.06844100	-0.24848600
N	2.41520200	-2.26930000	-1.15852800
C	3.66876800	-0.65272600	-2.62812700
H	4.54914800	-0.15641200	-2.19538800
H	3.99275300	-1.50723300	-3.22124100
C	1.20448800	-3.08318000	0.74969200
C	0.32154700	-4.13516500	0.49627800
C	1.96780000	-3.02255000	1.92018700
C	0.20894900	-5.14285600	1.45331100
C	1.81917600	-4.04786000	2.85401700
C	0.94799300	-5.11569900	2.63679500
H	-0.47741800	-5.96681100	1.27149500
H	2.40400400	-4.01369600	3.77069600
C	2.90884200	-1.87414500	2.17336600
H	2.34987800	-0.98153200	2.47455300
H	3.47633200	-1.61652600	1.27305400
H	3.61512900	-2.12149300	2.96827200
C	0.83306400	-6.23047200	3.64513800
H	0.95875200	-5.85521300	4.66360800
H	1.60465900	-6.98899200	3.47664200
H	-0.13798900	-6.72622800	3.57698200

C	-0.50840200	-4.15195400	-0.75813000
H	0.11097000	-3.98523300	-1.64424500
H	-1.25521200	-3.34946100	-0.72314600
H	-1.02710300	-5.10677500	-0.86637500
C	0.12272700	-0.19710700	0.74478000
O	-0.77754100	-1.10463200	1.26908400
C	-0.07487600	1.19100600	1.03513100
C	-1.13477900	1.67171500	1.73058900
H	0.68672100	1.89161700	0.70392600
H	-1.89580600	0.96254600	2.04803200
C	-1.36085200	3.07382600	2.07183100
C	-2.61467400	3.46449700	2.57551100
C	-0.38365500	4.07677400	1.92185100
C	-2.89002200	4.79013200	2.89188500
H	-3.38184200	2.70601700	2.71152100
C	-0.66071900	5.40187000	2.23430900
H	0.61158800	3.81462700	1.57227800
C	-1.91594800	5.77172900	2.71874200
H	-3.87032900	5.05835200	3.27491200
H	0.11334900	6.15309400	2.10763500
H	-2.12735500	6.80729100	2.96454000
C	-5.91600900	1.14622100	0.11264100
C	-5.89897300	1.14378200	-1.41573600
C	-5.69511500	-0.24865200	-2.02278700
C	-4.63096600	0.63674200	0.76329800
C	-4.25111700	-0.80384500	0.37665800
C	-3.54838100	-0.86827300	-0.95966600
H	-6.75383400	0.52105800	0.45083500
H	-5.11268500	1.80957300	-1.79350400
H	-6.05689600	-0.25532400	-3.05339400

H	-4.74845400	0.67796500	1.85177100
H	-5.13993600	-1.44524600	0.38515600
C	-3.66233700	-0.67017500	-3.39812500
H	-3.46230100	0.36511500	-3.70919500
C	-1.52619700	-0.99690300	-2.19053000
C	-2.37067700	-1.47225000	-3.36487500
H	-1.83836100	-1.35746500	-4.31231900
H	-2.60380500	-2.53500400	-3.23363400
H	-1.18657800	0.03566500	-2.36139000
H	-4.36388300	-1.10084300	-4.11899600
H	-0.62420900	-1.60964700	-2.08448600
N	-2.26761100	-1.05186600	-0.93674300
N	-4.30066700	-0.68458600	-2.08241700
H	-6.29764300	-0.98554500	-1.47704400
H	-6.85372800	1.53891400	-1.77910700
H	-6.11927600	2.16117200	0.47058100
H	-3.79101000	1.29818300	0.51395700
H	-3.54717400	-1.20264200	1.10936900
H	-1.43616700	-1.21892700	0.51264000

Re-M02-DBUH

C	5.26000400	-1.94443200	-0.70952300
C	4.17757200	-1.12929600	-0.38231800
C	4.32135300	-0.03945000	0.47184500
C	5.59193800	0.25183500	0.96528600
C	6.68563200	-0.54344900	0.61659000
C	6.52670000	-1.64998100	-0.21560500
C	4.83190100	-3.09283400	-1.58765500
C	3.29165800	-3.10100300	-1.50447500
C	2.91905200	-1.64405700	-1.05344000

H	3.46747200	0.56810300	0.76377200
H	5.72799400	1.09825700	1.63007700
H	7.66781900	-0.30614100	1.01207500
H	7.37517600	-2.27987200	-0.46386400
H	5.22920000	-4.05812500	-1.26275300
H	2.82995200	-3.32814700	-2.46575200
H	5.15159200	-2.93581100	-2.62313600
H	2.63251900	-1.05533000	-1.92819000
N	1.78770900	-1.67200500	-0.12641000
O	2.79516300	-4.10085800	-0.62554600
C	0.74364800	-0.84468000	0.05965000
C	1.72520000	-2.64194200	0.83644300
N	0.09494300	-1.33465600	1.11736900
N	0.69733000	-2.46267800	1.60811400
C	2.72310500	-3.75130700	0.74593800
H	3.69456500	-3.43900200	1.14915400
H	2.36889300	-4.62291500	1.29531800
C	-1.09024800	-0.87413300	1.80481300
C	-2.24881500	-1.63961600	1.68063200
C	-0.98275500	0.23612500	2.64388500
C	-3.35322600	-1.24463700	2.43631600
C	-2.11716800	0.59420400	3.36806600
C	-3.30710700	-0.13289600	3.27728800
H	-4.27347300	-1.81846300	2.35711100
H	-2.06737800	1.45773700	4.02636400
C	0.30230000	1.00869900	2.74625400
H	0.51298900	1.51968100	1.80129200
H	1.14790300	0.34842000	2.96603800
H	0.23860200	1.75821800	3.53618400
C	-4.52745700	0.30547200	4.04315100

H	-5.23609800	-0.51577800	4.16668400
H	-5.04120200	1.11369600	3.51092900
H	-4.25820400	0.68528400	5.03156300
C	-2.30339900	-2.84819300	0.78662700
H	-1.76668500	-3.69082900	1.23278000
H	-1.84906200	-2.63729200	-0.18623500
H	-3.33998500	-3.14886900	0.62274900
C	0.36272900	0.34693300	-0.82342200
O	-0.79660700	0.93232100	-0.37380700
C	1.50951700	1.33505200	-0.88099200
C	1.36781900	2.61310700	-0.52279500
H	2.45694000	0.96682000	-1.26397600
H	0.38396500	2.93546300	-0.18766100
C	2.42190100	3.64189000	-0.53910600
C	2.07128200	4.96124400	-0.22797400
C	3.76372400	3.35751900	-0.83407800
C	3.02744000	5.97230700	-0.21737900
H	1.03575500	5.19188200	0.00699300
C	4.71914800	4.36566100	-0.82086400
H	4.07190600	2.34226200	-1.06675700
C	4.35514000	5.67722800	-0.51389300
H	2.73562800	6.98905200	0.02471700
H	5.75348400	4.12792600	-1.04795400
H	5.10437200	6.46219000	-0.50346800
H	-1.59700500	0.40946800	-0.78233200
C	-5.94102400	2.55060000	-0.72480400
C	-6.55641000	1.54035800	-1.69421500
C	-6.41515100	0.08444100	-1.23757900
C	-4.44201700	2.37542700	-0.48027900
C	-4.06070700	0.99151700	0.07301700

C	-3.96011800	-0.04414200	-1.02211200
H	-6.46244400	2.46653200	0.23863500
H	-6.10857800	1.64048900	-2.69112200
H	-7.16296200	-0.53422600	-1.73815900
H	-4.11215800	3.13338000	0.23682300
H	-4.78415000	0.67550500	0.83276700
C	-5.07454100	-1.40715300	-2.71339800
H	-5.14117800	-0.81883100	-3.63926600
C	-2.60669100	-1.28843500	-2.54101500
C	-3.79536300	-2.22723700	-2.69298700
H	-3.71490200	-2.81487100	-3.61045200
H	-3.82526400	-2.92210000	-1.84731600
H	-2.46672900	-0.70686300	-3.46225600
H	-5.95034200	-2.06033500	-2.67246600
H	-1.68560100	-1.86374300	-2.39192600
N	-2.76708900	-0.37338200	-1.41570700
N	-5.11813100	-0.51947800	-1.55136200
H	-6.61454900	0.00460900	-0.16248500
H	-7.62329500	1.76263200	-1.80185000
H	-6.12941400	3.56423300	-1.09345700
H	-3.88016000	2.55418600	-1.40587100
H	-3.08554500	1.03463900	0.56356700
H	0.23845600	-0.09391500	-1.83145700

Re-TS2-tBuOH

C	3.71497200	2.74292100	0.27858300
C	2.77857500	1.79600600	-0.13220500
C	2.95618900	1.06173800	-1.30159000
C	4.11900700	1.26618700	-2.04294000
C	5.07285800	2.19479800	-1.62127800

C	4.87484500	2.94359500	-0.46260200
C	3.26644600	3.44259800	1.53649300
C	1.77898700	3.06333900	1.69289700
C	1.61707700	1.75393500	0.84085700
H	2.20439600	0.35377400	-1.64385000
H	4.27883100	0.70549200	-2.95782500
H	5.97120100	2.34576700	-2.21108200
H	5.60786800	3.68102700	-0.14989800
H	3.37316600	4.52972000	1.48909300
H	1.51412000	2.86762800	2.73240400
H	3.83724700	3.09296100	2.40321100
H	1.65542600	0.88589000	1.50446500
N	0.32729500	1.73898200	0.16339300
O	0.90617600	4.11211800	1.29426200
C	-0.55591300	0.74225100	-0.06846700
C	-0.20041600	2.89311400	-0.35043300
N	-1.57301600	1.33508700	-0.70376300
N	-1.36411800	2.68286200	-0.87996600
C	0.55541700	4.15197200	-0.07911400
H	1.43660200	4.22927400	-0.72872500
H	-0.08492700	5.01950600	-0.23466700
C	-2.79734800	0.76632800	-1.20535600
C	-3.95029200	0.92158800	-0.43914700
C	-2.76605900	0.10438600	-2.43144500
C	-5.13565600	0.41322300	-0.97146600
C	-3.97379800	-0.38699700	-2.91973300
C	-5.16700500	-0.23089200	-2.20895400
H	-6.05377100	0.51414200	-0.39804700
H	-3.98275400	-0.91340500	-3.87103000
C	-1.45922800	-0.12191500	-3.14129900

H	-0.82614500	-0.79324300	-2.54753200
H	-0.91064900	0.81475100	-3.28278400
H	-1.62107300	-0.57880100	-4.11862900
C	-6.46413300	-0.74439100	-2.77891000
H	-6.31687400	-1.69500400	-3.29731500
H	-6.87445300	-0.03459200	-3.50443000
H	-7.21132800	-0.88927500	-1.99596500
C	-3.88536100	1.54735300	0.92818500
H	-3.43325000	2.54304400	0.88690000
H	-3.27834200	0.92440000	1.60028400
H	-4.88674700	1.64240500	1.35182400
C	-0.47874800	-0.64347600	0.44021000
O	-1.62604600	-1.37234000	0.10212600
C	0.79153400	-1.35193700	0.11302900
C	0.83034900	-2.63444700	-0.27086900
H	1.72132400	-0.80345300	0.24469300
H	-0.11712900	-3.16128100	-0.35901600
C	2.04711000	-3.40947300	-0.56432700
C	1.94365800	-4.79920400	-0.70965700
C	3.31214400	-2.82055100	-0.71803000
C	3.06334600	-5.57989300	-0.98137700
H	0.96952700	-5.26850800	-0.60088500
C	4.43079100	-3.59891300	-0.98881100
H	3.42556900	-1.74236000	-0.64061600
C	4.31356900	-4.98280200	-1.11998400
H	2.95778800	-6.65523600	-1.08596300
H	5.39948100	-3.12310600	-1.10642200
H	5.18874300	-5.58708200	-1.33556700
H	-2.10455300	-1.34008600	0.97766700
C	-1.35977200	-2.96676400	3.01975700

C	-1.59927200	-1.55673900	3.58621800
H	-2.24889800	-3.30453200	2.47519800
H	-0.51912400	-2.94757600	2.31585200
H	-1.13843600	-3.69838300	3.80518700
C	-0.34898100	-1.11110700	4.36317500
C	-2.80202000	-1.59133300	4.54031400
H	-0.49572000	-0.09481700	4.74311200
H	-0.12297700	-1.77061800	5.20876700
H	0.52006100	-1.10376800	3.69388200
H	-2.65332400	-2.29305400	5.36905000
H	-2.97212800	-0.59235000	4.95496800
H	-3.70024000	-1.88838400	3.98932000
O	-1.86139200	-0.65322700	2.55844600
H	-0.72676600	-0.50878800	1.63770600

Re-TS2-DBU

C	1.45695500	-3.91390000	-2.17083300
C	1.11789100	-3.06536000	-1.12015400
C	1.18769400	-3.49321500	0.20494600
C	1.63755000	-4.78549000	0.46410100
C	2.00041600	-5.63294200	-0.58601700
C	1.90708900	-5.20569300	-1.90829100
C	1.24636800	-3.25553000	-3.50901400
C	0.60294200	-1.88045400	-3.20171100
C	0.64281200	-1.72224700	-1.63126200
H	0.88742400	-2.83948000	1.02057900
H	1.70119400	-5.13793700	1.48822000
H	2.34710700	-6.63818500	-0.36877900
H	2.17165000	-5.87279400	-2.72331500
H	0.58963400	-3.83822600	-4.16374200

H	1.18025700	-1.07230100	-3.65244800
H	2.19182100	-3.12351200	-4.04337600
H	1.32674600	-0.90692500	-1.38175500
N	-0.66284300	-1.37022200	-1.09504800
O	-0.69084700	-1.73535500	-3.76185000
C	-1.00230300	-0.69898500	0.06151500
C	-1.82272400	-1.74137200	-1.72009700
N	-2.36140000	-0.71597800	0.04270300
N	-2.87257100	-1.35695000	-1.07453500
C	-1.70205600	-2.41956600	-3.04231000
H	-1.45414400	-3.48303400	-2.91496500
H	-2.63427100	-2.33606100	-3.60021200
C	-3.27495300	-0.34063600	1.07745700
C	-4.23137800	0.63068300	0.78434800
C	-3.21558300	-0.98820400	2.31551500
C	-5.19117000	0.91476200	1.75737700
C	-4.18822000	-0.66693400	3.25745600
C	-5.19183900	0.26945700	2.99259800
H	-5.94405600	1.67139200	1.54882900
H	-4.16033400	-1.15773700	4.22811600
C	-2.09773000	-1.94174600	2.63436500
H	-1.17435700	-1.35914600	2.73668800
H	-1.95337300	-2.68221300	1.84043200
H	-2.29360200	-2.46987000	3.56964500
C	-6.23529900	0.58099700	4.03517600
H	-5.77239700	0.94632800	4.95676400
H	-6.81086000	-0.31299400	4.29396700
H	-6.93349300	1.34257300	3.68117800
C	-4.15857500	1.40138200	-0.50688000
H	-4.34164000	0.76114600	-1.37451200

H	-3.15157300	1.82464400	-0.61526000
H	-4.88474200	2.21642900	-0.51245400
C	-0.23153800	0.21820600	0.88982600
O	-0.88950800	0.89752000	1.80843600
C	1.17963300	-0.16184500	1.18397500
C	1.79479700	0.32138500	2.27657300
H	1.74354700	-0.78259200	0.49234400
H	1.20357400	0.97375200	2.91580300
C	3.19769700	0.09357500	2.64331100
C	3.81692400	0.96030200	3.55691600
C	3.96251700	-0.96314100	2.12169900
C	5.15123300	0.79861800	3.91672400
H	3.23580200	1.77508000	3.98204700
C	5.29591000	-1.12511700	2.47928100
H	3.50114100	-1.67789000	1.44464500
C	5.90055600	-0.24372600	3.37616900
H	5.60547100	1.48782600	4.62223500
H	5.86552100	-1.95138000	2.06419400
H	6.94062000	-0.37561100	3.65646500
C	3.11625100	4.36809400	-0.17084400
C	2.79987000	4.75844500	-1.61601000
C	1.33822600	5.15660300	-1.84823600
C	2.33083300	3.16821700	0.35762600
C	0.80420800	3.35603800	0.31137000
C	0.24675000	3.09160900	-1.06558200
H	2.90671900	5.23361400	0.47278700
H	3.05085000	3.93833900	-2.30100900
H	1.26150600	5.75404300	-2.75917000
H	2.62246700	2.97445300	1.39512500
H	0.54568100	4.37474800	0.62433800

C	-0.06413200	3.77856100	-3.38911800
H	0.73861800	3.36264700	-4.01388000
C	-0.88374400	1.59230200	-2.55342200
C	-1.25661100	2.83371900	-3.35269400
H	-1.55483800	2.57255100	-4.37067800
H	-2.10165100	3.33450000	-2.86811300
H	-0.13883300	0.99788700	-3.10202400
H	-0.35301400	4.74180800	-3.81920800
H	-1.75894100	0.94641600	-2.40861500
N	-0.36193700	1.95688800	-1.24447200
N	0.43202900	4.02150500	-2.03341500
H	0.98435700	5.79028000	-1.02612300
H	3.43006400	5.60967100	-1.89509900
H	4.18900100	4.16644300	-0.08112400
H	2.59304400	2.25996700	-0.20121500
H	0.30427100	2.66013400	0.99509200
H	-0.19569200	0.97608000	-0.20684200

Re-TS2-DBUH

C	-0.49781900	4.24460900	-1.87140300
C	-0.20249300	3.27533700	-0.91514000
C	-0.06702700	3.60437600	0.43110600
C	-0.27692000	4.92722600	0.81566300
C	-0.60182100	5.89684000	-0.13513700
C	-0.70653900	5.56489000	-1.48442700
C	-0.51377100	3.65653700	-3.25894500
C	0.10889600	2.25197700	-3.10764700
C	-0.01298200	1.92284000	-1.57392400
H	0.21455900	2.85847400	1.17091700
H	-0.17707300	5.20534400	1.85933000

H	-0.75685600	6.92379900	0.17902700
H	-0.93128300	6.32707500	-2.22413900
H	0.05863000	4.24341300	-3.98281900
H	-0.43068900	1.50841200	-3.69527900
H	-1.53677800	3.57487200	-3.64018400
H	-0.85836500	1.24650800	-1.41289900
N	1.19175700	1.25560600	-1.09147700
O	1.44100800	2.18299000	-3.59293600
C	1.37741600	0.28958500	-0.15841300
C	2.42527300	1.62713300	-1.55935500
N	2.70943600	0.12210000	-0.11147000
N	3.36990100	0.94785500	-0.99350000
C	2.44784500	2.60497800	-2.68773700
H	2.27588500	3.62706100	-2.32606400
H	3.40501300	2.56297100	-3.20619600
C	3.49446400	-0.71559500	0.75615900
C	4.17745700	-1.78939100	0.18692900
C	3.56461400	-0.39347400	2.11421500
C	4.97403900	-2.56133600	1.03424400
C	4.37172400	-1.19423000	2.91678100
C	5.08460900	-2.27758100	2.39470200
H	5.51710300	-3.40542900	0.61711300
H	4.44526100	-0.96883300	3.97793300
C	2.76384200	0.74481300	2.68470600
H	1.70137100	0.47533700	2.73020500
H	2.85597600	1.64745900	2.07218900
H	3.09770400	0.98071900	3.69622100
C	5.94918300	-3.11958900	3.29675900
H	6.44381800	-3.91801200	2.74066900
H	5.35245700	-3.57510100	4.09233600

H	6.71925000	-2.50902700	3.77690800
C	4.03784100	-2.11411700	-1.27681200
H	4.42674300	-1.30531200	-1.90121900
H	2.98487800	-2.25629400	-1.54523500
H	4.57795100	-3.03054400	-1.51831400
C	0.32994100	-0.50837900	0.48230100
O	0.86029700	-1.51571800	1.31170800
C	-0.74813800	0.25020600	1.16021300
C	-1.32993200	-0.13728400	2.30500000
H	-1.12351100	1.13188600	0.64805800
H	-0.96235400	-1.03973100	2.78904900
C	-2.46278800	0.54106100	2.95553800
C	-3.15667400	-0.12726500	3.97372900
C	-2.88485600	1.83228200	2.60323800
C	-4.24722900	0.46213600	4.60685400
H	-2.83477000	-1.12363900	4.26587100
C	-3.97342100	2.42100200	3.23453300
H	-2.35022200	2.39331100	1.84117700
C	-4.66264200	1.73849700	4.23756200
H	-4.77047700	-0.07579300	5.39098600
H	-4.28149800	3.42186400	2.94891700
H	-5.51023200	2.20296000	4.73056300
H	0.98704300	-2.31214600	0.77830800
C	-4.75771100	-2.93091300	0.07923400
C	-4.82087900	-3.30636000	-1.40201800
C	-3.66791100	-4.20062100	-1.86765700
C	-3.50737100	-2.15654700	0.49530100
C	-2.19392500	-2.90172800	0.19969100
C	-1.77278600	-2.76145400	-1.24156700
H	-4.80874100	-3.85383100	0.67221400

H	-4.83924800	-2.40675200	-2.02958200
H	-3.94842000	-4.71151800	-2.79041500
H	-3.55096900	-1.95624400	1.57074600
H	-2.29347100	-3.96222900	0.45609400
C	-2.05362900	-3.38521100	-3.59166300
H	-2.73192700	-2.69952500	-4.11512700
C	-0.40652300	-1.68050700	-2.88728500
C	-0.60976900	-2.93032300	-3.73170400
H	-0.38598900	-2.73523600	-4.78236200
H	0.06285400	-3.71889000	-3.38019400
H	-1.00870600	-0.85726700	-3.29631700
H	-2.18411500	-4.37953500	-4.02657800
H	0.64028800	-1.35796100	-2.89784100
N	-0.79847200	-1.93266600	-1.50642700
N	-2.43555200	-3.46466500	-2.17693500
H	-3.46321300	-4.98094800	-1.12556100
H	-5.75735500	-3.84222400	-1.58719200
H	-5.64458200	-2.34458700	0.33903400
H	-3.47509900	-1.17556800	0.00353600
H	-1.39064000	-2.49294600	0.81471900
H	-0.25965700	-1.15866700	-0.55186700

Si-M02-tBuOH

C	-4.16307900	-2.02144900	0.56813600
C	-3.09109100	-1.19841500	0.22505000
C	-3.24838800	-0.14395700	-0.66846500
C	-4.51329100	0.08905300	-1.20635400
C	-5.59284800	-0.72446700	-0.85659600
C	-5.42470500	-1.78647400	0.03074900
C	-3.73068900	-3.09657300	1.53377000

C	-2.18980400	-3.06802800	1.48377400
C	-1.83827700	-1.63537200	0.95741500
H	-2.40646900	0.48528200	-0.94107800
H	-4.65726600	0.90910200	-1.90232700
H	-6.57098500	-0.53320900	-1.28631200
H	-6.26329600	-2.42514700	0.29139700
H	-4.09842700	-4.09297000	1.27394800
H	-1.74132400	-3.23475200	2.46354600
H	-4.07760300	-2.87028000	2.54787800
H	-1.54917100	-0.95729500	1.76644400
N	-0.67700500	-1.70986300	0.07314400
O	-1.66262300	-4.11412000	0.66994700
C	0.37777100	-0.89537900	-0.07135300
C	-0.54187700	-2.72952100	-0.82719900
N	1.09459700	-1.43562800	-1.05469500
N	0.54099700	-2.59395700	-1.53623100
C	-1.53640600	-3.83974800	-0.71542300
H	-2.49324500	-3.55497100	-1.17128800
H	-1.15967500	-4.74009600	-1.19981500
C	2.32298500	-0.91615500	-1.58970600
C	3.50506200	-1.14791800	-0.88266600
C	2.26471700	-0.19910900	-2.78783400
C	4.67357400	-0.59804500	-1.41171600
C	3.46086300	0.32118400	-3.27572400
C	4.66948800	0.13485900	-2.59927200
H	5.61041700	-0.75397800	-0.88267000
H	3.44910600	0.88772100	-4.20330600
C	0.96135600	-0.02158800	-3.52117100
H	0.17933300	0.37461100	-2.86460200
H	0.60102000	-0.98011500	-3.90663100

H	1.08353200	0.66454500	-4.36012800
C	5.95046700	0.68993100	-3.16556500
H	6.35559900	0.01602600	-3.92719400
H	6.70830700	0.80882900	-2.38875800
H	5.78329700	1.65973700	-3.63997100
C	3.51204500	-1.94822600	0.39157900
H	2.91790800	-2.86083900	0.28313200
H	3.11017900	-1.37415300	1.23844700
H	4.53450900	-2.23459100	0.64615400
C	0.66556400	0.34627400	0.78302100
O	0.30253200	0.10806900	2.05600100
C	-0.05353100	1.50091000	0.09272200
C	-1.06178100	2.12989000	0.69928800
H	0.26896700	1.76342100	-0.91622900
H	-1.32482900	1.77331400	1.69484700
C	-1.88900500	3.20261400	0.12220200
C	-3.19294400	3.38017000	0.60228400
C	-1.43476000	4.03997400	-0.90610500
C	-4.02838800	4.35159000	0.05978300
H	-3.55235100	2.73804900	1.40212800
C	-2.26731000	5.01416500	-1.44580400
H	-0.41636400	3.93794100	-1.27004100
C	-3.56813900	5.17203700	-0.96762400
H	-5.03726400	4.47031500	0.44211000
H	-1.89823700	5.65964700	-2.23670000
H	-4.21512300	5.93506400	-1.38828200
H	1.63837700	-0.04910800	2.75358700
C	4.07113700	0.95260700	4.54885100
C	3.30365500	1.00737700	3.22592100
H	3.36806500	0.87867000	5.38386000

H	4.71679700	0.06909900	4.56574500
H	4.69349300	1.84199000	4.69118200
C	4.30015000	1.11957500	2.06460900
C	2.35900900	2.21287200	3.22586600
H	3.77581900	1.15609300	1.10263500
H	4.91806100	2.01981800	2.15036600
H	4.95895400	0.24465100	2.05621500
H	2.92003300	3.14206300	3.36786200
H	1.80366200	2.27977100	2.28494800
H	1.63009300	2.11849200	4.03703700
O	2.58245700	-0.20422700	3.11450400
H	1.75785400	0.51765000	0.64406300

Si-M02-DBU

C	-0.98471200	-3.27700000	-2.24106900
C	-0.99133500	-1.90095400	-1.99240300
C	-0.35290500	-1.01679000	-2.85866700
C	0.30919200	-1.53526500	-3.97176500
C	0.33010700	-2.90982800	-4.21253800
C	-0.32331900	-3.79056200	-3.35139100
C	-1.74950100	-4.02723300	-1.18147600
C	-2.55601400	-2.90208400	-0.49577500
C	-1.73687000	-1.60067600	-0.70646800
H	-0.37784600	0.04879000	-2.65726400
H	0.81367800	-0.86202100	-4.65778500
H	0.85003600	-3.29601000	-5.08394200
H	-0.32130900	-4.85870900	-3.54818700
H	-1.05577300	-4.50996000	-0.48288500
H	-3.50823400	-2.77706000	-1.01661900
H	-2.39982700	-4.80757000	-1.58378000

H	-2.36791800	-0.71088400	-0.75342000
N	-0.82061500	-1.46247900	0.44357000
O	-2.89731100	-3.12594200	0.85793300
C	0.35031900	-0.70040100	0.46805700
C	-0.64307300	-2.48340600	1.35520900
N	1.17775600	-1.38708800	1.35858900
N	0.52272300	-2.48965700	1.90131100
C	-1.78792200	-3.39365100	1.69240000
H	-1.47232400	-4.44202800	1.63284800
H	-2.11706400	-3.19799400	2.71640200
C	2.60282700	-1.37231800	1.35164600
C	3.26867500	-0.79486400	2.43638400
C	3.28805800	-1.88773400	0.24374800
C	4.66056500	-0.72211000	2.38908300
C	4.67827200	-1.78575100	0.23277800
C	5.37841400	-1.19952100	1.29028300
H	5.19485000	-0.27000400	3.22142400
H	5.22909700	-2.17355000	-0.62149400
C	2.53178200	-2.49384400	-0.90812000
H	2.03727200	-1.71717200	-1.50382500
H	1.74589000	-3.16961700	-0.55359200
H	3.20383100	-3.05323900	-1.56187100
C	6.87754800	-1.05686700	1.22778200
H	7.33726500	-1.91924800	0.73888300
H	7.30870000	-0.95315800	2.22581000
H	7.15441100	-0.16734000	0.65172800
C	2.47879200	-0.24262400	3.59167800
H	1.86647800	-1.02226400	4.05391400
H	1.79375500	0.53787000	3.24415800
H	3.13990400	0.18219700	4.34906600

C	0.50212400	0.52684700	-0.12908900
O	-0.59670400	1.08814900	-0.74351500
C	1.74444600	1.24005900	-0.18844600
C	1.90720900	2.45147700	-0.76768300
H	2.60324900	0.75017700	0.25956900
H	1.03985400	2.92932200	-1.21646800
C	3.17009400	3.18455900	-0.84803300
C	3.19156200	4.44061300	-1.47797200
C	4.38585300	2.70093500	-0.32591700
C	4.36361500	5.18153700	-1.58492800
H	2.26528900	4.83482100	-1.88843900
C	5.55594600	3.44177700	-0.43264200
H	4.42009000	1.73383200	0.17012700
C	5.55669300	4.68719800	-1.06252600
H	4.34439200	6.14880100	-2.07846600
H	6.47874400	3.04319500	-0.02069700
H	6.47394900	5.26145300	-1.14272300
C	-5.83701500	2.46252800	-1.70516200
C	-6.54966900	2.05890100	-0.41438000
C	-5.95961400	2.71393600	0.83888900
C	-4.35034800	2.10812500	-1.75655400
C	-3.51523000	2.72627800	-0.62143500
C	-3.62130000	1.93378200	0.66155800
H	-5.94001700	3.54923200	-1.83003100
H	-6.52746300	0.96940200	-0.28401200
H	-6.70012800	2.70578600	1.64176800
H	-3.94135200	2.45276600	-2.71123100
H	-3.81473800	3.76779500	-0.45728100
C	-4.97272400	1.21684600	2.56830300
H	-5.49128100	0.28283400	2.30859800

C	-2.69317900	0.33927600	2.16165300
C	-3.62920200	0.91888200	3.21337600
H	-3.76168000	0.22324300	4.04572500
H	-3.20616800	1.84724700	3.61126100
H	-3.03317100	-0.66427500	1.86569200
H	-5.61617800	1.77167100	3.25731700
H	-1.68118800	0.22096600	2.56429400
N	-2.61180300	1.18441600	0.97423900
N	-4.77901300	2.03654300	1.37318800
H	-5.73051200	3.76723600	0.63733400
H	-7.60314500	2.34910400	-0.48997300
H	-6.34511000	2.00145700	-2.55859400
H	-4.21975000	1.01818500	-1.73601700
H	-2.45998900	2.72908200	-0.89863700
H	-1.34874200	1.13540000	-0.06062400

Si-M02-DBUH

C	5.18016200	-1.43157100	-0.88527500
C	4.07855400	-0.84471700	-0.26488700
C	4.22271900	-0.08369900	0.89031000
C	5.50036200	0.09498800	1.41525300
C	6.60840000	-0.48349800	0.79267700
C	6.45613600	-1.25186400	-0.35956400
C	4.76793600	-2.20377900	-2.11231900
C	3.23475600	-2.32077100	-2.00844700
C	2.81413400	-1.15563800	-1.03956500
H	3.36252500	0.36225100	1.37847500
H	5.63292200	0.68916100	2.31346100
H	7.59726600	-0.33797400	1.21508600
H	7.31739100	-1.70954300	-0.83631500

H	5.21646000	-3.19875500	-2.17536700
H	2.74482600	-2.20268000	-2.97501400
H	5.04249300	-1.66002600	-3.02232200
H	2.44419400	-0.29641600	-1.60425900
N	1.71807200	-1.60815000	-0.18011700
O	2.82320800	-3.60669900	-1.55687200
C	0.59300100	-1.00210600	0.21691900
C	1.69601000	-2.87855500	0.32848000
N	-0.05734900	-1.90092100	0.95037700
N	0.61382300	-3.08911900	1.02268400
C	2.76930000	-3.79962700	-0.15300500
H	3.72693700	-3.58459100	0.33698700
H	2.49159300	-4.83650800	0.03203700
C	-1.40572600	-1.76820900	1.44348200
C	-2.43471200	-2.01678800	0.53276700
C	-1.61672700	-1.39751700	2.77303500
C	-3.74304200	-1.85514400	0.99080800
C	-2.94044800	-1.25640100	3.18189800
C	-4.01046100	-1.47521300	2.30783000
H	-4.56527100	-2.03955200	0.30276500
H	-3.14381000	-0.97616300	4.21237700
C	-0.46491000	-1.17063800	3.71480200
H	0.08195900	-0.25709400	3.46078000
H	0.24391100	-2.00211900	3.67746800
H	-0.82613600	-1.07015000	4.73877600
C	-5.42497100	-1.30236400	2.79728400
H	-6.14816700	-1.64306400	2.05365500
H	-5.63159300	-0.24980200	3.01935600
H	-5.58781500	-1.86528600	3.72017800
C	-2.12466200	-2.45498600	-0.87304100

H	-1.71936300	-1.62179000	-1.45986700
H	-3.02783300	-2.81907300	-1.36318900
H	-1.38654800	-3.26255300	-0.87929400
C	0.12757500	0.39541300	-0.12875700
O	-0.06612100	0.46703000	-1.50225200
C	1.13166100	1.39432400	0.40018600
C	1.80420700	2.22319000	-0.40149200
H	1.27658600	1.38583500	1.47910400
H	1.57846900	2.17722700	-1.46566800
C	2.84302100	3.18419900	0.00279700
C	3.46650900	3.94973500	-0.98989800
C	3.25617600	3.34985400	1.33309000
C	4.47541400	4.85306500	-0.66940400
H	3.15509000	3.82985000	-2.02399500
C	4.26358200	4.25042500	1.65407400
H	2.78836100	2.77670700	2.12846200
C	4.87801600	5.00524900	0.65414500
H	4.94728400	5.43555700	-1.45399900
H	4.57186200	4.36604600	2.68816000
H	5.66589600	5.70685900	0.90797600
H	-1.05739100	0.70185400	-1.65766300
C	-5.44349500	3.01654900	0.75126800
C	-6.38473600	2.24462200	-0.16983600
C	-5.95292800	0.78970400	-0.36313900
C	-3.98837600	3.04400600	0.28623800
C	-3.30487600	1.66536200	0.19605700
C	-3.59815100	0.94864400	-1.10289600
H	-5.48302000	2.56160600	1.75096700
H	-6.44828800	2.72790800	-1.15261600
H	-6.79863100	0.18819200	-0.70405800

H	-3.41099900	3.65435600	0.98723000
H	-3.57057100	1.04248800	1.06013000
C	-5.27705300	0.18697500	-2.69661300
H	-5.52137800	1.07009200	-3.30243000
C	-2.86138200	0.20560200	-3.25413600
C	-4.14777500	-0.60417400	-3.33563000
H	-4.39037700	-0.83577200	-4.37547200
H	-4.03378100	-1.55023400	-2.79951400
H	-2.88782100	1.02200600	-3.98724400
H	-6.17984100	-0.42343700	-2.62137400
H	-1.99751500	-0.41641900	-3.51514200
N	-2.61364400	0.78393200	-1.93379300
N	-4.88928100	0.59654100	-1.34770700
H	-5.63608400	0.36462600	0.59707900
H	-7.39288400	2.25386500	0.25765600
H	-5.80230300	4.04487400	0.86238900
H	-3.91312100	3.53789700	-0.69068300
H	-2.22713000	1.82317900	0.21930100
H	-0.81560200	0.51006900	0.42553100

Si-TS2-tBuOH

C	-4.88413600	-1.02431800	-0.04539200
C	-3.51761700	-0.93904000	-0.29437400
C	-2.66525000	-2.01702200	-0.07212900
C	-3.21167800	-3.19961600	0.41899600
C	-4.58323100	-3.29434900	0.67268400
C	-5.42811300	-2.21157900	0.44066600
C	-5.58882000	0.26626900	-0.37460700
C	-4.46831700	1.26678800	-0.75590500
C	-3.13491400	0.42957100	-0.80320500

H	-1.60026800	-1.93708900	-0.27902100
H	-2.56917800	-4.05433300	0.60413900
H	-4.99359400	-4.22310400	1.05607500
H	-6.49264000	-2.29029700	0.63998800
H	-6.17349800	0.65799400	0.46464300
H	-4.64510100	1.70162800	-1.73924200
H	-6.28335400	0.13673500	-1.20964300
H	-2.71684700	0.39275200	-1.80632600
N	-2.10392500	1.03338600	0.05993400
O	-4.41580300	2.38758100	0.11277500
C	-0.76317200	0.86775200	0.08026800
C	-2.43932300	1.75524800	1.17738200
N	-0.35552500	1.51707900	1.17940000
N	-1.39442700	2.07612600	1.87445400
C	-3.87765300	2.09349100	1.38484900
H	-4.40113000	1.25609900	1.86759900
H	-3.97129400	2.97932900	2.01273000
C	1.00194100	1.72374600	1.59851100
C	1.73945500	2.73256500	0.97680500
C	1.51565000	0.89309400	2.60057400
C	3.07318400	2.86968600	1.36941300
C	2.84971900	1.07155800	2.95370000
C	3.64234900	2.04956200	2.34256000
H	3.67786100	3.64253600	0.90139700
H	3.28207900	0.43415300	3.72113100
C	0.65295200	-0.16171500	3.24063800
H	0.26980800	-0.86697600	2.49350000
H	-0.21351800	0.28929200	3.73311000
H	1.22121900	-0.72477800	3.98229500
C	5.07810000	2.23157200	2.76068800

H	5.13656500	2.79838400	3.69536300
H	5.64471700	2.77553500	2.00253200
H	5.56200100	1.26686100	2.93111100
C	1.12358500	3.63341400	-0.06029900
H	0.13392900	3.97359600	0.26038200
H	1.01660000	3.12226600	-1.02800500
H	1.75414900	4.51239100	-0.21073600
C	0.11067700	0.19395100	-0.90658900
O	-0.62286000	-0.24061400	-2.02559600
C	0.97852200	-0.86097900	-0.30924900
C	1.13768900	-2.07847300	-0.84336100
H	1.54412700	-0.57218800	0.57237800
H	0.55587100	-2.32679700	-1.72904700
C	2.02509500	-3.13128200	-0.32178100
C	1.94566100	-4.41594100	-0.87530800
C	2.94729300	-2.91325400	0.71408700
C	2.74690500	-5.45309500	-0.40704000
H	1.23991100	-4.59881300	-1.68134800
C	3.74671100	-3.94830200	1.18311600
H	3.05134500	-1.92382000	1.15175900
C	3.65067300	-5.22439100	0.62680400
H	2.66419100	-6.44006700	-0.85140200
H	4.45542700	-3.75829600	1.98325500
H	4.27942100	-6.02916300	0.99360900
H	-0.24056600	0.36699100	-2.71556700
C	2.44399900	2.49437700	-4.42537800
C	2.17757100	1.46632100	-3.31610900
H	1.67009800	2.41478300	-5.19586500
H	2.40439700	3.50560100	-4.00696000
H	3.42242000	2.35029900	-4.89788600

C	3.27134500	1.59177900	-2.23985800
C	2.22890700	0.05103200	-3.91486200
H	3.08529200	0.87685900	-1.42808200
H	4.27164200	1.39701500	-2.64353500
H	3.26254400	2.60057200	-1.81159000
H	3.19706300	-0.17092600	-4.37823900
H	2.04187400	-0.69041200	-3.12975900
H	1.44919700	-0.05439700	-4.67786600
O	0.92121800	1.71738700	-2.76465100
H	0.76937100	1.05830600	-1.48137800

Si-TS2-DBU

C	5.49491600	0.97641000	-0.67349100
C	4.15139200	0.87141800	-1.03187200
C	3.36748900	1.99961300	-1.25918700
C	3.95942900	3.25213700	-1.10476400
C	5.30409400	3.36675800	-0.74224000
C	6.08277000	2.23050800	-0.53016500
C	6.12718400	-0.37783600	-0.48398800
C	5.06194100	-1.36239700	-1.02544200
C	3.71703400	-0.57440300	-1.12607300
H	2.33551300	1.85808400	-1.58042400
H	3.37317300	4.14973000	-1.27705900
H	5.74963100	4.35068000	-0.63059900
H	7.13049900	2.32213400	-0.25833200
H	6.35097200	-0.56106900	0.57216000
H	5.33350300	-1.65960400	-2.03995800
H	7.07048400	-0.48469800	-1.02569400
H	3.14448600	-0.77059200	-2.03105600
N	2.83576600	-0.95568900	-0.00636600

O	4.96229300	-2.58422600	-0.31249300
C	1.58728900	-0.47534500	0.26624400
C	3.23178100	-1.72081900	1.05911300
N	1.32733600	-0.94878300	1.51412900
N	2.33955800	-1.74689300	1.99737800
C	4.54512400	-2.43700100	1.02680200
H	5.28550500	-1.90301400	1.63487500
H	4.42533500	-3.43782500	1.44436000
C	0.08260100	-0.89262600	2.21372400
C	-0.82676600	-1.93850400	2.03754800
C	-0.16659100	0.18919300	3.06610800
C	-2.04906200	-1.85084200	2.70609300
C	-1.40575600	0.24038700	3.70065600
C	-2.36257000	-0.76346800	3.52068700
H	-2.77678400	-2.64899000	2.57694500
H	-1.62767300	1.07846300	4.35705800
C	0.88577300	1.24244300	3.29472700
H	1.19219800	1.71813200	2.35728400
H	1.78278200	0.79628900	3.73490700
H	0.51575500	2.01602700	3.96952200
C	-3.71497400	-0.65734000	4.17549100
H	-3.64572600	-0.16948800	5.15057900
H	-4.16890300	-1.64142900	4.31013900
H	-4.39180700	-0.05956500	3.55552500
C	-0.47931200	-3.14326600	1.20489200
H	0.14371900	-3.83470300	1.78144000
H	0.07828800	-2.86621600	0.30598000
H	-1.38713900	-3.66885300	0.89988400
C	0.69880300	0.15921000	-0.71704600
O	1.11988300	0.17730100	-1.98020400

C	-0.09063600	1.29460800	-0.19458300
C	-0.69857100	2.18003800	-1.00762300
H	-0.30561500	1.30676600	0.86984400
H	-0.48338700	2.10950400	-2.07176600
C	-1.66420000	3.19518900	-0.57895300
C	-2.23912700	4.05011900	-1.53357800
C	-2.08804100	3.33886600	0.75603500
C	-3.19208900	4.99992700	-1.17952500
H	-1.93078200	3.95559900	-2.57184700
C	-3.03825500	4.28827400	1.11063700
H	-1.67970800	2.68881000	1.52637700
C	-3.59975000	5.12674100	0.14631600
H	-3.61856700	5.64387700	-1.94312300
H	-3.34750000	4.37349200	2.14846600
H	-4.34316500	5.86609100	0.42649200
C	-5.38564500	0.18180400	-1.28183900
C	-5.49227100	-1.09715300	-2.11385400
C	-4.89019300	-2.32572200	-1.42306100
C	-3.95974700	0.61320800	-0.93737500
C	-3.15486900	-0.44532100	-0.16242300
C	-2.59174900	-1.50016100	-1.08435200
H	-5.94029900	0.02924300	-0.34541000
H	-5.00298500	-0.96572800	-3.08751100
H	-5.31443400	-3.23825300	-1.84752600
H	-3.99845500	1.52373400	-0.33074900
H	-3.77644400	-0.90602700	0.61430500
C	-2.96225800	-3.35916800	-2.61365000
H	-3.13322300	-2.91962200	-3.60678300
C	-0.72027500	-2.33991900	-2.33599500
C	-1.48320800	-3.65464600	-2.41362400

H	-1.11434800	-4.27346500	-3.23531200
H	-1.35210600	-4.21710800	-1.48321200
H	-0.65954200	-1.86095200	-3.31947100
H	-3.55137400	-4.27810100	-2.55184400
H	0.31556900	-2.48820900	-2.00919900
N	-1.33971100	-1.41277100	-1.40175100
N	-3.43911000	-2.44816100	-1.57252900
H	-5.15517600	-2.32403200	-0.35926300
H	-6.54969500	-1.29983900	-2.31469200
H	-5.88821300	0.99854900	-1.81039400
H	-3.40394300	0.87734800	-1.84612800
H	-2.30697300	0.02787300	0.33747500
H	-0.34795800	-0.65704800	-0.75294800

Si-TS2-DBUH

C	5.61411400	0.43618700	-0.91100700
C	4.22525400	0.52298600	-0.94678300
C	3.57030900	1.75042700	-0.87720300
C	4.34016100	2.90425100	-0.75885700
C	5.73531100	2.82491100	-0.71953500
C	6.38103900	1.59391100	-0.79857900
C	6.08798700	-0.98932700	-1.02061000
C	4.80273000	-1.85424400	-1.03046400
C	3.59260400	-0.84409500	-1.05651200
H	2.48505400	1.80947500	-0.92073800
H	3.85416700	3.87260200	-0.69982600
H	6.32092500	3.73407300	-0.62793700
H	7.46495100	1.53662000	-0.76968000
H	6.73859800	-1.28553700	-0.19086300
H	4.75647300	-2.47502800	-1.92472300

H	6.65922000	-1.14830900	-1.93959200
H	3.00221600	-0.95777300	-1.96250900
N	2.68059000	-1.09096900	0.07772300
O	4.75203300	-2.78400000	0.03864100
C	1.41105900	-0.67202000	0.29084100
C	3.12968000	-1.63291000	1.25796200
N	1.15182700	-1.00192800	1.56850600
N	2.22059800	-1.60451600	2.17951500
C	4.51478300	-2.18609900	1.29526400
H	5.23812900	-1.38810100	1.51357200
H	4.59566200	-2.95445000	2.06378400
C	-0.11863500	-0.92485000	2.23228000
C	-1.01878800	-1.97724400	2.04548100
C	-0.38706300	0.17621900	3.05179400
C	-2.26855300	-1.86485600	2.65493900
C	-1.65265800	0.24569200	3.63162800
C	-2.60834300	-0.75487200	3.43041900
H	-2.99126000	-2.66620600	2.52274700
H	-1.89489900	1.09656900	4.26324800
C	0.66370100	1.22359600	3.31104500
H	1.08249300	1.62329700	2.38152400
H	1.49538600	0.79496500	3.87854000
H	0.24634100	2.05328400	3.88324400
C	-3.98342400	-0.62977000	4.03146300
H	-4.44451100	-1.60936400	4.17234100
H	-4.63507700	-0.04499400	3.37345900
H	-3.94742100	-0.11897800	4.99618000
C	-0.62551200	-3.21108200	1.27794400
H	-0.23882500	-2.97006900	0.28344400
H	-1.48370600	-3.87493400	1.16005200

H	0.15980200	-3.75501000	1.81219000
C	0.46916600	-0.05278000	-0.63704500
O	1.01599900	0.01162500	-1.93822100
C	-0.13086600	1.22356000	-0.18428500
C	-0.44013500	2.24202600	-0.99944200
H	-0.41879000	1.27159300	0.86057800
H	-0.13421500	2.19211400	-2.04244100
C	-1.15437900	3.45963300	-0.58247500
C	-1.18777700	4.56079600	-1.44772600
C	-1.81838300	3.56641700	0.65085900
C	-1.84580000	5.73490700	-1.09293400
H	-0.68479700	4.49191800	-2.40872300
C	-2.47495000	4.73852900	1.00586200
H	-1.83777300	2.72109400	1.33575000
C	-2.49112300	5.82999400	0.13702800
H	-1.85525700	6.57569900	-1.77927300
H	-2.98387300	4.79971900	1.96281300
H	-3.00841900	6.74208700	0.41576900
H	0.31231300	-0.23198600	-2.55713700
C	-5.31181500	0.67028400	-1.40532400
C	-5.61244400	-0.59782900	-2.20599300
C	-5.21694300	-1.89486800	-1.49379700
C	-3.83839800	0.88383300	-1.05791400
C	-3.22345700	-0.27604700	-0.25642500
C	-2.82809000	-1.42659500	-1.14835000
H	-5.88687200	0.63220500	-0.47024300
H	-5.11064400	-0.56826900	-3.18125800
H	-5.76244600	-2.73489100	-1.92729400
H	-3.74152200	1.79809600	-0.46395700
H	-3.92210300	-0.62417200	0.51233300

C	-3.46003100	-3.34915400	-2.51608100
H	-3.59488300	-3.04051000	-3.56063800
C	-1.10475800	-2.61534500	-2.33611800
C	-2.03469400	-3.81750800	-2.26994600
H	-1.75842700	-4.56666300	-3.01469000
H	-1.96616500	-4.28033400	-1.28036100
H	-1.05543200	-2.23617400	-3.36528400
H	-4.16791900	-4.15623400	-2.31214100
H	-0.08235400	-2.88291400	-2.04271500
N	-1.56270900	-1.55479600	-1.44609700
N	-3.79347600	-2.23070500	-1.62734800
H	-5.49331500	-1.85294800	-0.43407100
H	-6.68831000	-0.63836900	-2.40422300
H	-5.67794000	1.53970600	-1.96041500
H	-3.24133600	1.04234700	-1.96553800
H	-2.32312500	0.05886400	0.26221300
H	-0.60744900	-0.86468300	-0.82539900

Re-TS2^D

C	-3.00982000	3.05092400	0.27343800
C	-2.19736000	1.91973000	0.30493600
C	-2.27193500	1.00478800	1.35184600
C	-3.21003600	1.22208000	2.35960600
C	-4.04509200	2.34073400	2.31878000
C	-3.94578800	3.26567500	1.28097100
C	-2.70094900	3.91060200	-0.92614700
C	-1.38223700	3.34434300	-1.49921100
C	-1.27121800	1.89663900	-0.89454900
H	-1.60683700	0.14547600	1.39570700
H	-3.28576000	0.52076900	3.18377300

H	-4.76914800	2.49842800	3.11145800
H	-4.58069900	4.14627100	1.26510100
H	-2.57785200	4.96914300	-0.67990600
H	-1.40613200	3.29085200	-2.58816800
H	-3.49771900	3.83864500	-1.67393100
H	-1.58260100	1.16956600	-1.64949000
N	0.10096600	1.58839800	-0.52749200
O	-0.26285800	4.17038700	-1.21066000
C	0.81920700	0.42974800	-0.60335700
C	0.92253200	2.55753600	-0.01742800
N	2.03859400	0.77046700	-0.12652500
N	2.10717500	2.10374700	0.22865400
C	0.36577700	3.94077500	0.03989500
H	-0.33837400	4.04509400	0.87615200
H	1.16657100	4.67090800	0.15121300
C	3.16168300	-0.06857200	0.17518400
C	4.37951200	0.21810300	-0.44505300
C	3.01095100	-1.10004900	1.10683200
C	5.48148600	-0.56304300	-0.09586700
C	4.14143500	-1.85122600	1.42081900
C	5.38328300	-1.59476800	0.83675100
H	6.43779300	-0.36326900	-0.57321900
H	4.04741900	-2.66060100	2.14103900
C	1.67491600	-1.41247600	1.72278200
H	1.04648200	-1.91778500	0.98067000
H	1.16095300	-0.50432900	2.05521800
H	1.79591500	-2.07215500	2.58408600
C	6.59286300	-2.40696700	1.22270700
H	6.33689500	-3.46254300	1.34363100
H	7.00529900	-2.05860900	2.17526300

H	7.37982300	-2.32613700	0.46974600
C	4.49680900	1.31000200	-1.47559000
H	4.41681600	2.29904400	-1.01698200
H	3.69544800	1.23178500	-2.21691400
H	5.45511700	1.24218900	-1.99322300
C	0.43232900	-0.82544200	-1.19363700
O	1.47639300	-1.78412100	-1.36377300
C	-0.91018000	-1.34900900	-0.90401800
C	-1.16237200	-2.66955000	-0.91293000
H	-1.71015000	-0.64872800	-0.67985700
H	-0.33563400	-3.32520600	-1.17349000
C	-2.45566100	-3.30194500	-0.62344600
C	-2.61917300	-4.66758800	-0.89853600
C	-3.54466700	-2.60896400	-0.06837300
C	-3.82460300	-5.31594500	-0.64854500
H	-1.78392600	-5.22137100	-1.31936400
C	-4.74992300	-3.25489700	0.17888900
H	-3.44539500	-1.55746800	0.18956200
C	-4.89894300	-4.61151000	-0.11128900
H	-3.92429800	-6.37337900	-0.87366700
H	-5.57708500	-2.69917300	0.61029900
H	-5.84057900	-5.11326700	0.08651800
H	0.90527900	-0.95090300	-2.26099600

Si-TS2^D

C	-4.31683400	-1.54459200	0.64230300
C	-3.10347400	-1.43095100	-0.03151000
C	-2.03854500	-2.29008700	0.22961200
C	-2.20711400	-3.26728300	1.20818200
C	-3.41808300	-3.38208900	1.89712700

C	-4.48224700	-2.52876700	1.61459700
C	-5.32073200	-0.52938900	0.16204300
C	-4.58941800	0.26845000	-0.94883600
C	-3.12169700	-0.28856500	-1.01863000
H	-1.12291400	-2.21137100	-0.35468400
H	-1.39490400	-3.95163800	1.43187000
H	-3.53363700	-4.15025500	2.65537600
H	-5.42579700	-2.63009900	2.14288500
H	-5.65976400	0.13390200	0.96475200
H	-5.06088900	0.08722400	-1.91499700
H	-6.21720800	-1.00856600	-0.24097600
H	-2.83259600	-0.61129900	-2.01718900
N	-2.15542700	0.75591600	-0.63183000
O	-4.66819600	1.67561700	-0.78568500
C	-0.79452900	0.70614800	-0.67133900
C	-2.49993200	1.85744800	0.10907800
N	-0.39886900	1.78882700	0.03950500
N	-1.46316100	2.51207000	0.52331700
C	-3.94615300	2.15905300	0.32541700
H	-4.28735500	1.70596000	1.26600700
H	-4.09977000	3.23682700	0.38636600
C	0.93923400	2.23422600	0.28083000
C	1.60782400	2.92529100	-0.72934800
C	1.53002800	1.91788800	1.50952500
C	2.93132100	3.29654000	-0.48609400
C	2.85014500	2.31111300	1.70722400
C	3.56584200	2.99606500	0.71846200
H	3.47725100	3.82960300	-1.26014300
H	3.33780700	2.06998900	2.64888600
C	0.76370900	1.13481800	2.54125700

H	0.43410100	0.17304000	2.13066900
H	-0.13299500	1.67515600	2.85809300
H	1.38289100	0.93986300	3.41785400
C	4.99569700	3.40115500	0.96558000
H	5.05468600	4.15066900	1.76051200
H	5.44908300	3.82248200	0.06653600
H	5.59339600	2.54187900	1.28231400
C	0.92398600	3.22935000	-2.03442900
H	-0.03689100	3.72501700	-1.86760000
H	0.72537600	2.30279900	-2.58394100
H	1.54612300	3.87375200	-2.65689400
C	0.00928500	-0.22411200	-1.42348000
O	-0.71044800	-1.15340400	-2.25108500
C	1.28735400	-0.67176700	-0.86390300
C	1.83961400	-1.85332900	-1.18943100
H	1.79395000	-0.00560600	-0.17242600
H	1.30064000	-2.48637100	-1.89020000
C	3.11975300	-2.35918500	-0.67665500
C	3.56469400	-3.62707200	-1.07922300
C	3.93553100	-1.62898700	0.20523600
C	4.77127800	-4.14929700	-0.62219900
H	2.94931200	-4.20748700	-1.76177000
C	5.13943400	-2.14940100	0.66203000
H	3.62987800	-0.64010700	0.53726900
C	5.56636700	-3.41329900	0.25221500
H	5.09072900	-5.13329300	-0.95151600
H	5.75179200	-1.56404800	1.34144300
H	6.50800500	-3.81617100	0.61079600
H	-0.08297100	-0.02348700	-2.58591700

Re-M2

C	0.13946000	3.15566000	1.26559700
C	-0.71977700	2.14308100	0.82304300
C	-1.35046000	1.30294800	1.73723600
C	-1.07568400	1.46084100	3.09590400
C	-0.19386200	2.44939600	3.53296400
C	0.41047900	3.31261300	2.61999900
C	0.65738000	3.97438700	0.11325100
C	-0.32828200	3.60113900	-1.01503700
C	-0.80517100	2.15888900	-0.69194700
H	-2.04956300	0.53998300	1.41206000
H	-1.55760700	0.81048400	3.81863500
H	0.00895100	2.55916700	4.59363100
H	1.07532400	4.10049700	2.96131800
H	1.68632300	3.68516200	-0.13338300
H	-1.20427500	4.25046300	-0.94909400
H	0.66105000	5.04844300	0.31217100
H	-1.80666500	1.97961700	-1.08805100
N	0.15001900	1.21705400	-1.32861900
O	0.14970200	3.74034800	-2.33259700
C	0.42837500	-0.09900400	-0.93977000
C	1.32086800	1.69169200	-1.90260000
N	1.78125200	-0.27552800	-1.23053500
N	2.30204700	0.86389200	-1.84037200
C	1.34496400	3.02977300	-2.58188300
H	2.23134500	3.59159800	-2.26418600
H	1.40373800	2.88785700	-3.66386000
C	2.69227600	-1.07749000	-0.46710000
C	3.23630900	-2.22183200	-1.05917700
C	3.02654700	-0.68272600	0.83405300

C	4.14385800	-2.97486000	-0.31820000
C	3.93397900	-1.47211400	1.54366900
C	4.50230900	-2.61636300	0.98405400
H	4.57926400	-3.86569600	-0.76493200
H	4.20859400	-1.17870200	2.55424500
C	2.41675700	0.55180400	1.44643500
H	1.35497600	0.40554700	1.68134900
H	2.47818500	1.40168600	0.75857100
H	2.93150900	0.82016100	2.37095100
C	5.46342000	-3.46707900	1.77408800
H	4.93697400	-4.29275000	2.26397200
H	5.96198400	-2.88442100	2.55179900
H	6.22657200	-3.90382200	1.12549300
C	2.81196200	-2.62408800	-2.44416000
H	2.98771100	-1.81652500	-3.15997600
H	1.73865200	-2.83764600	-2.45160100
H	3.35244600	-3.51293000	-2.77444000
C	-0.42484000	-1.07110900	-0.49883100
O	0.10386500	-2.32001200	-0.19122400
C	-1.85278200	-0.95221700	-0.49030100
C	-2.70391700	-1.90725800	-0.05502400
H	-2.25542100	-0.03440800	-0.91081800
H	-2.28094500	-2.83548800	0.32109600
C	-4.16532000	-1.81450500	-0.06174800
C	-4.92431900	-2.95838700	0.23533700
C	-4.86185500	-0.62436000	-0.33775700
C	-6.31475300	-2.92283100	0.24318000
H	-4.40671000	-3.88783000	0.45813000
C	-6.25041800	-0.58920700	-0.33352100
H	-4.31333600	0.29011600	-0.54554000

C	-6.98801200	-1.73789900	-0.04464500
H	-6.87379100	-3.82428700	0.47493100
H	-6.76245000	0.34368300	-0.54930800
H	-8.07254800	-1.70607400	-0.03851200
H	0.68099100	-2.24788500	0.57994800

Si-M2

C	3.79807800	1.05598800	1.30131400
C	2.89344600	1.61426700	0.39181700
C	1.94212300	2.53825000	0.81813200
C	1.88740300	2.86791300	2.17254000
C	2.77186900	2.28914300	3.08350100
C	3.74117700	1.38561900	2.65107500
C	4.76076300	0.12513400	0.61359200
C	4.58408700	0.50547100	-0.87344900
C	3.13928000	1.06296700	-1.00105800
H	1.25913600	2.98984600	0.10837700
H	1.14921500	3.58325000	2.52096100
H	2.71526300	2.55663200	4.13410000
H	4.44687700	0.95362500	3.35450700
H	4.48162100	-0.91828300	0.80132100
H	5.26979300	1.32024600	-1.11712800
H	5.79457100	0.24827000	0.94479200
H	3.03662100	1.80584600	-1.79113100
N	2.25033400	-0.08483800	-1.31237400
O	4.86576100	-0.51765600	-1.80431700
C	0.88210200	-0.14063200	-1.04882500
C	2.71530200	-1.38384200	-1.20718200
N	0.65074200	-1.46933100	-0.72402400
N	1.81063400	-2.22546900	-0.84727700

C	4.13155400	-1.70468700	-1.58593600
H	4.59144200	-2.34082800	-0.82040500
H	4.14002100	-2.25368800	-2.53096600
C	-0.42811000	-1.97501400	0.05849100
C	-1.36367900	-2.81667600	-0.55150100
C	-0.53951900	-1.57771800	1.39705100
C	-2.45078800	-3.24517500	0.20852200
C	-1.64878300	-2.02153300	2.11604000
C	-2.61660300	-2.84491100	1.53672400
H	-3.19156400	-3.89665000	-0.24911800
H	-1.75847700	-1.71830800	3.15478500
C	0.48729200	-0.67015500	2.01937200
H	0.34539800	0.36631900	1.69047700
H	1.50304900	-0.95772700	1.72771800
H	0.41636500	-0.69628400	3.10840500
C	-3.83201900	-3.26813500	2.32095100
H	-4.62734800	-2.52080300	2.22748300
H	-3.60148500	-3.37147200	3.38379700
H	-4.22738600	-4.21889400	1.95663000
C	-1.19800800	-3.20557100	-1.99547200
H	-0.24101000	-3.70949700	-2.15666400
H	-1.20294700	-2.31576200	-2.63343500
H	-2.00402100	-3.86808200	-2.31518400
C	-0.00192600	0.89607100	-1.20669800
O	0.52580100	2.08365900	-1.71539600
C	-1.39825200	0.85003800	-0.89155000
C	-2.25861700	1.88420900	-1.03027300
H	-1.77811700	-0.10348900	-0.53912400
H	-1.88185800	2.83695400	-1.39584800
C	-3.69000300	1.82875900	-0.72744400

C	-4.50293000	2.92550600	-1.05864800
C	-4.30755000	0.72366800	-0.11165400
C	-5.87013300	2.91947300	-0.80276000
H	-4.04648400	3.79260000	-1.52939700
C	-5.67333100	0.71727300	0.14121800
H	-3.71456600	-0.13855100	0.18360900
C	-6.46655300	1.81281300	-0.20307500
H	-6.47098400	3.78237900	-1.07375100
H	-6.12380700	-0.14898600	0.61705200
H	-7.53265600	1.80370800	-0.00131000
H	0.21284500	2.17598300	-2.62602200

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C	1.74090100	-4.48060400	1.85858400
C	1.63695700	-3.14511600	1.46067900
C	1.43762700	-2.13737400	2.40451000
C	1.32458600	-2.49255800	3.74758900
C	1.42071000	-3.82722100	4.14354700
C	1.63647200	-4.82957000	3.20105600
C	1.96263300	-5.39861700	0.68789400
C	2.32735000	-4.42853200	-0.45544800
C	1.77979900	-3.02603400	-0.04684700
H	1.39447100	-1.09713000	2.10320000
H	1.17127200	-1.71943400	4.49328600
H	1.33671300	-4.08456500	5.19467200
H	1.72538000	-5.86738900	3.50804500
H	1.05252500	-5.96757700	0.47175100
H	3.41336800	-4.33494800	-0.51205500
H	2.75873500	-6.12674400	0.85903600
H	2.43203200	-2.21483700	-0.36222200

N	0.46753700	-2.82257300	-0.71352600
O	1.92588200	-4.83110900	-1.74964000
C	-0.43204700	-1.81008000	-0.52152900
C	-0.19392100	-3.82103000	-1.38351400
N	-1.59597900	-2.28936600	-1.01817200
N	-1.44189000	-3.53324000	-1.57518100
C	0.53767500	-5.03111600	-1.88097800
H	0.19143000	-5.93120300	-1.36094400
H	0.33056500	-5.15714000	-2.94530500
C	-2.87666700	-1.65271900	-1.07328000
C	-3.68368200	-1.67542800	0.06942300
C	-3.26761100	-1.05717500	-2.27309600
C	-4.90353200	-1.00470500	0.00252500
C	-4.50702200	-0.42077000	-2.29713700
C	-5.31993600	-0.35804300	-1.16485000
H	-5.54273800	-0.98708600	0.88191600
H	-4.83464500	0.05793600	-3.21658900
C	-2.36902300	-1.10547600	-3.47849000
H	-2.13316300	-2.13866100	-3.74833300
H	-1.42109400	-0.59571700	-3.27386900
H	-2.84317500	-0.62226100	-4.33398600
C	-6.60375000	0.42740200	-1.19417400
H	-7.07117500	0.38601400	-2.18073400
H	-6.39914900	1.47994400	-0.96900900
H	-7.31612500	0.05811600	-0.45349000
C	-3.22577500	-2.37472900	1.32194400
H	-2.35693200	-1.87209900	1.76442000
H	-2.93001200	-3.40586100	1.10710800
H	-4.02284500	-2.38884700	2.06649300
C	-0.11849100	-0.52937200	0.02615400

O	1.24332200	-0.27805600	0.07690500
C	-1.03436800	0.30473500	0.62484700
C	-0.71243900	1.47767300	1.33676700
H	-2.07997900	0.05535800	0.49416300
H	0.31780900	1.58780600	1.67176100
C	-1.70643800	2.13000000	2.20003600
C	-1.26658200	3.14429800	3.06911600
C	-3.08438400	1.86079200	2.15050900
C	-2.16263400	3.85205100	3.86209800
H	-0.20342400	3.37589600	3.09458000
C	-3.97891700	2.56899900	2.94619000
H	-3.47421500	1.10016100	1.47875100
C	-3.52690700	3.56817800	3.80695600
H	-1.79524100	4.62981700	4.52492000
H	-5.03920600	2.34030100	2.88940000
H	-4.22812700	4.11972600	4.42472800
H	1.37242900	0.64465700	-0.19861500
C	5.67330600	2.59122200	-0.19661100
C	5.31773900	2.12729200	-1.49223100
C	6.33818900	1.73022800	-2.37592000
C	7.65381000	1.80409200	-1.95734100
C	7.98355400	2.26855900	-0.66550500
C	7.00579600	2.66633100	0.22900000
C	3.43849700	2.67203200	-0.37046100
C	3.89040300	2.18741100	-1.57746100
H	6.09191100	1.37317800	-3.37156900
H	8.45059200	1.50170300	-2.62928400
H	9.02648900	2.31382100	-0.36839000
H	7.25721700	3.02353200	1.22235200
H	3.28147500	1.91056200	-2.42605200

N	4.51211900	2.90991000	0.45250600
H	4.38727800	3.25673600	1.39279400
C	2.08443400	2.94172700	0.18090700
O	2.01537100	3.31428900	1.37594700
C	0.96327600	2.71341200	-0.65749400
C	-0.32017500	2.95110200	-0.13083100
H	1.11190600	2.37970200	-1.67857600
H	-0.34539700	3.65002900	0.70364500
C	-1.53752900	2.94582400	-0.96375000
C	-2.67462900	3.64261300	-0.53107500
C	-1.59695900	2.25871500	-2.18469000
C	-3.83817000	3.65382200	-1.29608100
H	-2.63751100	4.17828800	0.41371700
C	-2.75076600	2.29049400	-2.95832100
H	-0.73152100	1.70168500	-2.53162200
C	-3.87837600	2.98181600	-2.51502200
H	-4.70949000	4.19778300	-0.94420500
H	-2.77445000	1.77061400	-3.91147000
H	-4.78099000	2.99671200	-3.11869500

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C	6.63388600	-0.42916600	0.25253000
C	5.32761800	-0.11395700	0.61678400
C	4.97533700	0.11039400	1.94440300
C	5.96670600	0.01037500	2.91724600
C	7.28045200	-0.30514500	2.55933500
C	7.62406100	-0.52453900	1.22743200
C	6.75832400	-0.61787700	-1.23753500
C	5.30747800	-0.62119400	-1.77521000
C	4.42271500	-0.07214900	-0.59362500

H	3.95272200	0.36253900	2.21138100
H	5.71875700	0.17890800	3.95993700
H	8.04107100	-0.38382700	3.32949000
H	8.64549100	-0.77299400	0.95534300
H	7.26052800	-1.55012600	-1.51451800
H	5.19902000	0.03064600	-2.64305800
H	7.32756500	0.20009800	-1.68974900
H	4.07148800	0.93359100	-0.81486400
N	3.23640900	-0.91892900	-0.39386700
O	4.90826700	-1.89886200	-2.24588900
C	1.99068000	-0.65145600	0.08224900
C	3.31068500	-2.27122600	-0.60184300
N	1.38352400	-1.85964900	0.13417300
N	2.19806300	-2.86682900	-0.31096300
C	4.55839300	-2.80776900	-1.21992500
H	5.35571000	-2.91112600	-0.47119600
H	4.36620100	-3.77968300	-1.67344100
C	0.03686300	-2.16652300	0.52628900
C	-0.28039900	-2.20507400	1.88479800
C	-0.90909400	-2.35738500	-0.48736200
C	-1.61928200	-2.41247000	2.22162200
C	-2.22820700	-2.57481100	-0.09988400
C	-2.60357900	-2.58776500	1.24708300
H	-1.89848300	-2.42367600	3.27207400
H	-2.99099800	-2.71194600	-0.86133300
C	-0.50764100	-2.28841100	-1.93575100
H	0.22223300	-3.06516600	-2.18153700
H	-0.04203200	-1.32286700	-2.16466700
H	-1.37746800	-2.41214900	-2.58269200
C	-4.05194400	-2.77699600	1.61515600

H	-4.69138700	-2.12292700	1.01159900
H	-4.22383000	-2.56346100	2.67218500
H	-4.37057200	-3.80587900	1.41835400
C	0.77182200	-1.96954400	2.93447800
H	1.04650600	-0.90906600	2.97231600
H	1.67992700	-2.54066800	2.72199500
H	0.40184800	-2.25767000	3.91935300
C	1.48346800	0.63885800	0.46507300
O	2.46377700	1.59789900	0.59287000
C	0.16376300	0.88309600	0.70308000
C	-0.43128300	2.15212300	0.95447700
H	-0.51754000	0.05631400	0.54908000
H	0.25606000	2.95338600	1.22772100
C	-1.71418400	2.18720500	1.68535500
C	-2.05978200	3.33486900	2.41511900
C	-2.64011800	1.13436100	1.63348200
C	-3.28432300	3.43450200	3.06168700
H	-1.35241900	4.15955100	2.46605200
C	-3.86852300	1.23487300	2.28185100
H	-2.42462500	0.23210300	1.06900300
C	-4.20020100	2.38325100	2.99537100
H	-3.52795700	4.33356900	3.61966400
H	-4.57129800	0.40755600	2.22037100
H	-5.15744800	2.45868100	3.50168800
H	2.19841100	2.38982100	0.09767000
C	-6.00546600	-0.33160800	-0.73841100
C	-5.21435100	-1.14852400	-1.59453800
C	-5.63718800	-2.46340700	-1.85822800
C	-6.79658800	-2.93064300	-1.26211100
C	-7.55958600	-2.10673700	-0.40926000

C	-7.18008400	-0.80106700	-0.13988600
C	-4.19287000	0.84722600	-1.34118500
C	-4.06905800	-0.37259300	-1.96472600
H	-5.05380800	-3.10459800	-2.51396600
H	-7.12743900	-3.94687700	-1.45169800
H	-8.46342300	-2.50239500	0.04289000
H	-7.76725200	-0.16542800	0.51535000
H	-3.25338100	-0.68022400	-2.60384700
N	-5.37035700	0.87695300	-0.63681800
H	-5.60335800	1.67275000	-0.05846300
C	-3.29219900	2.02868900	-1.16901600
O	-3.81966400	3.08285000	-0.74408100
C	-1.92313200	1.80505500	-1.42199000
C	-0.95609100	2.70826400	-0.92068200
H	-1.62528000	0.82046100	-1.77149900
H	-1.38734600	3.65353200	-0.58737300
C	0.39692200	2.85011800	-1.51980500
C	1.17387000	3.98459200	-1.22654300
C	0.96259600	1.85532800	-2.32786700
C	2.47665600	4.10869000	-1.70153300
H	0.74479500	4.77070500	-0.60967900
C	2.27029000	1.97213800	-2.79769100
H	0.36759000	0.99120300	-2.60447000
C	3.03600200	3.09221700	-2.47980200
H	3.05618200	4.99438900	-1.46251500
H	2.68869800	1.18606700	-3.42010400
H	4.05353900	3.18184700	-2.84667400

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C	5.01193500	-1.73637800	1.37859000
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C	3.63288700	-1.55737900	1.45827000
C	2.86109800	-2.28150000	2.36386200
C	3.49933900	-3.20084400	3.19240100
C	4.88263000	-3.38494700	3.11678700
C	5.64786100	-2.65261300	2.21260400
C	5.62514700	-0.84002800	0.33611800
C	4.43484600	-0.20953100	-0.42280800
C	3.15799700	-0.52894300	0.45322500
H	1.78957300	-2.11783000	2.42626900
H	2.91823400	-3.77805400	3.90421500
H	5.36390400	-4.10708500	3.76873800
H	6.72236400	-2.79852800	2.15328500
H	6.27740300	-1.37397500	-0.36264900
H	4.55277900	0.86714300	-0.51624600
H	6.22798200	-0.05207900	0.80018500
H	2.78368400	0.37798800	0.92625300
N	2.06871100	-1.06748200	-0.37912500
O	4.34757200	-0.66231200	-1.76458200
C	0.71174600	-1.04339700	-0.24980300
C	2.36096400	-1.82426100	-1.48335200
N	0.26888800	-1.77251400	-1.30278300
N	1.29250900	-2.24808700	-2.07826200
C	3.78880300	-1.95252800	-1.89219000
H	4.31087600	-2.69127900	-1.26773000
H	3.85280200	-2.25768700	-2.93646000
C	-1.07574100	-1.96816700	-1.75792400
C	-1.80793000	-3.05110600	-1.27236200
C	-1.59546400	-1.02598800	-2.64803400
C	-3.13346400	-3.16305900	-1.69191400
C	-2.91871200	-1.18761900	-3.05018700

C	-3.70646900	-2.23475100	-2.56575600
H	-3.73624800	-3.98592000	-1.31613100
H	-3.34759900	-0.47019400	-3.74591800
C	-0.75991800	0.14862200	-3.07855300
H	0.16013900	-0.17452300	-3.57476500
H	-0.46911300	0.73790400	-2.19906700
H	-1.31775900	0.79618200	-3.75752500
C	-5.16227900	-2.32323000	-2.93930900
H	-5.75578100	-1.68029900	-2.27910700
H	-5.53972400	-3.34302600	-2.84166500
H	-5.32887900	-1.98417700	-3.96459700
C	-1.19370400	-4.00513100	-0.28490600
H	-0.97184300	-3.48602500	0.65490300
H	-0.25360700	-4.41482500	-0.66505900
H	-1.87366200	-4.82987400	-0.06829800
C	-0.04053200	-0.44822700	0.82921400
O	0.72366600	-0.05233900	1.88279200
C	-1.41827600	-0.42013900	0.85208300
C	-2.15683000	0.28130500	1.82261100
H	-1.95839800	-0.82324300	0.00465900
H	-1.58865000	0.65322800	2.67173900
C	-3.56604000	-0.02070800	2.10842000
C	-4.14241100	0.49179800	3.28030300
C	-4.39194700	-0.74962400	1.23580300
C	-5.48922900	0.29475000	3.57061800
H	-3.51810900	1.05879000	3.96744000
C	-5.73754000	-0.94133000	1.52304500
H	-3.98614100	-1.16594100	0.31707200
C	-6.29701900	-0.42052500	2.69039500
H	-5.90689200	0.70149600	4.48679500

H	-6.35611300	-1.50396300	0.82950800
H	-7.34811200	-0.57617500	2.91139800
H	0.53792000	0.93744200	2.09205700
C	3.59009100	3.10693700	0.06667000
C	3.16496100	2.90955300	-1.27605500
C	4.13291300	2.89835800	-2.29720400
C	5.46333700	3.07824100	-1.96239800
C	5.86016300	3.28306300	-0.62291600
C	4.93427300	3.30492600	0.40663700
C	1.36843600	2.77343400	0.08306300
C	1.74846800	2.70456200	-1.23930400
H	3.83858200	2.73645700	-3.32969300
H	6.21972700	3.06249800	-2.74045000
H	6.91201200	3.42474900	-0.39656800
H	5.23544800	3.45512700	1.43829900
H	1.10009500	2.51508300	-2.08282800
N	2.47893600	3.01633300	0.85894000
H	2.41369500	3.07346700	1.86562400
C	0.09607600	2.57636500	0.81091800
O	0.21557700	2.39467300	2.08117700
C	-1.11956500	2.51610500	0.14370100
C	-2.30397400	2.24168000	0.86383300
H	-1.13837500	2.60110700	-0.93872200
H	-2.33988200	2.61623800	1.88465500
C	-3.60006700	2.16380200	0.16976000
C	-4.77216500	2.59771000	0.80248400
C	-3.70519300	1.57839100	-1.09914200
C	-6.01024000	2.45791200	0.18470300
H	-4.70505100	3.03569700	1.79437300
C	-4.94257300	1.43692500	-1.71847500

H	-2.80886900	1.20289500	-1.58599200
C	-6.10063000	1.87622600	-1.07852300
H	-6.90767800	2.79515500	0.69424000
H	-5.00783700	0.97505600	-2.69964600
H	-7.06707700	1.76082000	-1.55911300

TS3RS

C	-4.59894400	0.17504900	2.64370800
C	-3.23608200	0.22487700	2.36117900
C	-2.30796300	0.57800900	3.33708900
C	-2.77001600	0.87890200	4.61578700
C	-4.13549700	0.82277200	4.90740300
C	-5.05780800	0.47002500	3.92537800
C	-5.39835200	-0.21291900	1.42805800
C	-4.40012000	-0.18176900	0.24710200
C	-2.96676800	-0.11368700	0.90955000
H	-1.24763500	0.60771000	3.10588200
H	-2.06496600	1.15871000	5.39173900
H	-4.48050800	1.06209600	5.90827900
H	-6.11922600	0.43538400	4.15229800
H	-6.23362600	0.46631900	1.22956300
H	-4.47740500	-1.07811300	-0.36529000
H	-5.82003400	-1.21724700	1.53764700
H	-2.44773600	-1.06429900	0.78355100
N	-2.14073000	0.92360900	0.27613900
O	-4.67017700	0.87807400	-0.65735200
C	-0.78906000	1.07190300	0.15708900
C	-2.72167800	2.06571900	-0.20922900
N	-0.64243500	2.29081100	-0.42097000
N	-1.84498400	2.90463600	-0.65858800

C	-4.21052800	2.13998000	-0.22245200
H	-4.59347700	2.39595100	0.77584500
H	-4.54412800	2.89358500	-0.93564800
C	0.56914400	3.01548400	-0.67003700
C	1.22064000	3.60853200	0.41635800
C	1.06522600	3.05342000	-1.97429200
C	2.44752400	4.21870300	0.16880800
C	2.29497900	3.68313100	-2.17094800
C	3.00658700	4.24792200	-1.11148200
H	2.98361500	4.67693200	0.99635300
H	2.71133500	3.71844100	-3.17443800
C	0.32234800	2.38617100	-3.09864900
H	-0.71422300	2.73285100	-3.14403500
H	0.31982000	1.30020800	-2.94443200
H	0.80351300	2.60043400	-4.05449000
C	4.36602800	4.85829200	-1.32974300
H	4.54877700	5.05665800	-2.38760800
H	5.14521200	4.17584800	-0.97419800
H	4.47212800	5.79459600	-0.77620100
C	0.64290500	3.53494700	1.80384500
H	0.81813900	2.54396100	2.23817100
H	-0.43691300	3.70909400	1.79734900
H	1.11060100	4.27582100	2.45408000
C	0.22923800	0.17473700	0.60831900
O	-0.20366000	-0.80365200	1.49290900
C	1.56097800	0.34369800	0.30893600
C	2.59474300	-0.50194900	0.76269000
H	1.82184600	1.12287500	-0.39418000
H	2.38034800	-1.07383600	1.66420200
C	3.99592300	-0.07184300	0.60441300

C	4.95464500	-0.41976800	1.56555700
C	4.42799600	0.62705900	-0.53563600
C	6.29018600	-0.06150700	1.41114700
H	4.64265800	-0.98642900	2.43969900
C	5.76323900	0.98557800	-0.68954900
H	3.71594300	0.87858700	-1.31926800
C	6.70239500	0.64738600	0.28443700
H	7.01229400	-0.34116400	2.17247900
H	6.07304800	1.52319300	-1.58109000
H	7.74406200	0.92554400	0.16141400
H	0.03115500	-1.65400000	1.09173900
C	-3.16147700	-1.59721800	-2.54602700
C	-3.20005900	-2.78082100	-1.75909100
C	-4.43103800	-3.43721900	-1.57352700
C	-5.56761400	-2.90251000	-2.15370600
C	-5.50649300	-1.72245200	-2.92653300
C	-4.31011500	-1.05874300	-3.13696900
C	-1.08175400	-2.00393100	-1.80344400
C	-1.86715000	-3.01446400	-1.29416100
H	-4.48390300	-4.34332600	-0.97741400
H	-6.52541700	-3.39369300	-2.01506600
H	-6.41790800	-1.32663200	-3.36267300
H	-4.26536900	-0.14441700	-3.71916000
H	-1.53450800	-3.83974100	-0.68128600
N	-1.86438600	-1.15439800	-2.54713900
H	-1.47033700	-0.36931700	-3.04649500
C	0.37037200	-1.69501300	-1.69275000
O	0.82904900	-0.76561800	-2.40313400
C	1.12237100	-2.46465100	-0.77735000
C	2.46910400	-2.12995600	-0.54776900

H	0.65155200	-3.28828700	-0.24878900
H	2.93123100	-1.54658400	-1.34303600
C	3.39102300	-3.05598500	0.15005800
C	4.73630200	-3.10871200	-0.23175600
C	2.96332300	-3.87324900	1.20550500
C	5.62576500	-3.97103700	0.40328000
H	5.08382400	-2.45689600	-1.02913700
C	3.85097600	-4.73098900	1.84446500
H	1.92887500	-3.82722500	1.53669500
C	5.18584800	-4.78719300	1.44177900
H	6.66460200	-3.99961200	0.08962700
H	3.50326500	-5.35671700	2.66052800
H	5.87775900	-5.45855700	1.94026900

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C	5.25793900	-2.87197000	-1.08613200
C	4.19356100	-2.54352400	-0.24058200
C	2.94440900	-3.13951800	-0.40497200
C	2.77231200	-4.05147100	-1.44508600
C	3.83083000	-4.37073400	-2.29635100
C	5.08389300	-3.78788000	-2.11769400
C	6.51267800	-2.13215600	-0.70631700
C	6.19338400	-1.65440800	0.72551400
C	4.64530200	-1.53936500	0.80319500
H	2.12750000	-2.91227300	0.26975300
H	1.80563200	-4.52339300	-1.58684700
H	3.68015100	-5.08871900	-3.09612900
H	5.91362600	-4.04912600	-2.76735900
H	6.67985200	-1.29422900	-1.39211900
H	6.48549200	-2.43378800	1.43239500

H	7.40934900	-2.75483000	-0.73199400
H	4.25074700	-1.72654800	1.80018400
N	4.28094300	-0.14539000	0.43475900
O	6.86153500	-0.48806000	1.15826400
C	3.04604000	0.36062000	0.16851300
C	5.19228500	0.81236600	0.06777400
N	3.27963000	1.56115300	-0.39648700
N	4.61433800	1.85345400	-0.44932500
C	6.65794500	0.63253700	0.32875200
H	7.20687200	0.55708600	-0.61670800
H	7.03160800	1.50482400	0.86835700
C	2.30567000	2.52440300	-0.81773700
C	1.80550100	2.43709700	-2.12031200
C	1.88736500	3.48748600	0.10136700
C	0.79261000	3.32411000	-2.47529300
C	0.86583900	4.34923600	-0.29890100
C	0.29615500	4.26823100	-1.57048600
H	0.37361200	3.27061200	-3.47708300
H	0.50572400	5.09847900	0.40137900
C	2.54524800	3.60200200	1.45017100
H	3.52975100	4.07036400	1.35368300
H	2.69507300	2.61896800	1.90577900
H	1.94079100	4.20958900	2.12675300
C	-0.85067800	5.16354800	-1.95684400
H	-0.81161200	5.42063100	-3.01766700
H	-0.84809200	6.08565100	-1.37224700
H	-1.80210400	4.65404900	-1.77330100
C	2.33196200	1.40162900	-3.07964800
H	2.11464000	0.38439800	-2.73191700
H	3.41784900	1.48280300	-3.18383800

H	1.87739300	1.52504900	-4.06344900
C	1.79576500	-0.26237500	0.51898300
O	1.89120800	-1.16870900	1.55852600
C	0.64384500	-0.09115700	-0.19346600
C	-0.61979200	-0.69897700	0.07627000
H	0.69160300	0.60773500	-1.01935500
H	-0.56157700	-1.56158700	0.74043800
C	-1.55764700	-0.88363400	-1.05524600
C	-2.59202400	-1.81738600	-0.91073500
C	-1.52455200	-0.11970800	-2.23277400
C	-3.56614600	-1.97783400	-1.89388300
H	-2.63404500	-2.41737800	-0.00577200
C	-2.48775000	-0.28579300	-3.21913800
H	-0.75552200	0.63405700	-2.38319600
C	-3.52011100	-1.21046000	-3.05256900
H	-4.36365400	-2.70037800	-1.74714500
H	-2.44145500	0.31877200	-4.12009000
H	-4.27590400	-1.33248600	-3.82210800
H	1.68252800	-0.71259400	2.39070200
C	-7.34835300	-0.18484000	-0.24265900
C	-7.22839800	-1.08753400	0.85050000
C	-8.34178400	-1.87145400	1.20442500
C	-9.51436300	-1.74299300	0.48073400
C	-9.60892000	-0.84199300	-0.60075500
C	-8.53370000	-0.05403200	-0.97583500
C	-5.26495600	-0.00772500	0.57635900
C	-5.89313100	-0.95585200	1.35228900
H	-8.27870100	-2.56767900	2.03584300
H	-10.37894800	-2.34318000	0.74630300
H	-10.54306700	-0.76458400	-1.14815900

H	-8.60368400	0.64091600	-1.80660600
H	-5.45824500	-1.49358900	2.18243900
N	-6.14407700	0.44918100	-0.37358400
H	-5.85209600	1.14388200	-1.04680300
C	-3.89147400	0.58041800	0.53481200
O	-3.70857200	1.49244900	-0.30762700
C	-2.93298000	0.06564300	1.42847100
C	-1.58084000	0.48312300	1.33458900
H	-3.22266400	-0.73073300	2.10570200
H	-1.45998800	1.41139800	0.77503400
C	-0.69341000	0.38435400	2.52311700
C	0.26265100	1.37739400	2.76431300
C	-0.74724400	-0.71304700	3.39499600
C	1.15055500	1.27453600	3.83573600
H	0.30824500	2.23259600	2.09479400
C	0.13744500	-0.82180000	4.46201900
H	-1.47365200	-1.50125300	3.21893100
C	1.09755700	0.16903100	4.68398700
H	1.88286000	2.05714100	4.01006800
H	0.08910600	-1.68534900	5.11753600
H	1.79283900	0.08159200	5.51215200

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C	6.63388600	-0.42916600	0.25253000
C	5.32761800	-0.11395700	0.61678400
C	4.97533700	0.11039400	1.94440300
C	5.96670600	0.01037500	2.91724600
C	7.28045200	-0.30514500	2.55933500
C	7.62406100	-0.52453900	1.22743200
C	6.75832400	-0.61787700	-1.23753500

C	5.30747800	-0.62119400	-1.77521000
C	4.42271500	-0.07214900	-0.59362500
H	3.95272200	0.36253900	2.21138100
H	5.71875700	0.17890800	3.95993700
H	8.04107100	-0.38382700	3.32949000
H	8.64549100	-0.77299400	0.95534300
H	7.26052800	-1.55012600	-1.51451800
H	5.19902000	0.03064600	-2.64305800
H	7.32756500	0.20009800	-1.68974900
H	4.07148800	0.93359100	-0.81486400
N	3.23640900	-0.91892900	-0.39386700
O	4.90826700	-1.89886200	-2.24588900
C	1.99068000	-0.65145600	0.08224900
C	3.31068500	-2.27122600	-0.60184300
N	1.38352400	-1.85964900	0.13417300
N	2.19806300	-2.86682900	-0.31096300
C	4.55839300	-2.80776900	-1.21992500
H	5.35571000	-2.91112600	-0.47119600
H	4.36620100	-3.77968300	-1.67344100
C	0.03686300	-2.16652300	0.52628900
C	-0.28039900	-2.20507400	1.88479800
C	-0.90909400	-2.35738500	-0.48736200
C	-1.61928200	-2.41247000	2.22162200
C	-2.22820700	-2.57481100	-0.09988400
C	-2.60357900	-2.58776500	1.24708300
H	-1.89848300	-2.42367600	3.27207400
H	-2.99099800	-2.71194600	-0.86133300
C	-0.50764100	-2.28841100	-1.93575100
H	0.22223300	-3.06516600	-2.18153700
H	-0.04203200	-1.32286700	-2.16466700

H	-1.37746800	-2.41214900	-2.58269200
C	-4.05194400	-2.77699600	1.61515600
H	-4.69138700	-2.12292700	1.01159900
H	-4.22383000	-2.56346100	2.67218500
H	-4.37057200	-3.80587900	1.41835400
C	0.77182200	-1.96954400	2.93447800
H	1.04650600	-0.90906600	2.97231600
H	1.67992700	-2.54066800	2.72199500
H	0.40184800	-2.25767000	3.91935300
C	1.48346800	0.63885800	0.46507300
O	2.46377700	1.59789900	0.59287000
C	0.16376300	0.88309600	0.70308000
C	-0.43128300	2.15212300	0.95447700
H	-0.51754000	0.05631400	0.54908000
H	0.25606000	2.95338600	1.22772100
C	-1.71418400	2.18720500	1.68535500
C	-2.05978200	3.33486900	2.41511900
C	-2.64011800	1.13436100	1.63348200
C	-3.28432300	3.43450200	3.06168700
H	-1.35241900	4.15955100	2.46605200
C	-3.86852300	1.23487300	2.28185100
H	-2.42462500	0.23210300	1.06900300
C	-4.20020100	2.38325100	2.99537100
H	-3.52795700	4.33356900	3.61966400
H	-4.57129800	0.40755600	2.22037100
H	-5.15744800	2.45868100	3.50168800
H	2.19841100	2.38982100	0.09767000
C	-6.00546600	-0.33160800	-0.73841100
C	-5.21435100	-1.14852400	-1.59453800
C	-5.63718800	-2.46340700	-1.85822800

C	-6.79658800	-2.93064300	-1.26211100
C	-7.55958600	-2.10673700	-0.40926000
C	-7.18008400	-0.80106700	-0.13988600
C	-4.19287000	0.84722600	-1.34118500
C	-4.06905800	-0.37259300	-1.96472600
H	-5.05380800	-3.10459800	-2.51396600
H	-7.12743900	-3.94687700	-1.45169800
H	-8.46342300	-2.50239500	0.04289000
H	-7.76725200	-0.16542800	0.51535000
H	-3.25338100	-0.68022400	-2.60384700
N	-5.37035700	0.87695300	-0.63681800
H	-5.60335800	1.67275000	-0.05846300
C	-3.29219900	2.02868900	-1.16901600
O	-3.81966400	3.08285000	-0.74408100
C	-1.92313200	1.80505500	-1.42199000
C	-0.95609100	2.70826400	-0.92068200
H	-1.62528000	0.82046100	-1.77149900
H	-1.38734600	3.65353200	-0.58737300
C	0.39692200	2.85011800	-1.51980500
C	1.17387000	3.98459200	-1.22654300
C	0.96259600	1.85532800	-2.32786700
C	2.47665600	4.10869000	-1.70153300
H	0.74479500	4.77070500	-0.60967900
C	2.27029000	1.97213800	-2.79769100
H	0.36759000	0.99120300	-2.60447000
C	3.03600200	3.09221700	-2.47980200
H	3.05618200	4.99438900	-1.46251500
H	2.68869800	1.18606700	-3.42010400
H	4.05353900	3.18184700	-2.84667400

TS3SR

C	-4.54397600	-1.24155300	-2.21069100
C	-3.29266600	-1.10081500	-1.61480700
C	-2.87290800	-1.93881800	-0.59299300
C	-3.73670600	-2.94590100	-0.16782200
C	-4.99107300	-3.09905800	-0.76068400
C	-5.40465400	-2.24861100	-1.78617800
C	-4.74097300	-0.21434000	-3.29751500
C	-3.59091600	0.79887300	-3.10383100
C	-2.51753600	0.02355700	-2.25611100
H	-1.90582100	-1.79757000	-0.11827800
H	-3.43506200	-3.60043000	0.64377200
H	-5.65622700	-3.88314000	-0.41301800
H	-6.38505000	-2.36601100	-2.23812200
H	-5.70369400	0.30162800	-3.24432100
H	-3.15920700	1.10922700	-4.05657800
H	-4.67077700	-0.67841400	-4.28716000
H	-1.73851600	-0.36350400	-2.91161700
N	-1.86523600	0.91340800	-1.28850000
O	-4.04757400	2.00916300	-2.51068100
C	-0.56247400	1.05180300	-0.90135100
C	-2.57161300	1.94257000	-0.72510200
N	-0.54450600	2.21322700	-0.17953600
N	-1.80968600	2.76211000	-0.07545400
C	-4.01173500	2.05570200	-1.09486900
H	-4.59874900	1.25028700	-0.63288100
H	-4.40842200	3.02076100	-0.78031100
C	0.58190200	3.07940800	0.05912500
C	1.28435700	3.55676400	-1.05820600
C	0.90175400	3.46779200	1.36489000

C	2.40863900	4.34643500	-0.82855400
C	2.02768500	4.27343300	1.53577100
C	2.81056700	4.69424300	0.46130500
H	2.97548800	4.70945400	-1.68241800
H	2.29819300	4.57806700	2.54358100
C	0.08356900	3.05225500	2.55684100
H	0.27524800	1.99832900	2.78148900
H	-0.98582900	3.19863200	2.37473200
H	0.35868700	3.65097600	3.42696300
C	4.05965200	5.50483200	0.68450700
H	4.20797400	6.23225300	-0.11701600
H	4.93798600	4.85127000	0.70311100
H	4.02158200	6.03807200	1.63670800
C	0.86217000	3.23666100	-2.46843900
H	-0.22726700	3.24751200	-2.57405500
H	1.21869800	2.24817900	-2.77599500
H	1.27690800	3.97397400	-3.15740200
C	0.48281200	0.11975600	-1.13511100
O	0.11528900	-1.02296900	-1.83520600
C	1.78019000	0.29978400	-0.71483400
C	2.75879900	-0.71559000	-0.82250300
H	2.03161800	1.21466100	-0.19474600
H	2.58923700	-1.44165400	-1.61618300
C	4.17528200	-0.36240300	-0.58706000
C	5.19096400	-0.94452400	-1.35380000
C	4.53666700	0.50337100	0.45694500
C	6.52922400	-0.65194300	-1.10545400
H	4.92293300	-1.63680100	-2.14813700
C	5.87382500	0.79711100	0.70320000
H	3.75932100	0.92445800	1.09237800

C	6.87639900	0.22339100	-0.07880800
H	7.30239300	-1.11166000	-1.71349300
H	6.13572700	1.46733100	1.51636700
H	7.91936300	0.45056600	0.11725200
H	0.19843300	-1.75779500	-1.20878200
C	-3.03707500	-0.02134700	2.35111100
C	-3.14218700	-1.39236500	2.70091200
C	-4.40247900	-1.89978100	3.06058300
C	-5.49624600	-1.05129900	3.05382100
C	-5.36565600	0.30838000	2.70149200
C	-4.13787000	0.84316700	2.34806000
C	-1.00463400	-0.95155900	2.12213000
C	-1.83428300	-1.96221300	2.54393900
H	-4.51629000	-2.94659500	3.32763400
H	-6.47498100	-1.43445800	3.32421900
H	-6.24343800	0.94653600	2.70951800
H	-4.02501300	1.89092300	2.08219800
H	-1.54245800	-2.98885000	2.71598800
N	-1.72867400	0.21477200	2.02064600
H	-1.30303700	1.10531200	1.80958000
C	0.43231000	-0.90354000	1.72962600
O	1.06943000	0.15844800	1.95800000
C	0.98387200	-2.02117500	1.07222500
C	2.36092600	-1.96525300	0.74019000
H	0.37046400	-2.89095600	0.85401900
H	2.93664100	-1.31726400	1.39950100
C	3.08913500	-3.18179500	0.30228500
C	4.41562100	-3.37432800	0.70520200
C	2.49480800	-4.14508800	-0.52350300
C	5.12201000	-4.50939400	0.31553100

H	4.89263400	-2.62128500	1.32730100
C	3.19917200	-5.27763700	-0.91615700
H	1.47324900	-4.00362300	-0.86815200
C	4.51553100	-5.46581300	-0.49422700
H	6.14789700	-4.64395900	0.64372700
H	2.72269100	-6.01459900	-1.55504400
H	5.06495300	-6.35046100	-0.79981000

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C	1.80577600	0.54571300	-1.03073900
O	2.56739600	1.70179500	-1.07292300
C	0.45564600	0.51177900	-1.24417700
C	-0.36673700	1.64629000	-1.49660100
H	-0.03348500	-0.44476800	-1.12716200
H	0.14139700	2.51284400	-1.92252600
C	-1.70711800	1.42582700	-2.05583700
C	-2.28033500	2.38201200	-2.90826100
C	-2.47856900	0.30311500	-1.70855000
C	-3.56741300	2.21928700	-3.40994400
H	-1.69997000	3.26077100	-3.17891200
C	-3.76493100	0.13899700	-2.21645300
H	-2.07220000	-0.44895800	-1.03787900
C	-4.31657600	1.09295600	-3.06949200
H	-3.98453000	2.96980900	-4.07465800
H	-4.34207200	-0.73676500	-1.93286800
H	-5.31960100	0.96300100	-3.46309500
H	1.98340500	2.46480100	-0.96092500
C	-4.18600900	-2.00675200	2.53259800
C	-5.10769200	-0.92748500	2.44509800
C	-6.45062100	-1.15395200	2.79782600

C	-6.83143200	-2.41506600	3.22065700
C	-5.89805300	-3.47020500	3.30220300
C	-4.56943700	-3.28336000	2.96110500
C	-3.07047200	-0.19886500	1.80399800
C	-4.37274700	0.20999600	1.97879200
H	-7.17564000	-0.34752600	2.73748800
H	-7.86487600	-2.60133200	3.49530600
H	-6.22924300	-4.44726100	3.63936100
H	-3.84928600	-4.09302800	3.02362600
H	-4.76224300	1.20094000	1.79528000
N	-2.96757600	-1.52932300	2.13414700
H	-2.08304600	-2.01370900	2.07675700
C	-1.82690200	0.46751200	1.33205900
O	-0.79263600	-0.25118800	1.26216200
C	-1.87888300	1.81446200	0.93628900
C	-0.71229200	2.39622900	0.39862700
H	-2.82969200	2.33502800	0.91370500
H	0.21109900	1.96864200	0.78894900
C	-0.65132600	3.85166100	0.11981800
C	0.54202300	4.55538400	0.32666300
C	-1.75684300	4.55024600	-0.38404000
C	0.63450500	5.91483200	0.04190600
H	1.40284000	4.03814200	0.74861000
C	-1.66467600	5.90849200	-0.67328400
H	-2.68770000	4.02054100	-0.56246700
C	-0.47021800	6.59630600	-0.46369300
H	1.56685500	6.44128300	0.22009000
H	-2.53040600	6.43329400	-1.06560600
H	-0.40261900	7.65548300	-0.68962300
C	4.28371200	-0.11284500	2.91455000

C	3.76947500	0.60533900	1.83238800
C	2.70442700	1.48169100	2.00745600
C	2.13090700	1.60899700	3.27018400
C	2.63617000	0.88173300	4.34858800
C	3.72192900	0.02403100	4.17981300
C	5.44597700	-0.97311800	2.49707800
C	5.82820700	-0.37795500	1.12474800
C	4.53893500	0.29140500	0.56616000
H	2.34114600	2.06322500	1.17220800
H	1.29217600	2.28357100	3.41234400
H	2.18609100	0.99316200	5.32975300
H	4.12583300	-0.52687600	5.02384000
H	5.13259600	-2.01986100	2.41996400
H	6.55451700	0.42281900	1.27692800
H	6.28495500	-0.93830300	3.19534200
H	4.74625900	1.16136100	-0.05576700
N	3.83817000	-0.70494200	-0.28282600
O	6.43877800	-1.26592500	0.21286800
C	2.59227700	-0.63089900	-0.83212500
C	4.27536300	-1.99430200	-0.46168200
N	2.33127200	-1.88343800	-1.26417700
N	3.37901700	-2.73243000	-1.03957200
C	5.66474800	-2.40722800	-0.07793000
H	5.63665600	-3.11554600	0.75772000
H	6.13374700	-2.90612400	-0.92773300
C	1.16331300	-2.33099800	-1.96642300
C	0.14472100	-2.94755000	-1.23605100
C	1.06644500	-2.04607000	-3.33064500
C	-1.03218600	-3.25299100	-1.91888100
C	-0.13099300	-2.36710600	-3.96590500

C	-1.19472600	-2.94839400	-3.27185300
H	-1.84956500	-3.71955200	-1.37429500
H	-0.24094600	-2.14560100	-5.02447500
C	2.19880000	-1.37657100	-4.06132600
H	3.15193500	-1.87118500	-3.85308600
H	2.29335600	-0.32999400	-3.75022400
H	2.02488600	-1.39532500	-5.13804600
C	-2.50874900	-3.20205200	-3.96168500
H	-3.05587300	-4.01909000	-3.48662700
H	-2.36387400	-3.44357900	-5.01705500
H	-3.13411900	-2.30389900	-3.90771900
C	0.28802500	-3.18711600	0.24256200
H	0.17581300	-2.23932900	0.78387000
H	1.26456900	-3.61393500	0.48550300
H	-0.48630200	-3.87416700	0.59071900

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C	-6.63573700	-0.15465700	-0.64459500
C	-5.28048100	0.13049800	-0.51023000
C	-4.57288600	0.80566800	-1.49742200
C	-5.25629500	1.20794900	-2.64201200
C	-6.61923600	0.93221900	-2.78403900
C	-7.31789800	0.25019800	-1.78950800
C	-7.15727800	-0.90034800	0.55710000
C	-5.90357300	-1.28063000	1.38200000
C	-4.73858900	-0.39381700	0.79822100
H	-3.51366700	1.01207600	-1.37141600
H	-4.73053400	1.73609300	-3.43151700
H	-7.13862300	1.24763400	-3.68330400
H	-8.37461000	0.03181000	-1.91035300

H	-7.71783300	-1.80299300	0.29502500
H	-6.03650000	-1.05857100	2.44076300
H	-7.82339700	-0.26773800	1.15199300
H	-4.48718700	0.40852200	1.48836800
N	-3.52392600	-1.19178200	0.58290000
O	-5.63779500	-2.67428800	1.34815800
C	-2.19880800	-0.88055400	0.62686800
C	-3.62435700	-2.50450800	0.20215100
N	-1.57607900	-2.03477500	0.28531400
N	-2.46241700	-3.04843100	0.03184100
C	-4.98611500	-3.11242700	0.17126600
H	-5.53018600	-2.81389600	-0.73522800
H	-4.91287400	-4.19893300	0.20470700
C	-0.16890800	-2.29763900	0.18101200
C	0.47948500	-2.86267600	1.28132200
C	0.49351200	-1.92219900	-0.98968100
C	1.86183500	-3.02575900	1.19431900
C	1.87349600	-2.10821100	-1.03014800
C	2.57441600	-2.63600100	0.05824800
H	2.39624300	-3.43984200	2.04567500
H	2.42345200	-1.81400500	-1.91937400
C	-0.26482500	-1.30130700	-2.13091400
H	-0.75018500	-0.37296700	-1.80686300
H	-1.04862200	-1.97144200	-2.49716000
H	0.40762700	-1.06553600	-2.95803100
C	4.07761800	-2.70519000	0.02785800
H	4.46041300	-3.40011500	0.77850600
H	4.49587500	-1.71140200	0.23219700
H	4.44885700	-3.00245300	-0.95665300
C	-0.28833100	-3.20655500	2.52874600

H	-1.11171000	-3.89259300	2.31104700
H	-0.72170600	-2.30314300	2.97347300
H	0.36642400	-3.66827900	3.26871300
C	-1.62821400	0.39392300	0.97355700
O	-2.55886900	1.40797600	1.05912300
C	-0.31300600	0.53134200	1.32484800
C	0.37619100	1.69235900	1.77419900
H	0.28865500	-0.36259400	1.23813700
H	-0.24785300	2.48883500	2.17974700
C	1.63934800	1.45394800	2.50197200
C	2.01655100	2.27929500	3.57095000
C	2.52121900	0.43386400	2.11050400
C	3.22653900	2.09112800	4.22881500
H	1.34689100	3.07603600	3.88662700
C	3.73276800	0.24736600	2.76836600
H	2.28044000	-0.20026800	1.26184000
C	4.09370300	1.07326900	3.82980300
H	3.49501100	2.73948300	5.05754900
H	4.39941900	-0.54815800	2.44509300
H	5.03809500	0.92567100	4.34405700
H	-2.18654300	2.21184400	0.66507700
C	6.20418800	-0.08611400	-1.14058000
C	5.38749800	-0.46750500	-2.24067000
C	5.86825300	-1.43917700	-3.13647200
C	7.11440400	-2.00021500	-2.91552500
C	7.90538400	-1.60891900	-1.81481100
C	7.46508900	-0.65094100	-0.91683800
C	4.27427000	1.05296500	-0.99793700
C	4.16677800	0.27270600	-2.12584500
H	5.26420500	-1.74797900	-3.98497100

H	7.49390900	-2.75382200	-3.59821800
H	8.87818900	-2.06775000	-1.66934300
H	8.06991100	-0.35092400	-0.06708900
H	3.32339900	0.25042400	-2.80165800
N	5.50057200	0.84070400	-0.41788700
H	5.78140100	1.35055900	0.40807400
C	3.36538700	2.02700300	-0.32083600
O	3.90242400	2.84960600	0.45343600
C	1.98614800	1.90846900	-0.61042000
C	1.04610400	2.67579300	0.10301100
H	1.66835600	1.11496600	-1.28157500
H	1.50960400	3.45069200	0.71517100
C	-0.25350900	3.08942600	-0.48586500
C	-1.00501600	4.10230300	0.13452400
C	-0.76112100	2.51703600	-1.65920500
C	-2.23384300	4.50678200	-0.37944300
H	-0.61405100	4.57147800	1.03418000
C	-1.98640100	2.92836500	-2.18072300
H	-0.17262100	1.77538900	-2.18850900
C	-2.73652700	3.91035600	-1.53715700
H	-2.79639500	5.28847900	0.12055700
H	-2.35344100	2.47847600	-3.09900000
H	-3.69634600	4.21731200	-1.93992800

TS3SS

C	0.38591700	0.43922400	-0.80305700
O	-0.87201300	0.24642800	-1.34604600
C	1.25574800	-0.59101600	-0.52929400
C	1.00559200	-1.96360100	-0.71022100

H	2.18977200	-0.30956300	-0.05922300
H	0.15165600	-2.25330600	-1.31981500
C	2.10550400	-2.93756200	-0.70913400
C	1.81255400	-4.26941300	-1.05321000
C	3.41858300	-2.63677300	-0.31053300
C	2.79015800	-5.25697600	-1.00751000
H	0.79187000	-4.51394400	-1.34132000
C	4.39466900	-3.62718500	-0.26445000
H	3.69386300	-1.62306600	-0.03310900
C	4.08998500	-4.94247000	-0.61199500
H	2.53602800	-6.27754500	-1.27815100
H	5.40164700	-3.36697400	0.05002400
H	4.85435700	-5.71191000	-0.57327000
H	-1.23874700	-0.55663900	-0.94586800
C	-5.65296900	-2.43227300	-1.16060300
C	-5.72315600	-1.45908100	-0.12720200
C	-6.94214900	-0.79188100	0.09523000
C	-8.03126600	-1.10315600	-0.69788300
C	-7.93748200	-2.07392300	-1.71899800
C	-6.75533200	-2.74911600	-1.96467800
C	-3.63497900	-2.31251800	-0.18847700
C	-4.42627700	-1.40150100	0.47664300
H	-7.02305600	-0.04456200	0.87902700
H	-8.97743700	-0.59684000	-0.53611500
H	-8.81205200	-2.29612200	-2.32206500
H	-6.67976700	-3.49615700	-2.74809300
H	-4.12773800	-0.77116400	1.30204100
N	-4.37761200	-2.92498100	-1.16799900
H	-3.97353400	-3.62854600	-1.76949700
C	-2.21201800	-2.72796800	-0.06695900

O	-1.80106700	-3.59780600	-0.87343700
C	-1.40045800	-2.08901700	0.90227900
C	-0.06706700	-2.51278800	1.04310500
H	-1.82053500	-1.32391000	1.54432700
H	0.12715700	-3.53490600	0.72153700
C	0.81273800	-2.02161600	2.11921900
C	1.87720800	-2.81889100	2.56048300
C	0.64179300	-0.75177800	2.69199900
C	2.74152600	-2.36718700	3.55407300
H	2.02490500	-3.79728100	2.11041200
C	1.50139300	-0.30484500	3.68973900
H	-0.15810500	-0.10605900	2.34039500
C	2.55541400	-1.10982300	4.12390300
H	3.56068800	-2.99897200	3.88294100
H	1.35215400	0.67793900	4.12767100
H	3.22583000	-0.75749200	4.90143100
C	-2.05529000	3.83867400	1.45978400
C	-1.90405700	2.68478300	0.68626800
C	-2.17836500	1.43256800	1.22323100
C	-2.55514900	1.34127200	2.56255100
C	-2.67935600	2.49095900	3.34394900
C	-2.44349800	3.74872400	2.79231500
C	-1.77273800	5.07667600	0.65396500
C	-1.84084100	4.54925600	-0.79579700
C	-1.47858100	3.03662400	-0.72426500
H	-2.11777100	0.54697900	0.60532000
H	-2.76053500	0.36846900	3.00229800
H	-2.97926500	2.40560100	4.38331700
H	-2.56803400	4.64621200	3.39057900
H	-0.78411500	5.47662000	0.90328400

S100

H	-2.87475600	4.60298600	-1.14288600
H	-2.49686700	5.87640700	0.82334800
H	-1.96810800	2.44558600	-1.49653000
N	-0.01074100	2.90826300	-0.92570700
O	-1.08673600	5.26471700	-1.74864400
C	0.79357900	1.80845400	-0.80162100
C	0.81808200	3.98894000	-1.10952100
N	2.05400600	2.30144500	-0.85654200
N	2.06824400	3.65484200	-1.05399800
C	0.28295300	5.35200200	-1.43305200
H	0.47770400	6.04845500	-0.60979700
H	0.79532200	5.72688000	-2.32091200
C	3.30099900	1.59238000	-0.89061600
C	4.01997700	1.46169800	0.29743900
C	3.72926100	1.05901700	-2.11005400
C	5.22391000	0.75736500	0.24466800
C	4.93279400	0.35875500	-2.11039100
C	5.69005500	0.19832300	-0.94628100
H	5.80057800	0.63326900	1.15756100
H	5.28749000	-0.07645800	-3.04149100
C	2.89700900	1.21537900	-3.35310000
H	2.63556100	2.26411500	-3.52311900
H	1.96258300	0.64982400	-3.26489000
H	3.43690500	0.84694600	-4.22635600
C	6.98092700	-0.57669200	-0.98918800
H	7.72984200	-0.05091300	-1.58920800
H	6.82526400	-1.55771100	-1.44701700
H	7.38987100	-0.72383300	0.01223400
C	3.47631900	2.02626400	1.58207500
H	2.50908000	1.56969500	1.82263800

H	3.32204000	3.10646000	1.50329300
H	4.15777500	1.82800800	2.41081600
TS3SS-180			
C	4.79763400	-0.68453000	-0.16786800
C	3.41536900	-0.62567100	0.00501800
C	2.83481100	-0.66340800	1.26531200
C	3.67518200	-0.76529000	2.37429000
C	5.06010200	-0.82081100	2.21046400
C	5.63333900	-0.77550500	0.93886300
C	5.14120900	-0.69022800	-1.63692500
C	3.82662200	-1.10329500	-2.33021700
C	2.70696400	-0.65983000	-1.33523700
H	1.75607900	-0.58024900	1.39326700
H	3.24665100	-0.80082500	3.37157300
H	5.69972500	-0.90216900	3.08401700
H	6.71122500	-0.82438000	0.81658400
H	5.94835700	-1.37791900	-1.90350600
H	3.70127200	-0.62699400	-3.30308900
H	5.43299800	0.31599900	-1.96004900
H	2.26332500	0.29446800	-1.61746300
N	1.64795500	-1.67506300	-1.29309400
O	3.77575100	-2.49990300	-2.61167400
C	0.35671500	-1.57261800	-0.86662100
C	2.03534300	-2.97903400	-1.10885000
N	0.04649000	-2.82170900	-0.43882700
N	1.09135300	-3.70205400	-0.59879300
C	3.42832900	-3.33836800	-1.52617100
H	4.12094900	-3.23167600	-0.68116300
H	3.45936000	-4.36918000	-1.88058400
C	-1.18803100	-3.26711300	0.13077300

C	-2.15784000	-3.80256100	-0.72042100
C	-1.39360300	-3.06995000	1.49870400
C	-3.38543500	-4.14286800	-0.15795000
C	-2.63837900	-3.42857000	2.01555200
C	-3.64525100	-3.95196900	1.20169400
H	-4.16274400	-4.55226400	-0.79815800
H	-2.83105600	-3.27804600	3.07490300
C	-0.34766100	-2.40108200	2.35087100
H	-0.33991400	-1.31610800	2.17010700
H	0.65409900	-2.78259400	2.13212600
H	-0.55685400	-2.56152900	3.40983100
C	-5.00626300	-4.26300800	1.76580300
H	-4.96615100	-4.40158200	2.84809200
H	-5.42621500	-5.16458400	1.31359800
H	-5.69477700	-3.43707000	1.55702300
C	-1.88369600	-3.94627200	-2.19256900
H	-0.97127300	-4.52224900	-2.37066700
H	-1.74591300	-2.96108400	-2.65180500
H	-2.71508100	-4.44337800	-2.69389800
C	-0.48576400	-0.43202200	-1.01649500
O	-0.01532100	0.48710000	-1.94247700
C	-1.75136000	-0.34551800	-0.47830500
C	-2.68983800	0.66021300	-0.77310500
H	-2.03260600	-1.09127300	0.25379400
H	-2.54210900	1.19549800	-1.70917900
C	-4.08923400	0.47992000	-0.35642100
C	-5.13039200	0.99436300	-1.14308400
C	-4.42893800	-0.14300700	0.85659300
C	-6.45818900	0.87369100	-0.74836300
H	-4.88452300	1.50728700	-2.06991500

C	-5.75780700	-0.26474700	1.25048700
H	-3.64703700	-0.52582500	1.50899600
C	-6.78198700	0.23940400	0.44981300
H	-7.24341100	1.28185800	-1.37768000
H	-5.99261300	-0.74612700	2.19563500
H	-7.81749800	0.14688700	0.76075400
H	-0.13868000	1.35781800	-1.53339600
C	3.89990000	2.50846000	1.26437200
C	3.75492500	2.76020800	-0.12631300
C	4.90530900	3.01044500	-0.89557900
C	6.14176800	2.99989800	-0.27396100
C	6.25966300	2.76070900	1.11171700
C	5.14711400	2.51914900	1.89797600
C	1.72279800	2.33393000	0.75779100
C	2.35686500	2.66158200	-0.42003400
H	4.82119600	3.20537200	-1.96109400
H	7.03825400	3.18899800	-0.85614900
H	7.24445600	2.76363700	1.56836400
H	5.23590300	2.32146000	2.96148400
H	1.88825100	2.79381900	-1.38593800
N	2.64824400	2.27555200	1.76870000
H	2.41203200	1.92417100	2.68532500
C	0.30694800	1.98459800	1.06768800
O	0.09187200	1.24516100	2.05588800
C	-0.67181600	2.57592500	0.22674500
C	-2.04102100	2.33323400	0.40982700
H	-0.34158300	3.31665100	-0.49622300
H	-2.30667400	1.82389700	1.33547900
C	-3.05308000	3.28975200	-0.09273100
C	-4.20963700	3.54119300	0.65256700

C	-2.89325400	3.94441300	-1.32208000
C	-5.17129400	4.43864400	0.19483900
H	-4.35709400	3.01866500	1.59410200
C	-3.85545200	4.83387100	-1.78412100
H	-2.01472000	3.74062500	-1.92909300
C	-4.99758000	5.08851500	-1.02401300
H	-6.06135600	4.62314100	0.78825700
H	-3.71719000	5.32795100	-2.74073300
H	-5.74841300	5.78392100	-1.38527200

TS3SS-270

C	-6.79121600	0.19834300	-0.28360600
C	-5.41522700	0.40240100	-0.25351900
C	-4.73343200	0.94807200	-1.33482900
C	-5.46216400	1.29647100	-2.46889500
C	-6.84586600	1.10073500	-2.50698900
C	-7.51953000	0.55335000	-1.41695300
C	-7.27959900	-0.41670400	1.00281700
C	-6.00085400	-0.82389900	1.77523400
C	-4.81990300	-0.07330700	1.05127300
H	-3.65863600	1.10185600	-1.29074700
H	-4.95375200	1.71916300	-3.33019300
H	-7.40121900	1.37313100	-3.39864500
H	-8.59323800	0.39660000	-1.45538400
H	-7.91604800	-1.29353000	0.84766900
H	-6.04518500	-0.51445400	2.81917300
H	-7.86062400	0.30408700	1.58654000
H	-4.44982300	0.74747500	1.66228700
N	-3.69673100	-0.98530000	0.79731200
O	-5.83053800	-2.23131300	1.83582300

C	-2.35923800	-0.77071700	0.67248600
C	-3.92958000	-2.30190000	0.49688000
N	-1.85884900	-1.97521500	0.31322000
N	-2.83547700	-2.93352700	0.21372900
C	-5.32619000	-2.80743100	0.64652700
H	-5.93449900	-2.54288100	-0.22928200
H	-5.32306500	-3.89048400	0.76534200
C	-0.52623100	-2.29932800	-0.10950500
C	0.35462800	-2.86654200	0.81653000
C	-0.18275000	-2.04085300	-1.43694800
C	1.63887200	-3.16767300	0.37260800
C	1.12064700	-2.35041100	-1.83172500
C	2.03787900	-2.91778500	-0.94503700
H	2.34710900	-3.60748800	1.07061200
H	1.41624000	-2.16408600	-2.86140200
C	-1.20442100	-1.49473100	-2.39889700
H	-1.67348200	-0.58507600	-2.00895500
H	-2.00036300	-2.22733000	-2.56687500
H	-0.74457400	-1.25793400	-3.36021200
C	3.42752700	-3.29048600	-1.38945900
H	3.59577200	-4.36366500	-1.25961600
H	4.18204800	-2.76051900	-0.80061100
H	3.58571800	-3.04499100	-2.44219400
C	-0.07528400	-3.10202700	2.23931200
H	-0.98356200	-3.70977200	2.28048200
H	-0.29249800	-2.15267400	2.74324100
H	0.71125800	-3.60945300	2.79910600
C	-1.66100200	0.46043800	0.91789300
O	-2.48224000	1.56727200	0.98176700
C	-0.33083600	0.49207400	1.23152600

C	0.43932600	1.62600900	1.62003900
H	0.19808300	-0.45040600	1.16767600
H	-0.14317600	2.47847800	1.97284200
C	1.66601200	1.34356400	2.39284500
C	2.06853300	2.18959900	3.43546600
C	2.49842700	0.26382400	2.05818500
C	3.25470200	1.96399200	4.12343100
H	1.43860300	3.03402800	3.70508800
C	3.69103600	0.04311100	2.74169200
H	2.23494000	-0.39562900	1.23527500
C	4.07632400	0.89011500	3.77655900
H	3.54315100	2.62956800	4.93157200
H	4.32443100	-0.79121000	2.45294900
H	5.00586800	0.71711800	4.30967000
H	-2.08611000	2.27991600	0.45535100
C	6.72215000	0.22716900	-0.64306800
C	5.95971600	-0.60245900	-1.51192200
C	6.60236200	-1.67336800	-2.16039400
C	7.95007500	-1.88911800	-1.93125300
C	8.68440400	-1.05478300	-1.06245100
C	8.08546100	0.00985000	-0.41031300
C	4.61336200	0.99608900	-0.66031300
C	4.62045300	-0.09242100	-1.50258000
H	6.04534500	-2.31949700	-2.83323000
H	8.45494000	-2.71238600	-2.42666600
H	9.74009100	-1.25049000	-0.90338700
H	8.64949800	0.65443600	0.25627300
H	3.77307100	-0.48068200	-2.05059700
N	5.87444800	1.18194000	-0.15280900
H	6.06074600	1.93471000	0.49504500

C	3.56390800	1.95048500	-0.19450700
O	3.95624400	2.89733800	0.52595600
C	2.23602800	1.70477900	-0.60805000
C	1.18932700	2.47353300	-0.06016500
H	2.03532800	0.84606600	-1.24172700
H	1.55998000	3.33262000	0.50046600
C	-0.05440500	2.76697200	-0.81661600
C	-0.80045600	3.91585800	-0.50648800
C	-0.51170800	1.94085300	-1.85135100
C	-1.96241100	4.23101400	-1.20826100
H	-0.45458100	4.56973100	0.29041800
C	-1.66815700	2.25882100	-2.56030900
H	0.05688200	1.05413400	-2.11629600
C	-2.39997900	3.40254700	-2.24108700
H	-2.51990500	5.12673100	-0.95461700
H	-1.99925400	1.60943700	-3.36689600
H	-3.30127800	3.64895800	-2.79297500

M3RR

C	-2.58822900	3.32417700	1.70333000
C	-2.25562500	2.27328500	0.84286800
C	-2.39927500	0.94789700	1.24100700
C	-2.84981900	0.68150700	2.53204000
C	-3.16750300	1.72905800	3.39844500
C	-3.04808400	3.05692600	2.98793700
C	-2.39510700	4.65945000	1.03107000
C	-2.36875400	4.26556200	-0.46129200
C	-1.80876100	2.81917400	-0.49506200
H	-2.17934200	0.13508200	0.56032700
H	-2.94341900	-0.35521600	2.83985700

H	-3.52329100	1.50926400	4.40026800
H	-3.31671500	3.86871900	3.65705000
H	-1.45021100	5.11369600	1.35083300
H	-3.39515100	4.21103100	-0.83003000
H	-3.19010800	5.37663500	1.24493900
H	-2.14313800	2.23672000	-1.35391900
N	-0.32806500	2.92618500	-0.60521100
O	-1.70459100	5.14883800	-1.34099700
C	0.58894800	1.94782400	-0.49106600
C	0.36210100	4.08982800	-0.82081700
N	1.77470200	2.54233800	-0.62767300
N	1.64860600	3.88336600	-0.83411600
C	-0.35334700	5.39037200	-1.02318800
H	-0.24287500	6.01968700	-0.13203300
H	0.09167300	5.91670900	-1.86890000
C	3.05642500	1.88924400	-0.69433800
C	3.92071100	1.99445200	0.39377300
C	3.34638700	1.15478600	-1.84851500
C	5.12664400	1.29562400	0.31422800
C	4.55283000	0.46120200	-1.86949800
C	5.44680700	0.51216300	-0.79500100
H	5.81721900	1.34635000	1.15193100
H	4.79828700	-0.13887200	-2.74220700
C	2.38968200	1.13247800	-3.01058700
H	2.10183700	2.14925800	-3.29632700
H	1.47324000	0.58461500	-2.76522600
H	2.85192500	0.65195000	-3.87365900
C	6.71845400	-0.29419500	-0.83898900
H	7.30378100	-0.05634400	-1.73150800
H	6.48609600	-1.36365200	-0.87566500

H	7.33906900	-0.10719400	0.03976900
C	3.55159800	2.81048800	1.60381000
H	2.59415900	2.48496300	2.02551300
H	3.44874300	3.86864600	1.34648600
H	4.31380200	2.71307200	2.37761700
C	0.31543400	0.51272000	-0.32251500
O	-0.62622400	0.09289100	-1.17828400
C	0.98465500	-0.13232000	0.64804900
C	0.86649500	-1.53081000	1.19382800
H	1.68545700	0.49286700	1.19568000
H	0.04819300	-1.51375000	1.92659700
C	2.14624900	-1.90473800	1.91629100
C	2.10268100	-2.69121800	3.06928200
C	3.39240800	-1.51736000	1.41472400
C	3.27717700	-3.07559500	3.71322800
H	1.13704600	-3.00233500	3.46176100
C	4.56781700	-1.88941800	2.06018000
H	3.43823800	-0.93181400	0.49778000
C	4.51361000	-2.67107300	3.21309500
H	3.22746100	-3.68442500	4.61075100
H	5.52596600	-1.57003800	1.65829100
H	5.42819600	-2.96363900	3.71930900
H	-0.88353100	-0.91913900	-0.88165000
C	-5.64304200	-2.16403000	-0.04151000
C	-5.27895700	-2.13487200	-1.41569600
C	-6.29366600	-2.02815400	-2.38405900
C	-7.61212000	-1.95714700	-1.97179100
C	-7.95017200	-1.98955200	-0.60187500
C	-6.97737900	-2.09234800	0.37760400
C	-3.40648200	-2.31097700	-0.17000200

C	-3.85076700	-2.22739900	-1.46881800
H	-6.04154900	-2.00351000	-3.44027400
H	-8.40335100	-1.87462900	-2.71018200
H	-8.99432700	-1.93274600	-0.31087000
H	-7.23531800	-2.11696000	1.43158000
H	-3.23198000	-2.22129000	-2.35469200
N	-4.48526800	-2.26771200	0.68003000
H	-4.36297400	-2.31615100	1.68144100
C	-2.05213200	-2.40527800	0.46075200
O	-2.02983300	-2.37037100	1.71876900
C	-0.93338300	-2.42743300	-0.39690100
C	0.44137200	-2.66973400	0.19395600
H	-1.10734900	-2.82727000	-1.39539600
H	0.41252800	-3.56180900	0.83910700
C	1.51801000	-2.90314200	-0.84768800
C	2.54949700	-3.81624000	-0.60120400
C	1.54961600	-2.18128300	-2.04465400
C	3.59026300	-3.99077600	-1.50936000
H	2.54175800	-4.38354800	0.32662300
C	2.58552300	-2.35706100	-2.96019200
H	0.74796400	-1.48285300	-2.26652900
C	3.61464300	-3.25673800	-2.69367200
H	4.38117200	-4.70274900	-1.29341800
H	2.58389700	-1.79252600	-3.88835600
H	4.42169600	-3.39286900	-3.40703300

M3RS

C	4.69606800	-0.78639500	2.23985500
C	3.31788300	-0.69250400	2.06130100
C	2.43278400	-0.99463400	3.09323900

C	2.95475400	-1.39717100	4.31953800
C	4.33669100	-1.49005900	4.50573200
C	5.21524100	-1.18319300	3.47008200
C	5.44285300	-0.41098700	0.98806300
C	4.36385200	-0.25029700	-0.10771500
C	2.97891000	-0.25943400	0.65100300
H	1.36063500	-0.90540700	2.94658500
H	2.28400800	-1.63905100	5.13735300
H	4.72803100	-1.80781400	5.46688900
H	6.28857500	-1.25936700	3.61604700
H	6.18083400	-1.16125000	0.68565400
H	4.47913900	0.69460000	-0.63401200
H	5.97985000	0.53438900	1.11714800
H	2.50923100	0.72403600	0.60266300
N	2.04639700	-1.22416400	0.03107100
O	4.46657100	-1.23388200	-1.12564400
C	0.69636500	-1.29866700	0.00552100
C	2.51932100	-2.36690300	-0.55640100
N	0.42353100	-2.46813900	-0.59075900
N	1.55271000	-3.13628100	-0.95793500
C	3.99421100	-2.50605800	-0.73620800
H	4.46815700	-2.85796800	0.19105000
H	4.20701100	-3.21552700	-1.53564300
C	-0.86934800	-3.04225400	-0.84469700
C	-1.50245600	-3.71813700	0.20040000
C	-1.45292300	-2.81701400	-2.09267000
C	-2.79639200	-4.17455600	-0.03484300
C	-2.74990800	-3.29646000	-2.27690200
C	-3.43704200	-3.96178400	-1.25891600
H	-3.32236000	-4.69746500	0.75985300

H	-3.24007800	-3.12833000	-3.23235900
C	-0.73465700	-2.00895600	-3.13944200
H	0.25284300	-2.42960000	-3.35193300
H	-0.59576700	-0.97260600	-2.79860100
H	-1.30942700	-1.99136000	-4.06663000
C	-4.86006200	-4.41334800	-1.45349900
H	-5.01202500	-5.41988900	-1.05589200
H	-5.13880000	-4.40911700	-2.50905000
H	-5.54101200	-3.74104100	-0.92043700
C	-0.82433300	-3.89118500	1.53266200
H	-0.74638100	-2.92867200	2.05136400
H	0.18775000	-4.28927100	1.41677000
H	-1.39413600	-4.57018300	2.16812100
C	-0.25066300	-0.32003000	0.54100000
O	0.32011800	0.59139200	1.38042400
C	-1.53669900	-0.27422900	0.16041200
C	-2.51451800	0.75323200	0.64918800
H	-1.89531100	-0.97741400	-0.57679700
H	-2.26587400	1.00587300	1.68863200
C	-3.92435900	0.20166100	0.58541300
C	-4.75633200	0.21348000	1.70538900
C	-4.42649500	-0.30602100	-0.61869700
C	-6.05715000	-0.28167700	1.63219800
H	-4.38057900	0.61683600	2.64228200
C	-5.72494100	-0.80028600	-0.69624800
H	-3.79622100	-0.31399300	-1.50611400
C	-6.54470100	-0.79312400	0.43218900
H	-6.68919600	-0.26811200	2.51461600
H	-6.09849300	-1.18856900	-1.63928100
H	-7.55712600	-1.17978100	0.37344100

H	0.01381900	1.46799600	1.00237000
C	3.34440300	2.26410000	-2.20802100
C	3.44876500	3.02562800	-1.00960800
C	4.72441700	3.43171000	-0.57658000
C	5.83450700	3.07551400	-1.32475400
C	5.70482300	2.32717500	-2.51411600
C	4.46370000	1.91716200	-2.97382500
C	1.28605500	2.45872000	-1.32878200
C	2.12469300	3.13906600	-0.47274200
H	4.83492500	4.00573900	0.33887600
H	6.82353600	3.37763300	-0.99522700
H	6.59451800	2.06571100	-3.07773200
H	4.36161900	1.33098900	-3.88142500
H	1.83660300	3.63850100	0.44158300
N	2.02391900	1.94417000	-2.36427000
H	1.57519200	1.37208500	-3.06685800
C	-0.16463400	2.08240100	-1.30991700
O	-0.52356400	1.26967900	-2.22164200
C	-0.94908200	2.55696300	-0.26947400
C	-2.38004100	2.09030500	-0.18681100
H	-0.61779800	3.40976000	0.31701100
H	-2.70266500	1.83434900	-1.20449600
C	-3.33529200	3.11681200	0.38089500
C	-4.51555700	3.43960000	-0.29266200
C	-3.08099800	3.73537600	1.60995000
C	-5.41400000	4.36394500	0.23645500
H	-4.73110300	2.95448900	-1.24127100
C	-3.97572500	4.65890000	2.14401700
H	-2.17015900	3.49221300	2.15279800
C	-5.14617500	4.97802300	1.45693700

H	-6.32383300	4.60318500	-0.30551400
H	-3.75982500	5.13156700	3.09744900
H	-5.84388300	5.69878800	1.87142300

M3SR

C	4.27579500	-1.51407100	-1.03706900
C	3.12342100	-0.96652300	-1.61563000
C	3.03137400	0.40886200	-1.81321300
C	4.05862700	1.22490000	-1.34754600
C	5.15847900	0.68447900	-0.68232200
C	5.28467700	-0.69606900	-0.54270800
C	4.27968400	-3.01187900	-1.17022300
C	3.30526600	-3.19035500	-2.35408800
C	2.23829600	-2.07601900	-2.15581000
H	2.19487900	0.83952400	-2.34608300
H	3.99402000	2.29720100	-1.48956800
H	5.92537300	1.34756900	-0.29070400
H	6.16930800	-1.12897300	-0.08532000
H	3.91302300	-3.49140000	-0.25558800
H	3.83136300	-2.94464200	-3.27915900
H	5.26619600	-3.42607300	-1.38837200
H	1.70654100	-1.81437500	-3.06965700
N	1.20939100	-2.63614200	-1.20472200
O	2.77488000	-4.47897500	-2.54471400
C	0.11561100	-2.08382600	-0.60953400
C	1.21587200	-3.96190700	-0.82769600
N	-0.41574700	-3.06198900	0.13678900
N	0.25380800	-4.23356800	-0.00027800
C	2.15996600	-4.98291100	-1.38614700
H	2.89143400	-5.28413100	-0.62723000

H	1.58242800	-5.86326600	-1.67224900
C	-1.57030000	-3.01396600	0.99113600
C	-2.80051800	-3.38526100	0.44610100
C	-1.40766200	-2.52693800	2.28956400
C	-3.92263000	-3.23634600	1.25745100
C	-2.56232500	-2.39989500	3.06047000
C	-3.82170900	-2.73921600	2.55899500
H	-4.89954100	-3.49413300	0.85702600
H	-2.47654400	-2.00997100	4.07154700
C	-0.06053100	-2.07839100	2.78562000
H	0.19106400	-1.10265600	2.34685500
H	0.71957500	-2.79806300	2.52051500
H	-0.07468700	-1.96813500	3.87130200
C	-5.05049000	-2.57665200	3.41415100
H	-4.99332100	-1.66315900	4.01149800
H	-5.15208600	-3.41755300	4.10769000
H	-5.95364700	-2.53588800	2.80151400
C	-2.90347200	-3.84347900	-0.98311000
H	-2.21764000	-4.67031100	-1.18726800
H	-2.64833200	-3.02273100	-1.66365500
H	-3.91940000	-4.16835400	-1.21045700
C	-0.47251400	-0.77031000	-0.87438800
O	0.20423300	-0.03860100	-1.79453300
C	-1.61706500	-0.33497900	-0.31977800
C	-2.30569800	0.91040000	-0.79761700
H	-2.08895800	-0.88655500	0.47761400
H	-2.10790100	1.00942700	-1.87375800
C	-3.80129100	0.79902400	-0.57703500
C	-4.69600100	1.06658900	-1.61426200
C	-4.31504100	0.47217500	0.68298700

C	-6.07187000	1.00076000	-1.40541400
H	-4.30737800	1.33838600	-2.59258500
C	-5.68916700	0.40237900	0.89527000
H	-3.63575100	0.27061600	1.50960300
C	-6.57286300	0.66498700	-0.15015900
H	-6.75251600	1.21163300	-2.22447100
H	-6.06954400	0.14567500	1.87958300
H	-7.64434300	0.61050600	0.01400200
H	0.22811200	0.88657300	-1.37737600
C	3.97753000	2.09258400	1.97531100
C	3.95606600	3.27205200	1.18110600
C	5.13735200	4.02459000	1.06027100
C	6.27774900	3.60338600	1.72456900
C	6.26962700	2.43777800	2.51956300
C	5.12488900	1.67003500	2.65555600
C	1.92857400	2.28539800	1.07436600
C	2.63757600	3.37684100	0.62994900
H	5.15368300	4.92373900	0.45073300
H	7.19464300	4.17805000	1.63774000
H	7.17813600	2.13676500	3.03178500
H	5.11816300	0.76575400	3.25607000
H	2.26352800	4.15788800	-0.01644400
N	2.73654200	1.52456200	1.88371100
H	2.36656900	0.72768800	2.38178000
C	0.51362600	1.82379300	0.90843100
O	0.09184500	1.02195200	1.79517800
C	-0.21143900	2.30051300	-0.18300900
C	-1.72388500	2.20259100	-0.11827500
H	0.22213800	3.11130200	-0.76285600
H	-2.00993300	2.12867600	0.94091800

C	-2.41004500	3.40701800	-0.72837900
C	-3.41270200	4.09579000	-0.04231000
C	-2.08491800	3.82463700	-2.02404400
C	-4.06629200	5.17908800	-0.62716300
H	-3.68763000	3.77254900	0.95853600
C	-2.73547600	4.90420000	-2.61379700
H	-1.30904100	3.29615300	-2.57368600
C	-3.72955600	5.58784100	-1.91487000
H	-4.84165000	5.70261400	-0.07603700
H	-2.46621500	5.21373000	-3.61915000
H	-4.23733400	6.43114200	-2.37219400

M3SS

C	-3.19694800	3.48725200	0.97979600
C	-2.32365800	2.46922400	0.60824100
C	-1.99479900	1.44000100	1.48658300
C	-2.54330500	1.45324000	2.76552500
C	-3.41177000	2.47970000	3.14923300
C	-3.74844500	3.49672500	2.25987200
C	-3.43545700	4.45690700	-0.14646300
C	-2.52746900	3.97664400	-1.30617900
C	-1.83270600	2.65025700	-0.80835900
H	-1.34750300	0.62809800	1.16958600
H	-2.29977800	0.65808600	3.46371300
H	-3.83304600	2.47925900	4.14934500
H	-4.43101000	4.28621500	2.55945100
H	-3.19481700	5.49039400	0.12431900
H	-3.11694000	3.73815700	-2.19065700
H	-4.48346100	4.45140300	-0.45824900
H	-2.08204000	1.80719000	-1.44685000

N	-0.35590100	2.78425900	-0.84113200
O	-1.62349500	4.97429200	-1.74803500
C	0.62569400	1.85300500	-0.80836800
C	0.25478900	4.00694900	-0.76536900
N	1.76788100	2.55149000	-0.73606100
N	1.54759800	3.89487800	-0.70790800
C	-0.58838400	5.23578800	-0.82614700
H	-0.97582100	5.48217100	0.17214000
H	0.00008600	6.07589500	-1.19420600
C	3.11880000	2.06221300	-0.65963000
C	3.68677900	1.92533400	0.60896000
C	3.76581900	1.70516000	-1.84292900
C	4.97462800	1.39576700	0.67200200
C	5.04998300	1.17676100	-1.72474700
C	5.66523800	1.01362700	-0.48136100
H	5.44168900	1.26498300	1.64459800
H	5.57806900	0.87581200	-2.62568500
C	3.07689300	1.83456800	-3.17388400
H	2.62499600	2.82303500	-3.29481700
H	2.27962300	1.08845900	-3.26607300
H	3.78444900	1.67401400	-3.98806100
C	7.05596500	0.44326100	-0.38931300
H	7.80421900	1.22919700	-0.53287300
H	7.21949300	-0.31403100	-1.15953800
H	7.23169500	-0.00990700	0.58873900
C	2.90337800	2.28223500	1.84334200
H	1.97882600	1.69476200	1.89471400
H	2.62634600	3.34046900	1.84451300
H	3.48400900	2.07004300	2.74189400
C	0.44275300	0.39520000	-0.84732100

O	-0.81596400	0.03077600	-1.16484500
C	1.43316200	-0.46567100	-0.54762000
C	1.27551600	-1.95617400	-0.63612000
H	2.38619300	-0.07016600	-0.23135500
H	0.61509800	-2.18516000	-1.48187900
C	2.59220900	-2.67209700	-0.85770700
C	2.58251400	-3.86438300	-1.58947800
C	3.80244100	-2.23960200	-0.30711400
C	3.74963600	-4.59761500	-1.78137600
H	1.63881000	-4.21576400	-2.00068500
C	4.97418200	-2.96810300	-0.50192800
H	3.84347500	-1.33814800	0.29929900
C	4.95355500	-4.14758700	-1.24179800
H	3.72062300	-5.51816400	-2.35602900
H	5.90396000	-2.61428600	-0.06612300
H	5.86715100	-4.71336300	-1.39452100
H	-1.01921900	-0.81015700	-0.58423800
C	-5.34582800	-2.92563100	-1.02187000
C	-5.38829300	-1.87501500	-0.06390500
C	-6.63107900	-1.29569600	0.24890400
C	-7.77086900	-1.76508600	-0.38033000
C	-7.70434000	-2.81038100	-1.32545500
C	-6.49784600	-3.40280200	-1.65802900
C	-3.24951200	-2.54881500	-0.31269400
C	-4.04062600	-1.65428400	0.37036400
H	-6.69227500	-0.49104500	0.97616800
H	-8.73505500	-1.32489100	-0.14586900
H	-8.61691400	-3.15663600	-1.80039000
H	-6.44282300	-4.20722400	-2.38466100
H	-3.69950200	-0.91771800	1.08475300

N	-4.03678400	-3.30480500	-1.14508400
H	-3.62529900	-4.00083300	-1.75083700
C	-1.77877900	-2.83092800	-0.34233400
O	-1.38500900	-3.64459700	-1.22349500
C	-0.95716300	-2.12870900	0.54855900
C	0.49677500	-2.54686000	0.60485600
H	-1.41703000	-1.69334500	1.43255900
H	0.55072100	-3.63509400	0.45281400
C	1.21171200	-2.21676500	1.89575100
C	2.15191500	-3.10854500	2.42339100
C	1.00473100	-1.00755800	2.56946700
C	2.86415300	-2.80523400	3.58133600
H	2.32924000	-4.05049200	1.91015200
C	1.71326600	-0.69819200	3.72862100
H	0.27940500	-0.29760500	2.18215800
C	2.64807700	-1.59642400	4.23900000
H	3.58635600	-3.51580000	3.97151100
H	1.53143600	0.24591100	4.23432800
H	3.19902900	-1.35820000	5.14326600

TS4RR

C	-2.58457000	3.32946300	1.70068600
C	-2.25103000	2.28034300	0.83858100
C	-2.40083900	0.95406200	1.23106000
C	-2.85884400	0.68457800	2.51881900
C	-3.17739600	1.73023200	3.38726900
C	-3.05165000	3.05915400	2.98208800
C	-2.38395100	4.66605300	1.03306500
C	-2.35321300	4.27596000	-0.46033100
C	-1.79614900	2.82860100	-0.49558300

H	-2.17944100	0.14491400	0.54645000
H	-2.95814600	-0.35247300	2.82391000
H	-3.53898300	1.50809900	4.38649700
H	-3.32111900	3.86932300	3.65283200
H	-1.43845900	5.11566300	1.35764700
H	-3.37854200	4.22455300	-0.83252500
H	-3.17699600	5.38570300	1.24591800
H	-2.12742700	2.24856700	-1.35726300
N	-0.31514900	2.93258800	-0.59841600
O	-1.68432000	5.16014600	-1.33551800
C	0.59868100	1.95128100	-0.48311900
C	0.37840200	4.09466400	-0.81152100
N	1.78621600	2.54305100	-0.61710600
N	1.66429600	3.88493000	-0.82282700
C	-0.33334500	5.39738200	-1.01307600
H	-0.22420200	6.02433800	-0.12007600
H	0.11550300	5.92471200	-1.85612800
C	3.06595700	1.88644000	-0.68456000
C	3.93020500	1.98633300	0.40398900
C	3.35421700	1.15398300	-1.84046000
C	5.13414000	1.28412900	0.32318000
C	4.55845900	0.45664300	-1.86269800
C	5.45225700	0.50234600	-0.78779300
H	5.82452800	1.33069900	1.16129700
H	4.80238000	-0.14217500	-2.73672000
C	2.39809700	1.13857400	-3.00316400
H	2.11969900	2.15780100	-3.28976300
H	1.47634200	0.59960100	-2.75804900
H	2.85681800	0.65345500	-3.86553900
C	6.72149800	-0.30776600	-0.83343000

H	6.48586600	-1.37615300	-0.87877400
H	7.33985000	-0.12919800	0.04867500
H	7.31060000	-0.06519200	-1.72222600
C	3.56273400	2.79995200	1.61613500
H	3.45700400	3.85825700	1.36066200
H	4.32711600	2.70291600	2.38786100
H	2.60701600	2.47177900	2.03970600
C	0.31931400	0.51541800	-0.31993500
O	-0.61759500	0.09860200	-1.17706500
C	0.98619800	-0.13057600	0.65287300
C	0.86354100	-1.53103200	1.19331200
H	1.68662500	0.49186000	1.20402700
H	0.04820800	-1.51468200	1.92919300
C	2.14281700	-1.91551700	1.91132800
C	2.09727600	-2.71277900	3.05684100
C	3.39004200	-1.52822300	1.41247100
C	3.27069500	-3.10825300	3.69595700
H	1.13074500	-3.02381400	3.44724100
C	4.56450700	-1.91124700	2.05330000
H	3.43720000	-0.93414300	0.50118700
C	4.50831900	-2.70403300	3.19847700
H	3.21932900	-3.72545900	4.58766200
H	5.52355900	-1.59182800	1.65359500
H	5.42224600	-3.00527500	3.70082300
H	-0.88008200	-0.93955500	-0.87330000
C	-5.65366400	-2.16314100	-0.04041100
C	-5.28860600	-2.12051600	-1.41384300
C	-6.30255300	-2.00802400	-2.38250600
C	-7.62134700	-1.94414800	-1.97087700
C	-7.96047800	-1.98941500	-0.60141400

C	-6.98874600	-2.09853600	0.37814300
C	-3.41712500	-2.30290200	-0.16838400
C	-3.86025500	-2.20857900	-1.46667600
H	-6.04928100	-1.97336100	-3.43812600
H	-8.41217200	-1.85720500	-2.70913800
H	-9.00506000	-1.93769600	-0.31101300
H	-7.24769400	-2.13307100	1.43156000
H	-3.24033600	-2.19301900	-2.35161400
N	-4.49665400	-2.27043700	0.68157300
H	-4.37757800	-2.32860000	1.68279200
C	-2.06204000	-2.39841700	0.45814600
O	-2.03452300	-2.37996900	1.71317700
C	-0.94059600	-2.39969100	-0.40631900
C	0.43135300	-2.66125800	0.18785000
H	-1.11832700	-2.82301600	-1.39526600
H	0.39165200	-3.55732400	0.82656600
C	1.50728400	-2.89822200	-0.85382000
C	2.53315000	-3.81820800	-0.60899900
C	1.54377500	-2.17368100	-2.04904400
C	3.57343300	-3.99672000	-1.51691000
H	2.52168400	-4.38758000	0.31755700
C	2.57925900	-2.35360000	-2.96430400
H	0.74683300	-1.46926900	-2.26899300
C	3.60287400	-3.25999200	-2.69945900
H	4.35998700	-4.71389000	-1.30221500
H	2.58156800	-1.78689900	-3.89114900
H	4.40951700	-3.39919700	-3.41270200

TS4RS

C	4.75725200	-1.01438600	0.99479200
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S124

C	3.38192200	-0.94017300	1.20205800
C	2.83608400	-0.91816900	2.48197900
C	3.70476900	-0.97722000	3.56933600
C	5.08635000	-1.04717800	3.37084700
C	5.62239100	-1.06267200	2.08483200
C	5.09259700	-0.99493800	-0.47273100
C	3.74412100	-1.17124900	-1.20331200
C	2.64742300	-0.86410100	-0.11756500
H	1.76132300	-0.84005200	2.61622300
H	3.30672500	-0.96394400	4.57873500
H	5.74910300	-1.08996300	4.22941300
H	6.69657200	-1.11607900	1.93437100
H	5.78653000	-1.78645200	-0.77265700
H	3.64032100	-0.47462900	-2.03641400
H	5.54430500	-0.03524700	-0.74633200
H	2.20241500	0.11947000	-0.27245900
N	1.56380000	-1.84925700	-0.20128700
O	3.61314900	-2.45714400	-1.80086500
C	0.23695500	-1.72181000	-0.03006100
C	1.80785200	-3.15343800	-0.52614300
N	-0.26343900	-2.94405400	-0.23964000
N	0.70680500	-3.84777800	-0.56544100
C	3.20750600	-3.49122700	-0.92271200
H	3.85840600	-3.56445400	-0.04146200
H	3.23179300	-4.43282100	-1.47016400
C	-1.64294900	-3.33235700	-0.12132600
C	-2.20312100	-3.38978800	1.15538300
C	-2.36535900	-3.56236400	-1.29479100
C	-3.56558300	-3.67429200	1.23617800
C	-3.72256000	-3.84281900	-1.15780800

C	-4.33965000	-3.88655200	0.09483300
H	-4.03343500	-3.72308600	2.21604800
H	-4.31526200	-4.01719300	-2.05224500
C	-1.70316100	-3.47269800	-2.64381700
H	-0.92692500	-4.23493500	-2.75381600
H	-1.22246600	-2.49795800	-2.78249100
H	-2.43785200	-3.60665200	-3.43853200
C	-5.82311800	-4.12107600	0.20483200
H	-6.36172900	-3.17456300	0.08966000
H	-6.08786400	-4.53917200	1.17822600
H	-6.17591100	-4.79984600	-0.57481000
C	-1.38128900	-3.11937200	2.38742300
H	-1.20778700	-2.04409000	2.51230100
H	-0.40464500	-3.60946400	2.33382400
H	-1.89978500	-3.47979700	3.27699400
C	-0.46776100	-0.49404100	0.36384200
O	0.23154700	0.27916900	1.20116200
C	-1.67701400	-0.19956000	-0.14433600
C	-2.45828700	1.01327400	0.30361100
H	-2.12403500	-0.87061400	-0.86957300
H	-2.31212300	1.10599600	1.39037000
C	-3.93704200	0.83111400	0.03082800
C	-4.87968600	1.03980600	1.03918700
C	-4.39049300	0.48381700	-1.24599400
C	-6.24171800	0.89437200	0.78539100
H	-4.53960500	1.32530500	2.03141400
C	-5.75040100	0.33602200	-1.50459300
H	-3.67203400	0.33017900	-2.04838500
C	-6.68154600	0.53834300	-0.48728900
H	-6.96010700	1.05809900	1.58269700

H	-6.08352100	0.06334700	-2.50124100
H	-7.74215300	0.42213200	-0.68662700
H	0.02948900	1.31551900	0.77756200
C	4.08895800	2.34343500	-1.51776300
C	4.06423600	2.51516200	-0.10644500
C	5.28478200	2.55674600	0.59284600
C	6.46850700	2.45344200	-0.11560800
C	6.46900900	2.30708100	-1.52102500
C	5.28701900	2.24584900	-2.23900400
C	1.94115500	2.45712800	-0.87034300
C	2.68563400	2.59135100	0.27870100
H	5.29219200	2.66590700	1.67336000
H	7.41609300	2.48624200	0.41247100
H	7.41572800	2.23298300	-2.04653400
H	5.28362800	2.12575200	-3.31758000
H	2.29328800	2.68169900	1.28172300
N	2.78838100	2.30378400	-1.94261600
H	2.42908000	2.13833400	-2.87243500
C	0.47562200	2.28383500	-1.13439700
O	0.17993500	1.83515800	-2.26226700
C	-0.40963200	2.50076900	-0.04389700
C	-1.90151700	2.34151100	-0.32129300
H	-0.11110600	3.29156900	0.64425500
H	-2.02897300	2.25103700	-1.40831600
C	-2.73631600	3.50711100	0.16597900
C	-3.66126500	4.12591900	-0.67729200
C	-2.64408500	3.95276700	1.48949200
C	-4.46715900	5.16673400	-0.22013600
H	-3.75416900	3.77946200	-1.70344400
C	-3.44866300	4.99013700	1.95302800

H	-1.93390400	3.48087400	2.16512200
C	-4.36363800	5.60271400	1.09812000
H	-5.17802000	5.63449900	-0.89461600
H	-3.36126600	5.32237400	2.98315700
H	-4.99101400	6.41215100	1.45781900

TS4SR

C	4.71381500	-1.80263700	-1.07743900
C	3.42255900	-1.38652800	-0.76311400
C	3.16258900	-0.56624800	0.33112900
C	4.24049400	-0.16380700	1.11678200
C	5.54240700	-0.55502300	0.79451900
C	5.78966500	-1.37741400	-0.30245500
C	4.71814900	-2.70453900	-2.28618200
C	3.23230800	-3.04860000	-2.54168900
C	2.42352300	-1.96943300	-1.73692300
H	2.14979300	-0.24949900	0.57407200
H	4.06782700	0.46438500	1.98268900
H	6.36870200	-0.21818800	1.41274900
H	6.80134500	-1.69103800	-0.54176900
H	5.29408100	-3.62351100	-2.14006300
H	2.97911800	-2.98929700	-3.60012200
H	5.14045200	-2.19206500	-3.15654300
H	1.99760400	-1.21601600	-2.39500300
N	1.31132800	-2.59448100	-1.00259800
O	2.91302700	-4.38684600	-2.18281600
C	0.12099000	-2.11521400	-0.58493800
C	1.47373700	-3.82968200	-0.43851500
N	-0.38179600	-3.07947100	0.20037300
N	0.45021000	-4.15801400	0.29103800

C	2.70270000	-4.59707800	-0.80077200
H	3.55746500	-4.26467700	-0.19615700
H	2.54307500	-5.66267200	-0.63816500
C	-1.58880100	-3.05090400	0.98169500
C	-2.71750200	-3.69680600	0.47361400
C	-1.57721600	-2.33485900	2.18053000
C	-3.89357700	-3.59650600	1.21406200
C	-2.77958800	-2.26871900	2.88427700
C	-3.94175900	-2.88506800	2.41533900
H	-4.79413000	-4.07504000	0.83844100
H	-2.80881000	-1.71245800	3.81790200
C	-0.34730600	-1.61038800	2.65411700
H	-0.25088200	-0.63831400	2.15168800
H	0.56115600	-2.18921700	2.46216500
H	-0.41088700	-1.42203100	3.72748600
C	-5.22188800	-2.79674800	3.20422900
H	-5.23069800	-3.54095400	4.00714900
H	-6.09059900	-2.98133400	2.56867800
H	-5.33070000	-1.81279300	3.66697100
C	-2.66136800	-4.41625100	-0.84681500
H	-1.89689900	-5.19835400	-0.83865100
H	-2.41096300	-3.71977600	-1.65479300
H	-3.62474200	-4.87272400	-1.07663200
C	-0.43371100	-0.79559000	-0.94150000
O	0.46200100	0.02146600	-1.49634700
C	-1.72486100	-0.49653000	-0.69940300
C	-2.37323600	0.81277400	-1.08108500
H	-2.35949200	-1.24155500	-0.24122000
H	-2.10642500	1.03894200	-2.12491000
C	-3.88142800	0.69443600	-0.97326900

C	-4.71481000	1.12676900	-2.00579000
C	-4.46831500	0.19879600	0.19619900
C	-6.10078900	1.06420400	-1.87810600
H	-4.27174000	1.52679800	-2.91418400
C	-5.85258900	0.13136200	0.32710100
H	-3.83634600	-0.13979000	1.01591400
C	-6.67465900	0.56474400	-0.71143700
H	-6.73286000	1.40448600	-2.69254500
H	-6.28824300	-0.25910200	1.24216100
H	-7.75424300	0.51333600	-0.61179100
H	0.20037600	1.05267900	-1.08260800
C	3.89530900	3.10288400	1.53671100
C	3.95690000	3.37553100	0.14357800
C	5.17047600	3.82894200	-0.40425800
C	6.26464800	3.99094900	0.42658400
C	6.17992200	3.71153500	1.80727400
C	5.00078700	3.26754900	2.38046100
C	1.88616600	2.63992400	0.65002000
C	2.66312000	3.07884100	-0.39519100
H	5.24476700	4.04501800	-1.46603200
H	7.20647000	4.33947000	0.01483700
H	7.05714500	3.84852900	2.43181500
H	4.93245600	3.05081000	3.44195900
H	2.35540900	3.15396600	-1.42820000
N	2.62955200	2.65901600	1.80624200
H	2.24338200	2.33809700	2.68279200
C	0.48443300	2.12934900	0.75808100
O	0.19728300	1.55085000	1.83187000
C	-0.34553300	2.24825700	-0.38581700
C	-1.84307800	2.01217400	-0.21708300

H	-0.06430300	3.04997000	-1.06766400
H	-2.01685000	1.74034800	0.83249200
C	-2.65505100	3.25405500	-0.53430600
C	-3.59003800	3.75721600	0.37250700
C	-2.52064400	3.89411700	-1.77160800
C	-4.36509200	4.87262200	0.05875600
H	-3.71638000	3.26275100	1.33233400
C	-3.29461900	5.00521700	-2.09233500
H	-1.80339600	3.51442200	-2.49588400
C	-4.22088300	5.50052000	-1.17537600
H	-5.08398300	5.24993600	0.77979900
H	-3.17459500	5.48592400	-3.05856800
H	-4.82415500	6.36827300	-1.42259800

TS4SS

C	-3.11877400	3.55904400	1.05321400
C	-2.26436200	2.52882100	0.67127400
C	-1.98328000	1.46703600	1.52722100
C	-2.55720700	1.46113600	2.79500400
C	-3.40558200	2.50017600	3.18979100
C	-3.69671400	3.54910600	2.32152500
C	-3.31003500	4.56440600	-0.05042600
C	-2.40375600	4.08249000	-1.21071000
C	-1.74244300	2.73209500	-0.73114300
H	-1.35392400	0.64729400	1.19688700
H	-2.34842600	0.64133400	3.47577800
H	-3.84772600	2.48417000	4.18078600
H	-4.36518400	4.34803400	2.62793600
H	-3.03727100	5.58154400	0.25061600
H	-2.99253200	3.87071700	-2.10273300

H	-4.35346900	4.60375300	-0.37486800
H	-1.99483400	1.90528200	-1.38986100
N	-0.26315600	2.83611900	-0.74431300
O	-1.47671200	5.06865500	-1.63088700
C	0.69644800	1.88141800	-0.74122700
C	0.37547600	4.04326600	-0.65981300
N	1.85513400	2.55416400	-0.67487700
N	1.66654900	3.90216000	-0.62516300
C	-0.44002600	5.29102600	-0.69991300
H	-0.82708500	5.52839600	0.30057100
H	0.16791100	6.12465600	-1.05057300
C	3.19424000	2.02863200	-0.68611600
C	3.83011600	1.82568900	0.53905400
C	3.75815500	1.68949100	-1.91804000
C	5.09497700	1.23809600	0.50733700
C	5.02009200	1.10296600	-1.89472000
C	5.69591600	0.86183100	-0.69504700
H	5.61160900	1.05448400	1.44571800
H	5.48309100	0.81440300	-2.83505200
C	2.99933200	1.89744200	-3.20019200
H	2.57974400	2.90579900	-3.25792200
H	2.16946800	1.18524900	-3.27115500
H	3.65107000	1.74255200	-4.06083100
C	7.04203800	0.18755500	-0.71427000
H	7.75254000	0.75235500	-1.32436800
H	6.95746900	-0.81305600	-1.14930400
H	7.45342000	0.08989600	0.29208900
C	3.13296100	2.15454400	1.83149500
H	2.25007200	1.51602100	1.95930300
H	2.79833600	3.19545000	1.85170400

H	3.79536800	1.98244100	2.68088600
C	0.46989500	0.42603700	-0.80062000
O	-0.78935100	0.09212800	-1.09297200
C	1.45486900	-0.45077400	-0.51551700
C	1.27657800	-1.94204800	-0.61762900
H	2.42484800	-0.07836700	-0.22526000
H	0.66859000	-2.15027500	-1.50815800
C	2.60190900	-2.66104400	-0.76808300
C	2.67945900	-3.77853300	-1.60405200
C	3.74507600	-2.28402100	-0.05447100
C	3.86738300	-4.49233900	-1.74013700
H	1.79127700	-4.08784700	-2.15013300
C	4.93609300	-2.99365100	-0.18936700
H	3.70978100	-1.43951000	0.62973000
C	5.00337000	-4.09784100	-1.03636200
H	3.90609200	-5.35460900	-2.39851100
H	5.81076400	-2.68611200	0.37659300
H	5.93231000	-4.64908900	-1.14265300
H	-1.00030400	-0.82958900	-0.47702000
C	-5.40540500	-2.89267600	-1.15080200
C	-5.44464000	-1.82822400	-0.20880500
C	-6.68368400	-1.23176700	0.08780000
C	-7.82302400	-1.69918200	-0.54218700
C	-7.75988000	-2.75922900	-1.47194900
C	-6.55819700	-3.36841800	-1.78813700
C	-3.31209700	-2.52530500	-0.43308400
C	-4.09844400	-1.61432600	0.23221900
H	-6.74106100	-0.41597700	0.80265000
H	-8.78459500	-1.24657100	-0.32155200
H	-8.67272200	-3.10313600	-1.94803300

H	-6.50649100	-4.18368100	-2.50267900
H	-3.75315500	-0.87023500	0.93687900
N	-4.10023000	-3.28687400	-1.26104500
H	-3.70006900	-3.99949400	-1.85443400
C	-1.84460600	-2.80984000	-0.43956100
O	-1.43778500	-3.63934800	-1.28247500
C	-1.02179300	-2.05484300	0.43878300
C	0.41887500	-2.53640800	0.56046400
H	-1.50830000	-1.70952500	1.35118900
H	0.43982300	-3.62261900	0.38888300
C	1.06306800	-2.26606100	1.90157500
C	1.88728400	-3.23070400	2.48989100
C	0.90028600	-1.04704200	2.57083500
C	2.53121500	-2.98968100	3.70166700
H	2.02930300	-4.18190100	1.98291400
C	1.54273000	-0.79859000	3.78196400
H	0.26462900	-0.28018500	2.13807700
C	2.36269800	-1.77000000	4.35254300
H	3.16432300	-3.75652800	4.13747500
H	1.39781400	0.15532400	4.28119100
H	2.86065600	-1.57984000	5.29804400

M4RR

C	3.27969700	3.93249000	0.42469400
C	2.16750300	3.18471200	0.82169100
C	2.26799500	2.19906000	1.80018300
C	3.51977200	1.95602700	2.36421900
C	4.63555000	2.69413100	1.96390100
C	4.52391600	3.69287300	0.99714800
C	2.90568600	4.94574200	-0.62701200

C	1.37325800	5.03214200	-0.46133800
C	0.93825300	3.64215300	0.07028100
H	1.38319200	1.64728000	2.10602600
H	3.62711300	1.18267000	3.11838100
H	5.60123400	2.49411000	2.41784200
H	5.39118300	4.27523400	0.70101100
H	3.18589000	4.57888500	-1.62146300
H	1.14397400	5.75651300	0.32316900
H	3.38398200	5.91792100	-0.49098900
H	0.02908300	3.65298800	0.67203600
N	0.64613600	2.79235000	-1.10814800
O	0.63929700	5.46440400	-1.58969100
C	0.37578200	1.47445500	-1.11599400
C	0.57409000	3.22824300	-2.40366700
N	0.16548200	1.16468100	-2.39315600
N	0.28152500	2.25264100	-3.21546100
C	0.80358300	4.66914600	-2.74278900
H	1.79581800	4.79479600	-3.19232000
H	0.05759500	4.99330600	-3.46991700
C	-0.32462500	-0.09021400	-2.89127400
C	0.52673300	-0.89624500	-3.64465000
C	-1.65248400	-0.42245300	-2.60257300
C	0.00841700	-2.10498700	-4.11077200
C	-2.11221600	-1.65339000	-3.06689600
C	-1.29508300	-2.50710700	-3.81436100
H	0.64496600	-2.75142500	-4.71019700
H	-3.13768200	-1.94589800	-2.85358600
C	-2.53707600	0.52671500	-1.83695100
H	-2.48944400	1.53059400	-2.27231000
H	-2.23491200	0.60887300	-0.78524900

H	-3.57525800	0.19185400	-1.86825300
C	-1.80336900	-3.85339200	-4.25799600
H	-1.68575100	-4.58395700	-3.44996400
H	-1.24863100	-4.22166200	-5.12378800
H	-2.86451900	-3.81262200	-4.51428500
C	1.94048700	-0.47061100	-3.93539200
H	2.48297800	-0.25363500	-3.00931600
H	1.95857500	0.43922900	-4.54225500
H	2.47511700	-1.25634800	-4.47047400
C	0.22460500	0.63424500	0.11558900
O	-0.57795900	1.13576600	0.97886900
C	1.02225000	-0.46798000	0.18513300
C	1.05711300	-1.25007500	1.46570800
H	1.63918300	-0.74405600	-0.66451200
H	0.64527600	-0.58488500	2.23364700
C	2.45319400	-1.63743800	1.91035900
C	2.79101400	-1.54040100	3.26371300
C	3.41875000	-2.11961500	1.02062200
C	4.06047900	-1.89316900	3.71781200
H	2.04440600	-1.17584400	3.96654800
C	4.68877800	-2.47392800	1.46824900
H	3.17124500	-2.23063400	-0.03209800
C	5.01703200	-2.35686400	2.81769000
H	4.30211400	-1.80216700	4.77256300
H	5.42458900	-2.84463800	0.76096000
H	6.00873400	-2.62962700	3.16458600
H	-1.37995800	-1.49911300	0.22269200
C	-4.99232700	0.74690100	2.38777100
C	-5.23833600	0.08536800	1.15440000
C	-6.43233000	0.35506000	0.45934100

C	-7.32831100	1.25818700	0.99706400
C	-7.06287700	1.90595000	2.22485500
C	-5.90181200	1.66392700	2.93437200
C	-3.24270200	-0.57784200	1.95605600
C	-4.10948400	-0.75540100	0.90470200
H	-6.63936900	-0.14004300	-0.48477600
H	-8.25224700	1.47860200	0.47267200
H	-7.78829900	2.61029000	2.61918000
H	-5.69805000	2.16175900	3.87651700
H	-3.95458400	-1.41181100	0.05976600
N	-3.78149800	0.31475000	2.85198000
H	-3.30601600	0.59884700	3.69591200
C	-1.93804500	-1.19663900	2.25355200
O	-1.43328800	-1.03956000	3.35360700
C	-1.33110800	-2.05589100	1.16723400
C	0.10199300	-2.49193500	1.47018400
H	-1.98080500	-2.93355700	1.04513800
H	0.12117500	-2.89038200	2.49224500
C	0.57867200	-3.57807700	0.53297100
C	1.25101800	-4.69181900	1.04334500
C	0.41501100	-3.47726100	-0.85422600
C	1.74869500	-5.68252100	0.20066100
H	1.39494000	-4.77347300	2.11806500
C	0.91552300	-4.46506400	-1.70026600
H	-0.09352500	-2.61433900	-1.27862000
C	1.58231700	-5.57151400	-1.17742100
H	2.26683100	-6.53898500	0.62112700
H	0.78526200	-4.36500700	-2.77414600
H	1.96877300	-6.33964300	-1.83988600

M4RS

C	4.84524800	-0.77357500	2.23402900
C	3.46481900	-0.69854600	2.06794600
C	2.58571200	-1.07655200	3.07870300
C	3.12187200	-1.55186400	4.27313900
C	4.50646300	-1.63529400	4.44712600
C	5.37716600	-1.24293600	3.43290500
C	5.57080200	-0.28539200	1.00727700
C	4.48181900	-0.12691200	-0.07838200
C	3.10894300	-0.17677500	0.69275200
H	1.51551500	-0.96809800	2.92430900
H	2.46082500	-1.85584700	5.07836400
H	4.90733300	-2.00943300	5.38396200
H	6.45222100	-1.30736700	3.57269700
H	6.35146800	-0.97016200	0.66111700
H	4.57759300	0.82143500	-0.60131200
H	6.04916900	0.68230600	1.19390200
H	2.61765800	0.79650100	0.73188900
N	2.17985800	-1.09486400	0.01812900
O	4.59904900	-1.10181800	-1.10753000
C	0.83325300	-1.11299000	-0.03880100
C	2.63612500	-2.22816400	-0.59475500
N	0.53774200	-2.25920300	-0.67281200
N	1.65618400	-2.95621500	-1.03857200
C	4.11177800	-2.38095600	-0.75414200
H	4.56946200	-2.75671500	0.17162600
H	4.33477400	-3.07130100	-1.56748800
C	-0.75061600	-2.85092500	-0.91934700
C	-1.42460800	-3.44531200	0.14964600
C	-1.26971100	-2.78006400	-2.21221400

C	-2.67775600	-3.99181000	-0.11627500
C	-2.52685800	-3.34448800	-2.42686200
C	-3.24185900	-3.95139000	-1.39310800
H	-3.23282000	-4.45103700	0.69828100
H	-2.96179000	-3.29420700	-3.42191300
C	-0.52167700	-2.05752300	-3.30107700
H	0.46855400	-2.49360800	-3.46048700
H	-0.37978400	-1.00236900	-3.03490500
H	-1.07577100	-2.09947100	-4.23983100
C	-4.59559200	-4.56298300	-1.64155100
H	-4.52302700	-5.65381300	-1.69954800
H	-5.02535000	-4.20464700	-2.57966100
H	-5.28485400	-4.31830600	-0.82891400
C	-0.84821500	-3.43239400	1.53890100
H	-0.96775300	-2.43687100	1.98277600
H	0.21938900	-3.67179400	1.53688700
H	-1.36352800	-4.15283700	2.17591800
C	-0.07772400	-0.08230800	0.57992300
O	0.42383800	0.57922800	1.54914000
C	-1.31911900	-0.02211900	0.01009600
C	-2.43447200	0.81328000	0.56263600
H	-1.53883700	-0.61497600	-0.86669200
H	-2.16207200	1.08924900	1.59022800
C	-3.71806300	0.00454600	0.59463900
C	-4.38680300	-0.24187200	1.79437100
C	-4.24770900	-0.52971400	-0.58585600
C	-5.54881400	-1.01215500	1.82121100
H	-3.99009900	0.17341500	2.71736700
C	-5.40778300	-1.29732500	-0.56493300
H	-3.73753300	-0.35668300	-1.53151300

C	-6.06212400	-1.54512100	0.64159400
H	-6.05218600	-1.19503900	2.76575800
H	-5.79985900	-1.70694000	-1.49163100
H	-6.96607200	-2.14614400	0.65943600
H	-0.68149000	2.70123400	0.57085200
C	3.10415600	2.35475200	-2.20585500
C	3.14639200	2.99828100	-0.93863800
C	4.38637600	3.42884000	-0.42713900
C	5.52720800	3.21134500	-1.17582200
C	5.46333600	2.56352500	-2.43161400
C	4.26348000	2.12754400	-2.96247800
C	1.01297600	2.45960400	-1.41359500
C	1.80337600	3.04548200	-0.45234000
H	4.43889600	3.92143900	0.53896000
H	6.49050400	3.53836000	-0.79870600
H	6.37967700	2.40360700	-2.99038600
H	4.21652900	1.62744900	-3.92389000
H	1.46627500	3.45544500	0.48817400
N	1.79904300	2.04166800	-2.46426100
H	1.41821800	1.62210000	-3.30010900
C	-0.45039700	2.30728200	-1.51008000
O	-0.94032000	1.85336400	-2.53424500
C	-1.26411000	2.83425600	-0.34808700
C	-2.62696700	2.14910800	-0.21716000
H	-1.38370900	3.91304800	-0.51584300
H	-2.97884700	1.91118700	-1.22799000
C	-3.66573600	3.01196200	0.46346300
C	-4.96363000	3.09763700	-0.04614700
C	-3.36827100	3.69711200	1.64651000
C	-5.93801000	3.85478000	0.60011100

H	-5.21056400	2.55712000	-0.95653800
C	-4.33837900	4.45588300	2.29573300
H	-2.36597900	3.63767800	2.06483800
C	-5.62788100	4.53805400	1.77342000
H	-6.94016900	3.91144300	0.18626800
H	-4.08745400	4.98439700	3.21028400
H	-6.38533300	5.12949100	2.27791300

M4SR

C	3.82562700	-1.86739300	-1.25310800
C	2.58359700	-1.54204500	-1.80503400
C	2.24435200	-0.22369600	-2.09970700
C	3.17816300	0.77230600	-1.81700700
C	4.41572900	0.45489900	-1.25170200
C	4.74941600	-0.86804400	-0.96744500
C	3.96448000	-3.35610100	-1.06729100
C	2.86840800	-3.89994200	-2.00858400
C	1.77787400	-2.79654100	-2.05375300
H	1.27771100	-0.00588000	-2.54607700
H	2.94792700	1.80884700	-2.04363900
H	5.12939500	1.24580600	-1.04129200
H	5.71817700	-1.11276500	-0.54161700
H	3.77462400	-3.62740100	-0.02211500
H	3.27841300	-3.97987900	-3.01759600
H	4.95237900	-3.74058900	-1.32950100
H	1.19712000	-2.77168500	-2.97543200
N	0.81626900	-3.07930500	-0.96333700
O	2.36583000	-5.18682700	-1.70964200
C	-0.20938600	-2.30902300	-0.54976500
C	0.80980200	-4.21271700	-0.19687600

N	-0.77811200	-2.99189200	0.44543500
N	-0.15374200	-4.18607200	0.67762600
C	1.80402600	-5.30935400	-0.42215400
H	2.56787800	-5.29303800	0.36460300
H	1.29335100	-6.27253200	-0.37931700
C	-1.99320700	-2.68266400	1.15243200
C	-3.20463400	-2.89586200	0.49546500
C	-1.89784400	-2.21659800	2.46580800
C	-4.37147000	-2.63896000	1.21650000
C	-3.09164700	-1.96343700	3.13734800
C	-4.33398100	-2.17282200	2.52992400
H	-5.33166500	-2.79102900	0.73033100
H	-3.05158000	-1.59465500	4.15953700
C	-0.55648600	-1.97616500	3.10579700
H	-0.01806600	-1.17022100	2.59358600
H	0.06658700	-2.87399800	3.06380800
H	-0.67990200	-1.68847500	4.15107100
C	-5.60411500	-1.87796700	3.28585900
H	-5.65312500	-0.81988900	3.56182600
H	-5.65213000	-2.45744500	4.21227700
H	-6.48612200	-2.11606700	2.68762100
C	-3.24270500	-3.35675600	-0.93687700
H	-2.66391500	-4.27656100	-1.07107000
H	-2.81713200	-2.59895500	-1.60500100
H	-4.27050400	-3.54961700	-1.24763100
C	-0.69086700	-1.05958100	-1.23690200
O	-0.67951800	-1.13888800	-2.51176500
C	-1.05274000	-0.05854000	-0.38707400
C	-1.69355000	1.21142400	-0.86528600
H	-0.97887600	-0.21693700	0.68301600

H	-1.34438700	1.41759400	-1.88759500
C	-3.20992600	1.08312700	-0.91888900
C	-3.93359500	1.56635100	-2.01113700
C	-3.91167500	0.52189700	0.15158900
C	-5.32496100	1.50108500	-2.03274500
H	-3.39850000	2.01160400	-2.84656700
C	-5.30251400	0.45790200	0.13623600
H	-3.36081700	0.11599100	0.99849800
C	-6.01546600	0.94992000	-0.95562800
H	-5.86994800	1.88068100	-2.89196700
H	-5.82856200	0.01225900	0.97665000
H	-7.09968500	0.89788500	-0.97006200
H	0.65629800	2.29710600	-0.96776700
C	4.57970600	1.95583200	1.77308600
C	4.56912000	3.07450800	0.89731000
C	5.78637200	3.71048600	0.58405100
C	6.95424900	3.21948200	1.13285200
C	6.94128500	2.10164400	1.99954700
C	5.76554700	1.45803400	2.33318000
C	2.46916700	2.29639100	1.11686000
C	3.21439600	3.26893900	0.49014600
H	5.80086800	4.56745100	-0.08224700
H	7.90129800	3.69469000	0.89961900
H	7.87876300	1.74203700	2.41140300
H	5.75581600	0.59873000	2.99526500
H	2.84074900	4.02603700	-0.18458100
N	3.29207500	1.51852200	1.89705200
H	2.95577600	0.74178600	2.44711700
C	1.02683300	1.98850600	1.08024200
O	0.55580500	1.22648000	1.90910900

C	0.23134900	2.65565900	-0.01898400
C	-1.28545300	2.42217900	0.02705400
H	0.46151900	3.72707900	0.02686300
H	-1.55620400	2.16194000	1.05859000
C	-2.06059400	3.66360600	-0.36401400
C	-3.16182500	4.07193100	0.39128500
C	-1.74209200	4.38239000	-1.52062600
C	-3.92917800	5.16763200	0.00504900
H	-3.42830500	3.51010000	1.28279200
C	-2.50580700	5.47990800	-1.91142000
H	-0.89255200	4.07724000	-2.12807900
C	-3.60338200	5.87568100	-1.14939100
H	-4.78317800	5.46708700	0.60469800
H	-2.24460700	6.02567100	-2.81286300
H	-4.19964900	6.73003600	-1.45352700

M4SS

C	-4.19236100	0.86082000	1.84422300
C	-2.91950100	0.57062800	1.36564700
C	-1.97671000	-0.08652200	2.15134500
C	-2.34223700	-0.48895900	3.43277200
C	-3.63072400	-0.22819100	3.91062800
C	-4.55910300	0.45222100	3.12619900
C	-5.00241300	1.62942800	0.83293700
C	-4.04257500	1.88381400	-0.35593800
C	-2.73371700	1.06902000	-0.04652800
H	-0.97499200	-0.27032800	1.76539800
H	-1.62609700	-1.00698500	4.06270800
H	-3.90591200	-0.54927300	4.91009400
H	-5.55102200	0.66855200	3.51194400

H	-5.37021000	2.58268800	1.22805600
H	-4.47189100	1.53061800	-1.29469600
H	-5.87381100	1.05878100	0.50109100
H	-2.55389300	0.26243400	-0.76396900
N	-1.56114500	1.94446500	-0.12099500
O	-3.79866900	3.26903100	-0.57093900
C	-0.27506200	1.60604000	-0.30324000
C	-1.60100800	3.26694200	0.21081300
N	0.41042100	2.73116000	-0.08613000
N	-0.40698000	3.78540400	0.23006700
C	-2.95648700	3.87006800	0.39471100
H	-3.31796100	3.69680600	1.41807200
H	-2.92946000	4.94256300	0.20420900
C	1.83041800	2.91856900	-0.21498700
C	2.58567900	3.04090400	0.95126100
C	2.38237000	2.94145100	-1.49797400
C	3.96312700	3.20890900	0.80456000
C	3.76242700	3.10488000	-1.58984700
C	4.56457500	3.24482100	-0.45469500
H	4.57839700	3.30202400	1.69595400
H	4.22395400	3.11980300	-2.57404800
C	1.51853700	2.78025700	-2.72014400
H	0.67955200	3.48318900	-2.70224300
H	1.09897500	1.76990500	-2.78063200
H	2.10082000	2.96362100	-3.62421500
C	6.05083800	3.44660700	-0.59575800
H	6.27931200	4.49751300	-0.80049500
H	6.44823100	2.85551600	-1.42474000
H	6.57795800	3.16300600	0.31801200
C	1.93253200	2.96200000	2.30564300

H	1.36391500	2.03043300	2.41160900
H	1.23171500	3.78819700	2.45571400
H	2.68349000	2.99547500	3.09602100
C	0.19622000	0.27313100	-0.81886600
O	-0.53845800	-0.19252200	-1.75360300
C	1.33843900	-0.22031300	-0.25838800
C	1.95098600	-1.46050300	-0.83493700
H	1.81037700	0.31487200	0.55811100
H	1.47506800	-1.59963900	-1.81293400
C	3.44961800	-1.36362800	-1.07605800
C	4.06601000	-2.32296100	-1.88972400
C	4.24846000	-0.36118500	-0.52309400
C	5.43574400	-2.29390300	-2.13010300
H	3.45535100	-3.09853600	-2.34798500
C	5.62238400	-0.32617400	-0.76192900
H	3.80175200	0.41902700	0.08534400
C	6.22362000	-1.29349400	-1.56127100
H	5.88817500	-3.04703100	-2.76831100
H	6.22041900	0.46500700	-0.31736200
H	7.29264500	-1.26605100	-1.74747700
H	-0.31926200	-2.07570900	0.70101200
C	-4.01097300	-1.93510400	-2.07687200
C	-4.19683700	-1.99021100	-0.66850800
C	-5.44231200	-1.62215200	-0.12791700
C	-6.44592800	-1.20752700	-0.98483000
C	-6.23607700	-1.14910800	-2.38077300
C	-5.02603500	-1.51007600	-2.94537600
C	-2.08725400	-2.60112300	-1.15385300
C	-2.95371300	-2.41812600	-0.10351800
H	-5.60148100	-1.65302500	0.94675200

H	-7.41212600	-0.91804300	-0.58329100
H	-7.04407300	-0.81579200	-3.02402300
H	-4.86438400	-1.46706600	-4.01727700
H	-2.73173200	-2.56141600	0.94448200
N	-2.73284500	-2.34469600	-2.33853800
H	-2.24940600	-2.31324400	-3.22404600
C	-0.66101400	-2.98461800	-1.18567600
O	-0.15160600	-3.35934100	-2.22805600
C	0.09090800	-2.91058500	0.12693100
C	1.60523600	-2.76610000	-0.03988000
H	-0.14087700	-3.82510000	0.69035400
H	1.95011400	-3.60815600	-0.65106400
C	2.33295200	-2.82929900	1.28626900
C	3.49868700	-3.59339100	1.40288600
C	1.90298100	-2.10855600	2.40636100
C	4.21314000	-3.64202300	2.59673100
H	3.85014200	-4.15251500	0.53928100
C	2.61489800	-2.15302300	3.60342800
H	1.00274100	-1.50323800	2.34664100
C	3.77254400	-2.92054400	3.70383900
H	5.11384500	-4.24477200	2.66123700
H	2.26213500	-1.58716900	4.46057200
H	4.32549900	-2.95730500	4.63709200

TS5RR

C	-4.38158200	-2.76310200	-0.16152200
C	-3.32170400	-2.27145800	-0.93037500
C	-2.67225900	-3.07870900	-1.85738200
C	-3.05275300	-4.41603700	-1.95171500
C	-4.07511000	-4.92361100	-1.14750400

C	-4.75845200	-4.09768800	-0.25620900
C	-5.02760000	-1.65316600	0.62427900
C	-4.57372400	-0.41554000	-0.18219000
C	-3.16359900	-0.78151800	-0.71743400
H	-1.88655300	-2.66542100	-2.47732100
H	-2.55761200	-5.06639700	-2.66534000
H	-4.35944400	-5.96751500	-1.23679300
H	-5.58374000	-4.48313200	0.33478800
H	-4.65136700	-1.62775200	1.65442300
H	-5.22027600	-0.31321700	-1.05718900
H	-6.11571900	-1.72973000	0.67439500
H	-2.84006900	-0.25024300	-1.61290200
N	-2.19700400	-0.41412000	0.36539600
O	-4.63775500	0.82111600	0.48250800
C	-0.88327400	-0.67949400	0.48035200
C	-2.54917500	0.26458200	1.50750400
N	-0.52182300	-0.25876600	1.68860600
N	-1.55347900	0.33694300	2.34692300
C	-3.90357000	0.88407400	1.68204800
H	-4.43231000	0.40283500	2.51391100
H	-3.76795500	1.94533300	1.91452300
C	0.71993100	-0.59621800	2.33950700
C	0.98649300	-1.96408100	2.51654800
C	1.59203100	0.40753700	2.76841600
C	2.20580400	-2.30858200	3.09369300
C	2.79497700	0.00173300	3.34932000
C	3.12378700	-1.34256100	3.51048400
H	2.43741300	-3.36106600	3.23497400
H	3.49205200	0.76667000	3.68313100
C	1.31226100	1.87859700	2.61164400

H	0.25632100	2.08573600	2.43775100
H	1.89616900	2.28416400	1.77613100
H	1.62482600	2.41162800	3.51251100
C	4.41883700	-1.74578200	4.16549700
H	5.19988300	-1.00370900	3.98490100
H	4.76382800	-2.71401100	3.79505700
H	4.28843500	-1.83370700	5.24893300
C	-0.00705800	-3.03445800	2.13698700
H	-0.03655700	-3.20255800	1.05596500
H	-1.01815500	-2.76733900	2.46137700
H	0.26404500	-3.97528800	2.61786800
C	0.08257800	-1.14091100	-0.59854400
O	-0.09152400	-2.23399400	-1.13363900
C	0.97153000	-0.11869000	-1.00261700
C	2.01887600	-0.47757900	-2.01430000
H	1.23341000	0.63087300	-0.25799900
H	1.51216300	-1.09142300	-2.77157200
C	3.20793500	-1.26301000	-1.50566800
C	3.98697500	-1.98677700	-2.41474200
C	3.58389500	-1.26120200	-0.16050700
C	5.12323600	-2.67376400	-1.99819500
H	3.69716600	-2.00437600	-3.46340800
C	4.71930200	-1.95026200	0.26153200
H	2.98853500	-0.71555900	0.56772400
C	5.49600600	-2.65444200	-0.65457700
H	5.71488200	-3.22914200	-2.71960300
H	4.99512900	-1.93309400	1.31242300
H	6.38031900	-3.19136900	-0.32587500
H	0.99266800	2.52699300	-3.14211800
C	-2.73246900	3.02484200	-0.72012200

C	-1.70713300	3.28118000	0.22459600
C	-1.98453700	4.10929700	1.32790400
C	-3.24987700	4.65625000	1.45143700
C	-4.25249100	4.39805900	0.49083500
C	-4.00908900	3.58686000	-0.60377800
C	-0.89664000	1.87781400	-1.36010100
C	-0.55439900	2.54921400	-0.20974200
H	-1.21535000	4.31669400	2.06654700
H	-3.47975200	5.29711900	2.29668200
H	-5.23427900	4.84328300	0.61562200
H	-4.78333900	3.37559000	-1.33378400
H	0.40047400	2.51509100	0.28487800
N	-2.20774800	2.17429400	-1.66114300
H	-2.66735400	1.78630100	-2.47263200
C	-0.20372400	0.89134700	-2.28985800
O	-0.99970000	0.10748900	-2.89490000
C	0.99999000	1.43317400	-3.12974900
C	2.37366400	0.86481900	-2.72157500
H	0.76982300	1.09375800	-4.14286100
H	2.95480700	0.63481800	-3.62242900
C	3.23797500	1.76827800	-1.85723000
C	4.60540700	1.48651100	-1.72446400
C	2.73345100	2.87557100	-1.17179800
C	5.42780500	2.26498600	-0.91708500
H	5.02792500	0.63921600	-2.25827700
C	3.55262000	3.65793300	-0.35579800
H	1.68950800	3.14675600	-1.27961200
C	4.90272200	3.35270500	-0.22033700
H	6.48299800	2.02328100	-0.83387900
H	3.12913800	4.51248400	0.16417100

H	5.54291100	3.96178900	0.40989400
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TS5RS

C	-0.05456400	-0.04470000	0.51659300
O	0.28835300	0.35129400	1.62509900
C	-1.23638500	0.31873100	-0.22499500
C	-2.38001900	0.87830200	0.60258600
H	-1.56882200	-0.46545600	-0.90281100
H	-1.95256800	1.54056000	1.36673400
C	-3.16172800	-0.20801000	1.30170700
C	-3.07629000	-0.35389900	2.68918900
C	-3.92627000	-1.12893500	0.57804600
C	-3.73880500	-1.39243700	3.34108600
H	-2.47427300	0.35013900	3.25807600
C	-4.59366600	-2.16404400	1.22672800
H	-3.98925400	-1.04901500	-0.50538800
C	-4.50117000	-2.30101800	2.61107100
H	-3.65914100	-1.49067300	4.41940800
H	-5.18240800	-2.86930600	0.64684200
H	-5.01956000	-3.10965500	3.11638700
H	-1.65424400	3.30636100	-0.34728300
C	2.59216800	2.54223900	-1.87839300
C	2.40262300	3.17548600	-0.61758700
C	3.47605500	3.88302500	-0.04771100
C	4.67553300	3.95976800	-0.73800500
C	4.83576500	3.33612500	-1.99329600
C	3.80216400	2.61946000	-2.57678800
C	0.48140700	2.15021300	-1.21538700
C	1.05048500	2.90508900	-0.21556000
H	3.36130500	4.36748600	0.91762000

H	5.50842000	4.50750200	-0.30838500
H	5.78759600	3.41437700	-2.50863200
H	3.92549800	2.13099200	-3.53790500
H	0.56464900	3.23233900	0.69336100
N	1.41285700	1.91777800	-2.19362400
H	1.11929800	1.45989900	-3.04806700
C	-0.90033700	1.56362700	-1.47253400
O	-1.00660900	1.03330800	-2.65201000
C	-2.03023600	2.55937800	-1.05670800
C	-3.15309000	1.75464300	-0.39986500
H	-2.35311100	3.07640700	-1.96366000
H	-3.58908200	1.10357700	-1.16902400
C	-4.25802000	2.56935500	0.22690600
C	-5.57647500	2.43264900	-0.21215500
C	-3.99384000	3.46644600	1.26832700
C	-6.60622400	3.17391200	0.36444800
H	-5.79574600	1.73440900	-1.01613800
C	-5.01833200	4.20765600	1.84855600
H	-2.97597300	3.58918900	1.63083200
C	-6.32992900	4.06461300	1.39765400
H	-7.62387000	3.05288200	0.00621200
H	-4.79366700	4.89853500	2.65537200
H	-7.12914300	4.64253800	1.85074900
C	4.89521700	-0.60462800	2.19267800
C	3.51477200	-0.64168400	2.01041200
C	2.68043400	-1.29683200	2.91202400
C	3.25795000	-1.92556700	4.01208000
C	4.64171700	-1.88976700	4.20329800
C	5.46833400	-1.22826000	3.29843300
C	5.57443300	0.16455300	1.09021100

C	4.48113900	0.41073200	0.02592100
C	3.11784600	0.09106200	0.74642300
H	1.60531900	-1.30303300	2.76229500
H	2.62859600	-2.44462700	4.72740900
H	5.07722100	-2.38427400	5.06568300
H	6.54346700	-1.20520500	3.44834700
H	6.41960000	-0.37039600	0.64592900
H	4.47885000	1.44206300	-0.31960800
H	5.95627900	1.12208300	1.45912500
H	2.54471400	1.00110600	0.93540800
N	2.28746100	-0.77517400	-0.10658500
O	4.69085500	-0.35323700	-1.15480400
C	0.95623600	-0.90772400	-0.21292000
C	2.84912400	-1.73825700	-0.89269700
N	0.75982200	-1.94384400	-1.02979400
N	1.93734100	-2.47068000	-1.46635600
C	4.33483000	-1.71671300	-1.04419800
H	4.82009700	-2.20699900	-0.18911100
H	4.62810400	-2.22560700	-1.96209900
C	-0.47706800	-2.59838700	-1.38103300
C	-1.21292900	-3.22731700	-0.37513700
C	-0.86177200	-2.57951500	-2.72848500
C	-2.38592900	-3.87734000	-0.76438800
C	-2.04439400	-3.23567900	-3.05349800
C	-2.81597400	-3.89103500	-2.08839700
H	-2.97906000	-4.37432400	-0.00156600
H	-2.37730200	-3.22868300	-4.08839100
C	-0.06681100	-1.81843000	-3.75257300
H	0.95383600	-2.20007500	-3.83338700
H	-0.04091700	-0.76134800	-3.45558700

H	-0.54549400	-1.89518300	-4.73025400
C	-4.08922800	-4.59210200	-2.48276600
H	-3.87967600	-5.42699800	-3.15812000
H	-4.76152700	-3.90850800	-3.00896600
H	-4.61217800	-4.98448400	-1.60830000
C	-0.82043500	-3.18222300	1.07804600
H	-1.17547400	-2.25323700	1.54319800
H	0.26262100	-3.24870500	1.22140700
H	-1.28600500	-4.00951700	1.61641100

TS5SR

C	5.30992000	-0.26559800	0.00731900
C	3.97679700	-0.38454500	0.39221100
C	3.60439100	-0.48745300	1.72786700
C	4.60697600	-0.41350300	2.69479300
C	5.94435000	-0.25943300	2.31983800
C	6.30730900	-0.19287300	0.97466100
C	5.42286700	-0.25872800	-1.49773700
C	4.08353400	-0.85761600	-1.96397400
C	3.08841100	-0.45040500	-0.83599600
H	2.55543500	-0.59125000	2.01026400
H	4.34673200	-0.48183000	3.74585400
H	6.71189500	-0.20793900	3.08541600
H	7.35058100	-0.10110900	0.68841500
H	6.26327000	-0.83987000	-1.88450400
H	3.76283000	-0.47464300	-2.93337000
H	5.51603100	0.76888000	-1.87009700
H	2.58354900	0.49556900	-1.05760900
N	2.07785500	-1.48929400	-0.67540700
O	4.15583200	-2.27406100	-2.13492000

C	0.76564700	-1.43839500	-0.40915300
C	2.46663700	-2.79549800	-0.59901100
N	0.41407400	-2.69758200	-0.15422400
N	1.46317400	-3.56410600	-0.28265900
C	3.87463600	-3.09526600	-1.01240100
H	4.57053300	-2.92636600	-0.18267300
H	3.95117900	-4.13194300	-1.34027400
C	-0.88954200	-3.20457300	0.18958800
C	-1.73485400	-3.60831500	-0.84207400
C	-1.21013900	-3.30159800	1.54736300
C	-2.96085600	-4.16128200	-0.47294200
C	-2.45811200	-3.83609500	1.85921400
C	-3.33894800	-4.27529600	0.86474000
H	-3.64196700	-4.49211400	-1.25275100
H	-2.74623100	-3.92165300	2.90394600
C	-0.25043400	-2.82477900	2.60478800
H	-0.10445200	-1.73494000	2.55904200
H	0.73106800	-3.29352800	2.47908600
H	-0.62562200	-3.07871000	3.59741800
C	-4.68773400	-4.83116000	1.24003400
H	-5.16410600	-5.32317500	0.38975100
H	-5.35012600	-4.02888900	1.58153300
H	-4.60268200	-5.55354000	2.05583800
C	-1.35353600	-3.40738600	-2.28336100
H	-1.34528700	-2.33885100	-2.52880800
H	-2.07177500	-3.89714200	-2.94199000
H	-0.35773500	-3.80704100	-2.49574500
C	-0.13658300	-0.24730000	-0.70175000
O	0.13305000	0.31350300	-1.76552300
C	-1.09445400	0.12117700	0.27648000

C	-2.23785100	1.01119400	-0.13739600
H	-1.35123000	-0.66190700	0.98749100
H	-1.83621200	1.80668800	-0.77559000
C	-3.35680400	0.32707300	-0.89393000
C	-3.96803400	0.95994700	-1.97939400
C	-3.84790900	-0.91532400	-0.48121400
C	-5.04277200	0.36791900	-2.63927800
H	-3.59955300	1.93048500	-2.30265700
C	-4.92422400	-1.50803200	-1.13560500
H	-3.38323400	-1.43076600	0.35774300
C	-5.52591900	-0.86861600	-2.21783200
H	-5.50390700	0.87370800	-3.48196200
H	-5.29098100	-2.47394000	-0.79927400
H	-6.36400000	-1.33167100	-2.72892700
H	-1.29553400	3.06898300	1.97047200
C	2.82054900	2.79563400	0.26257000
C	1.94005000	3.40353500	-0.67169700
C	2.48611700	4.22788300	-1.67145400
C	3.85748400	4.41544400	-1.71435300
C	4.71112200	3.79936200	-0.77518500
C	4.20733000	2.98414600	0.22630000
C	0.72845000	2.11083700	0.73531900
C	0.61339000	2.96463900	-0.33940400
H	1.83995700	4.70448800	-2.40288200
H	4.28842900	5.04758800	-2.48438300
H	5.78166200	3.96799800	-0.83764700
H	4.85606000	2.50098000	0.95210800
H	-0.28956100	3.22153000	-0.87275400
N	2.05089900	2.02470300	1.08941100
H	2.32217700	1.49707200	1.90676300

C	-0.19919800	1.24094400	1.56689700
O	0.40742100	0.51475600	2.42982700
C	-1.49278100	1.99378900	2.01461000
C	-2.74159400	1.63289200	1.18863700
H	-1.63779800	1.72931200	3.06467200
H	-3.28070400	0.83236700	1.71142200
C	-3.71273100	2.76485300	0.94664700
C	-5.08134200	2.58477700	1.15611400
C	-3.27307400	3.99304100	0.43978600
C	-5.98947900	3.60470300	0.87822200
H	-5.43821600	1.63010500	1.53462400
C	-4.17548200	5.01419800	0.15907800
H	-2.21128500	4.15296400	0.26375400
C	-5.53902000	4.82409300	0.38017700
H	-7.04931700	3.44480500	1.05080500
H	-3.81395800	5.96056000	-0.23116400
H	-6.24372900	5.62103100	0.16505600

TS5SS

C	-2.16346000	-0.48849400	3.90499200
C	-1.71195000	-0.85907700	2.64190500
C	-1.90788000	-2.14276500	2.13931700
C	-2.57331000	-3.06900100	2.93721100
C	-3.02706300	-2.70682000	4.20923400
C	-2.82894000	-1.41867100	4.70047900
C	-1.84930100	0.95440300	4.20546600
C	-0.96691400	1.44212900	3.03002600
C	-1.02149100	0.29322400	1.95211900
H	-1.56141600	-2.41694700	1.14466500
H	-2.74040700	-4.07555700	2.56903100

H	-3.54115100	-3.44062900	4.82141200
H	-3.18452500	-1.14481900	5.68895200
H	-1.32189900	1.09079300	5.15508900
H	-1.35749800	2.36221600	2.59367400
H	-2.76440400	1.55095100	4.26139900
H	-1.57128500	0.63335200	1.07571700
N	0.33871600	-0.09901900	1.53826000
O	0.35197400	1.77316300	3.42468400
C	0.79318700	-0.74650700	0.44414800
C	1.36025700	-0.08856900	2.44689300
N	2.03255800	-1.12755600	0.74817100
N	2.40891300	-0.70524400	1.98772000
C	1.15537800	0.65016300	3.72893300
H	0.68631700	0.00090800	4.48072400
H	2.11080600	1.00757300	4.11174600
C	2.94232200	-1.98326300	0.02094700
C	2.82555900	-3.36011700	0.23137600
C	3.92198500	-1.40247500	-0.77604300
C	3.77030500	-4.17536800	-0.38122700
C	4.84733100	-2.26514900	-1.36828400
C	4.79070300	-3.64387100	-1.17754500
H	3.70935500	-5.25130700	-0.23730200
H	5.62657500	-1.84228200	-1.99706400
C	3.91352300	0.07108900	-1.05617000
H	3.69011700	0.66359400	-0.16271000
H	3.13014000	0.27619500	-1.79644100
H	4.87391700	0.39972600	-1.45880000
C	5.79117300	-4.55922300	-1.83421900
H	6.19707700	-5.27616300	-1.11559000
H	6.62037800	-3.99563100	-2.26610600

H	5.31821900	-5.13304800	-2.63715000
C	1.68923800	-3.92232900	1.04009800
H	0.74980700	-3.76875100	0.49731800
H	1.59892700	-3.43339700	2.01541500
H	1.82238900	-4.99258700	1.20325600
C	0.12327700	-0.99153400	-0.89666600
O	0.46192800	-2.01409900	-1.49363800
C	-0.70808800	0.04659700	-1.38199100
C	-1.64052600	-0.26131700	-2.52109200
H	-1.08490700	0.75031000	-0.65168500
H	-1.02531900	-0.70834000	-3.31300300
C	-2.78311400	-1.20730700	-2.22754000
C	-3.31749800	-1.97968800	-3.26285300
C	-3.35805900	-1.31386700	-0.95874900
C	-4.39427100	-2.83386900	-3.03914900
H	-2.87782500	-1.90948300	-4.25526000
C	-4.42785600	-2.17383400	-0.72447500
H	-2.96758800	-0.71214500	-0.14178000
C	-4.95172100	-2.93634700	-1.76588900
H	-4.79183900	-3.42727900	-3.85681500
H	-4.84928700	-2.24756900	0.27385700
H	-5.78448200	-3.60887600	-1.58634200
H	-0.82374100	2.94431200	-2.96924000
C	2.90322000	3.36865700	-0.82205400
C	2.01736400	3.29903400	0.28281600
C	2.37174300	3.93589500	1.48412300
C	3.57593200	4.61704500	1.54817700
C	4.44154200	4.67579400	0.43652300
C	4.12101300	4.05465100	-0.75955700
C	1.13884900	2.10423300	-1.43157700

C	0.89996200	2.50118200	-0.13584500
H	1.71332500	3.87580900	2.34613200
H	3.86511800	5.11275100	2.46952100
H	5.37987000	5.21465300	0.52119500
H	4.78705100	4.09367800	-1.61557300
H	0.03330200	2.26825200	0.46433300
N	2.32914500	2.65652300	-1.84455300
H	2.75388000	2.39053900	-2.72177400
C	0.45472800	1.22031100	-2.46630900
O	1.25159300	0.53384000	-3.17245100
C	-0.73922300	1.88610800	-3.23339100
C	-2.07422500	1.14034400	-3.04609700
H	-0.43630500	1.83122700	-4.28175900
H	-2.57502800	1.00978600	-4.01157800
C	-3.06231200	1.81224300	-2.11026500
C	-4.42594400	1.51811800	-2.22954500
C	-2.66765400	2.68380300	-1.08926800
C	-5.36062400	2.05987900	-1.35240200
H	-4.75374500	0.84283600	-3.01646800
C	-3.59905400	3.22324100	-0.20165000
H	-1.62144200	2.95945200	-0.98523800
C	-4.94951800	2.91160500	-0.32858200
H	-6.41215700	1.81629200	-1.46868100
H	-3.26454200	3.89756100	0.58136600
H	-5.67659300	3.33417900	0.35749900

M5RR

C	-4.08155900	-2.81976800	-0.71131500
C	-3.08493900	-2.09144700	-1.36923400
C	-2.24228200	-2.67653600	-2.30558800

C	-2.38961400	-4.04155000	-2.55160000
C	-3.36504500	-4.78316700	-1.88141600
C	-4.22517500	-4.17893700	-0.96299200
C	-4.89614600	-1.91752200	0.18444700
C	-4.58254000	-0.52594000	-0.41361900
C	-3.14191300	-0.64375900	-0.95772300
H	-1.49796200	-2.06551400	-2.80828600
H	-1.74641000	-4.53149300	-3.27530200
H	-3.46649700	-5.84382000	-2.08937700
H	-4.99781600	-4.75766200	-0.46597900
H	-4.55527500	-1.99373200	1.22522900
H	-5.23151700	-0.36090800	-1.27702000
H	-5.96553900	-2.13768000	0.17410300
H	-2.84414500	0.04079500	-1.74863700
N	-2.23510300	-0.38056900	0.19900000
O	-4.78075300	0.59167800	0.42117000
C	-0.94013900	-0.68643700	0.34722600
C	-2.66271400	0.07277100	1.42169800
N	-0.64634100	-0.48338200	1.62793000
N	-1.71695300	-0.00712000	2.31890900
C	-4.05813600	0.58026500	1.62980300
H	-4.55345100	-0.02645600	2.39857600
H	-4.00345300	1.61795600	1.97604900
C	0.53852100	-1.00445000	2.26815400
C	0.65019400	-2.40590700	2.30260200
C	1.50055500	-0.15190200	2.80948300
C	1.81947100	-2.93861200	2.83207000
C	2.65108500	-0.74419000	3.33748100
C	2.83922800	-2.12351800	3.33362200
H	1.93622900	-4.01879300	2.86342100

H	3.41962900	-0.09861100	3.75546700
C	1.35478500	1.34524200	2.83095800
H	0.30949900	1.65248500	2.77776400
H	1.89945500	1.80006200	1.99300700
H	1.78751400	1.74569600	3.75014600
C	4.10513300	-2.74013400	3.86621000
H	4.77305300	-1.98261100	4.28065500
H	4.63651800	-3.26500300	3.06614200
H	3.88497200	-3.47278000	4.64749100
C	-0.46420900	-3.30348400	1.82382100
H	-0.52127300	-3.33157200	0.73083000
H	-1.43306600	-2.96597400	2.20714200
H	-0.29730800	-4.32135200	2.17853800
C	0.15278800	-0.99599500	-0.68174700
O	0.35530500	-2.12400700	-1.04937600
C	0.92474900	0.22639900	-1.06501100
C	2.06024700	-0.07142200	-2.03069500
H	1.27621100	0.73442000	-0.15520800
H	1.61429500	-0.65459400	-2.84545800
C	3.23925600	-0.83602600	-1.48203300
C	3.99497300	-1.64120300	-2.33962800
C	3.63368800	-0.74172200	-0.14432900
C	5.11593900	-2.32672600	-1.87888600
H	3.69653800	-1.72865400	-3.38186000
C	4.74928800	-1.43073700	0.32400000
H	3.07679300	-0.11356500	0.54571100
C	5.49696600	-2.22478200	-0.54229700
H	5.68915000	-2.94612600	-2.56187200
H	5.03385800	-1.33956100	1.36886600
H	6.36801700	-2.76171200	-0.17984100

H	0.92092500	3.00432800	-2.69846000
C	-2.77893800	3.08295000	-0.41504200
C	-1.86482400	3.25215500	0.65784000
C	-2.29358800	3.91799200	1.81886600
C	-3.59602400	4.38713900	1.88168500
C	-4.48679800	4.20952200	0.80237200
C	-4.09137800	3.56229700	-0.35737400
C	-0.84707400	2.06986000	-0.98737200
C	-0.64386000	2.60783000	0.26274100
H	-1.61285400	4.05760500	2.65397800
H	-3.94014400	4.90109800	2.77376600
H	-5.50167300	4.58534000	0.88319300
H	-4.77929200	3.41218100	-1.18308400
H	0.26246800	2.54796500	0.84188800
N	-2.11786200	2.38537900	-1.39611400
H	-2.47257500	2.00978500	-2.26532800
C	-0.05990100	1.13470700	-1.91011300
O	-0.91591600	0.34231600	-2.60142800
C	0.94840300	1.92021200	-2.84204900
C	2.36375700	1.34298100	-2.62431500
H	0.60764100	1.70359000	-3.85727500
H	2.89078000	1.21553700	-3.57617800
C	3.26311100	2.14586600	-1.70534400
C	4.65006800	1.96925400	-1.78064500
C	2.76453500	3.01513600	-0.73075300
C	5.50912500	2.62177300	-0.90292600
H	5.05633900	1.29355100	-2.52958300
C	3.62085800	3.66705400	0.15721500
H	1.69633600	3.19911100	-0.66631200
C	4.99618300	3.47009100	0.07739700

H	6.58070700	2.46645300	-0.98243700
H	3.20748200	4.33724800	0.90542800
H	5.66390000	3.97916000	0.76523400

M5RS

C	-0.17499600	-0.48484000	0.45977900
O	0.09854000	-0.23212600	1.61624500
C	-1.21899400	0.10554500	-0.38163600
C	-2.25503400	0.98271600	0.28504500
H	-1.67874100	-0.66646900	-1.00758000
H	-1.74362500	1.70931000	0.92622700
C	-3.29486200	0.27044300	1.12062800
C	-3.96519600	0.96570200	2.13334900
C	-3.64790300	-1.06113400	0.88170700
C	-4.95883500	0.34709700	2.88716200
H	-3.70100800	2.00246300	2.32856100
C	-4.63620500	-1.68489400	1.63934500
H	-3.15087500	-1.63029700	0.10062200
C	-5.29751600	-0.98284300	2.64393300
H	-5.46599500	0.90237600	3.67008800
H	-4.88247100	-2.72489000	1.44180500
H	-6.06772000	-1.46786800	3.23510900
H	-1.45040800	2.88783200	-2.17508600
C	2.55513400	2.95605200	-1.12205100
C	2.03457800	3.28696300	0.15751600
C	2.80254800	4.10266900	1.00732600
C	4.03920100	4.55239500	0.57468900
C	4.53643100	4.20970900	-0.69910400
C	3.80363500	3.41225300	-1.56365500
C	0.56129200	1.93041300	-0.90330900

C	0.76105500	2.62730200	0.27056900
H	2.43030700	4.37304200	1.99116200
H	4.63930200	5.18132200	1.22457400
H	5.50755500	4.58073700	-1.01083400
H	4.17857400	3.15165900	-2.54911300
H	0.11341700	2.64752400	1.13465600
N	1.63593100	2.14184000	-1.72897200
H	1.67879000	1.59693800	-2.58474200
C	-0.49407600	0.99628300	-1.52972200
O	0.07964200	0.24198900	-2.46336900
C	-1.73947400	1.85004200	-1.98569300
C	-2.87129600	1.74602600	-0.93209200
H	-2.06027300	1.41453800	-2.93566200
H	-3.65995900	1.09652200	-1.33037100
C	-3.51032700	3.04813200	-0.51397700
C	-4.89912800	3.18371300	-0.47328300
C	-2.72049200	4.12939300	-0.10464200
C	-5.49024000	4.37070700	-0.04246200
H	-5.52276000	2.34722200	-0.77857500
C	-3.30608700	5.31482300	0.32756400
H	-1.63580200	4.03541100	-0.12612800
C	-4.69511200	5.44023400	0.35864300
H	-6.57216200	4.45780500	-0.02017500
H	-2.67875400	6.14432600	0.63913700
H	-5.15175400	6.36609300	0.69395500
C	5.10316500	-0.57332200	1.18563600
C	3.72836100	-0.75889600	1.30833200
C	3.16056000	-1.29741300	2.45756500
C	4.00839900	-1.66027600	3.50179900
C	5.38896400	-1.47778800	3.38861400

C	5.94630000	-0.93158600	2.23363700
C	5.44793300	0.03896100	-0.14867900
C	4.16582200	-0.10009600	-0.99508300
C	3.01562400	-0.29604500	0.05661600
H	2.08366400	-1.42120100	2.53524300
H	3.59431700	-2.08538100	4.40998500
H	6.03543800	-1.76754700	4.21074000
H	7.02018100	-0.79485100	2.15046000
H	6.28865100	-0.44552000	-0.65284200
H	3.97657100	0.78978700	-1.59246200
H	5.69531100	1.10084900	-0.03470600
H	2.45497300	0.63082200	0.21509200
N	2.07516100	-1.31453600	-0.41720600
O	4.25088000	-1.15302500	-1.94852200
C	0.75380100	-1.43582400	-0.27809700
C	2.50588100	-2.42509500	-1.08916800
N	0.43086500	-2.60294700	-0.81989200
N	1.51843300	-3.23550100	-1.34581500
C	3.94872700	-2.45169100	-1.47585800
H	4.57258700	-2.74026800	-0.61968500
H	4.11059200	-3.15468100	-2.29228300
C	-0.86359100	-3.23188600	-0.77395700
C	-1.28471900	-3.77187100	0.44274400
C	-1.62909100	-3.25785400	-1.94652000
C	-2.55613300	-4.34835300	0.47262800
C	-2.89312000	-3.83424100	-1.85458900
C	-3.37280300	-4.37753800	-0.65704900
H	-2.91550000	-4.77498700	1.40545900
H	-3.52156500	-3.85932200	-2.74123100
C	-1.10140200	-2.66647300	-3.22401200

H	-0.23108000	-3.23204500	-3.57270400
H	-0.77928200	-1.62493600	-3.07014100
H	-1.86718200	-2.70417600	-4.00069900
C	-4.75698200	-4.96845500	-0.59694700
H	-4.89501100	-5.72225000	-1.37670500
H	-5.51175500	-4.19202800	-0.75674700
H	-4.94738600	-5.43499500	0.37169200
C	-0.42250800	-3.72469800	1.67782200
H	-0.47021100	-2.73916100	2.15415200
H	0.62562700	-3.93657400	1.44639300
H	-0.76752300	-4.46057800	2.40534000

M5SR

C	-4.94916600	1.25173500	-0.61187400
C	-3.65479500	1.04673600	-0.13675200
C	-3.39323800	0.62907000	1.16121900
C	-4.49146800	0.36558200	1.98180100
C	-5.79523600	0.52849000	1.50965500
C	-6.03595900	0.98119500	0.21151400
C	-4.91935900	1.79581100	-2.02046900
C	-3.46929800	2.28613400	-2.20052600
C	-2.65151600	1.39350900	-1.21523500
H	-2.36526100	0.51870600	1.52106800
H	-4.32987700	0.03414100	3.00346800
H	-6.63363300	0.31787000	2.16636200
H	-7.05121600	1.13548000	-0.14111300
H	-5.62151400	2.61554200	-2.19169000
H	-3.11200500	2.17115600	-3.22466100
H	-5.13805000	1.00953800	-2.75176600
H	-2.24660000	0.50857500	-1.71330400

N	-1.52973300	2.15890600	-0.67595100
O	-3.33165100	3.68025100	-1.92405100
C	-0.26924600	1.82516400	-0.38766000
C	-1.71089300	3.44636100	-0.25805900
N	0.27428500	2.89936500	0.17407000
N	-0.61451100	3.93157100	0.25418800
C	-3.03143300	4.06528000	-0.59225600
H	-3.79911500	3.74200100	0.12079100
H	-2.95312000	5.15187900	-0.57391700
C	1.64377900	3.06705300	0.59328600
C	2.64603700	3.12813300	-0.37718800
C	1.89088100	3.14193500	1.97044100
C	3.95507900	3.29564400	0.07834400
C	3.21688700	3.29462000	2.36458300
C	4.25889300	3.37298700	1.43526600
H	4.75478400	3.35430400	-0.65553300
H	3.44267800	3.34708000	3.42654000
C	0.77411200	2.98926700	2.96487600
H	0.30453500	2.00469900	2.82391800
H	0.01121800	3.76066600	2.82663600
H	1.16337300	3.06693400	3.98141000
C	5.68777100	3.49700800	1.89506700
H	6.11464300	2.50540100	2.08010100
H	5.75657300	4.06424700	2.82586700
H	6.30499100	3.98824700	1.13973900
C	2.38171300	2.97200900	-1.85205400
H	2.51519900	1.92460300	-2.15196900
H	3.09566600	3.56757100	-2.42401300
H	1.37362000	3.28333300	-2.13648600
C	0.42488000	0.55885800	-0.85123600

O	0.25355200	0.26984500	-2.01899400
C	1.15979000	-0.19121100	0.17141800
C	2.02239100	-1.33674700	-0.32973600
H	1.74317600	0.50819800	0.78285900
H	1.42227000	-1.95672300	-1.00380600
C	3.24609300	-0.86536100	-1.08019700
C	3.40340300	-1.15721700	-2.43751600
C	4.21525600	-0.07529600	-0.45086500
C	4.50062700	-0.67777000	-3.15011700
H	2.65080900	-1.75966700	-2.93912500
C	5.31336100	0.40412200	-1.15874600
H	4.10712500	0.18059800	0.60197300
C	5.45974500	0.10513900	-2.51247100
H	4.60466100	-0.91505100	-4.20430200
H	6.05465800	1.01548000	-0.65178900
H	6.31583300	0.47915500	-3.06498800
H	0.67451200	-2.63895700	2.39308700
C	-2.92084600	-2.71214500	0.81691200
C	-2.55094400	-2.74093700	-0.55172900
C	-3.40342400	-3.37248300	-1.47077900
C	-4.58661800	-3.93428300	-1.01621200
C	-4.94163000	-3.87835800	0.34548800
C	-4.11634800	-3.26956500	1.27873100
C	-0.95194700	-1.62981200	0.61014700
C	-1.29473700	-2.04505300	-0.65636900
H	-3.13994300	-3.41558800	-2.52387100
H	-5.25477500	-4.42253400	-1.71877800
H	-5.87821300	-4.32040400	0.67076800
H	-4.38662400	-3.22344400	2.32917300
H	-0.72627600	-1.89101600	-1.56167800

N	-1.91703500	-2.06454900	1.49205700
H	-1.95675100	-1.67692100	2.42501100
C	0.15661500	-0.80042500	1.27015700
O	-0.38933400	0.12098800	2.06806100
C	1.18150100	-1.76880900	1.96566600
C	2.30361700	-2.15845900	0.97109600
H	1.59595100	-1.18536800	2.79336300
H	3.26129200	-1.81132500	1.37356300
C	2.45400100	-3.63153000	0.66489600
C	3.72639000	-4.19488800	0.54116000
C	1.33822100	-4.44737100	0.44351900
C	3.88649600	-5.54026900	0.21426000
H	4.60065000	-3.56925500	0.70527200
C	1.49452800	-5.79146000	0.11787400
H	0.33919200	-4.02320700	0.52195000
C	2.76969300	-6.34389200	0.00375100
H	4.88402500	-5.95981000	0.12637900
H	0.61763300	-6.40992500	-0.04826800
H	2.89036200	-7.39292500	-0.24741100

M5SS

C	-2.36143300	-0.33041500	3.78135400
C	-1.83976700	-0.76190800	2.56518200
C	-2.04337100	-2.05795700	2.09961100
C	-2.79126400	-2.93161400	2.88410900
C	-3.31779700	-2.50669600	4.10745700
C	-3.10915500	-1.20751000	4.56356800
C	-2.02013300	1.11172300	4.05172100
C	-1.03093600	1.52145900	2.93477200
C	-1.07473300	0.34719900	1.88195900

H	-1.64246800	-2.38526400	1.14258000
H	-2.96679700	-3.94598400	2.54223300
H	-3.89670700	-3.19935500	4.70956700
H	-3.51968800	-0.88365000	5.51487200
H	-1.56424900	1.27000200	5.03415300
H	-1.33528900	2.45131900	2.45265200
H	-2.91500100	1.73953800	4.01028100
H	-1.56934400	0.68796200	0.97244200
N	0.28994400	-0.10062300	1.54353100
O	0.27344100	1.78510000	3.41592200
C	0.79518800	-0.75520300	0.47817400
C	1.25361400	-0.12346800	2.51292600
N	2.00328000	-1.17017600	0.85245400
N	2.31339300	-0.76412700	2.11211400
C	0.99401200	0.62462600	3.77986200
H	0.44104800	0.00190700	4.49607300
H	1.93726600	0.93466800	4.22869700
C	2.94184800	-2.01911900	0.15331800
C	2.85429900	-3.39274000	0.39603200
C	3.90438500	-1.43110600	-0.66017100
C	3.81382200	-4.20057200	-0.20282000
C	4.84491500	-2.28829700	-1.23685600
C	4.81794500	-3.66358000	-1.01632500
H	3.77815900	-5.27388700	-0.03414500
H	5.61247400	-1.86331000	-1.87828800
C	3.86202200	0.03485800	-0.97175900
H	3.62836800	0.64198600	-0.09015900
H	3.07257800	0.20718200	-1.71941300
H	4.81618900	0.37434800	-1.38054900
C	5.83335300	-4.57098000	-1.66068700

H	6.23539800	-5.28542700	-0.93765300
H	6.66317100	-4.00083500	-2.08256700
H	5.37397400	-5.14719700	-2.46984100
C	1.74230600	-3.95831100	1.23650200
H	0.77910700	-3.79109400	0.74150400
H	1.69875200	-3.48652600	2.22315600
H	1.87204500	-5.03235200	1.37488300
C	0.21490500	-0.98078100	-0.91261000
O	0.50009200	-2.02875500	-1.45360000
C	-0.53544400	0.12627600	-1.50821400
C	-1.49857100	-0.26961800	-2.61639800
H	-1.02659800	0.73014500	-0.74732500
H	-0.87634000	-0.71680100	-3.40009200
C	-2.59770300	-1.23814100	-2.25892000
C	-2.99832300	-2.20035000	-3.18993000
C	-3.25674500	-1.19981200	-1.02576700
C	-4.02451200	-3.09695100	-2.90134000
H	-2.49272700	-2.24727400	-4.15136600
C	-4.27406600	-2.10117700	-0.72500300
H	-2.98793600	-0.44292200	-0.29176000
C	-4.66323100	-3.05365800	-1.66426000
H	-4.31808700	-3.83652200	-3.63996800
H	-4.76054600	-2.05633900	0.24499600
H	-5.45669200	-3.75735600	-1.43356400
H	-0.74663600	2.95057100	-2.91508200
C	2.89776300	3.40080400	-0.79830600
C	2.00875500	3.38204300	0.30860400
C	2.35388300	4.09065100	1.47096300
C	3.55272700	4.78536000	1.50160100
C	4.42218300	4.78823500	0.39279400

C	4.10917100	4.09852700	-0.76854600
C	1.14646700	2.09681900	-1.34820000
C	0.89949700	2.55113400	-0.07168700
H	1.69285800	4.07976500	2.33291400
H	3.83198100	5.33635000	2.39424700
H	5.35552300	5.33939900	0.44951200
H	4.77690100	4.09721600	-1.62425300
H	0.02710000	2.34750700	0.53173800
N	2.32768300	2.63616000	-1.78490300
H	2.74118100	2.28295300	-2.63870800
C	0.47381900	1.14890200	-2.34450400
O	1.35954600	0.50946300	-3.08003800
C	-0.62064400	1.90541600	-3.21286300
C	-1.94950800	1.12712100	-3.15448000
H	-0.21417300	1.88990500	-4.22606100
H	-2.37840900	0.99493800	-4.15318000
C	-3.01931400	1.74098400	-2.27228800
C	-4.36179000	1.42482300	-2.50999500
C	-2.72313300	2.55961900	-1.17537000
C	-5.37281700	1.88873900	-1.67465800
H	-4.61182800	0.79001600	-3.35679600
C	-3.73165500	3.01816200	-0.32753200
H	-1.69530100	2.85900600	-0.98236900
C	-5.06032300	2.68154900	-0.57165700
H	-6.40603600	1.62847100	-1.88287700
H	-3.47494200	3.64952300	0.51817100
H	-5.84608500	3.04193200	0.08451700

TS6RR

C	-3.84717900	-2.92095500	-0.64189000
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C	-3.05016300	-2.03420900	-1.37554800
C	-2.26127100	-2.45755100	-2.43665200
C	-2.25711600	-3.81794500	-2.74316700
C	-3.02966900	-4.71492300	-2.00297500
C	-3.83639700	-4.27558400	-0.95152600
C	-4.66589600	-2.17597500	0.38680000
C	-4.63488700	-0.74397400	-0.19269500
C	-3.24728300	-0.63198400	-0.86494800
H	-1.65933500	-1.73460800	-2.98075900
H	-1.64945500	-4.18317600	-3.56450100
H	-3.01389500	-5.76995400	-2.25807600
H	-4.45286200	-4.97699700	-0.39772700
H	-4.19188000	-2.21578700	1.37693600
H	-5.37005000	-0.67773700	-0.99840800
H	-5.68402100	-2.55494500	0.49424900
H	-3.17852800	0.14894000	-1.61294300
N	-2.27821800	-0.32224400	0.23025300
O	-4.93843900	0.31984500	0.67324600
C	-0.96841200	-0.59693100	0.32972700
C	-2.67856200	0.07279700	1.48305700
N	-0.64047500	-0.42127500	1.60511800
N	-1.70193000	-0.00473200	2.34507400
C	-4.08745200	0.48164300	1.78436600
H	-4.43734900	-0.09367200	2.65047800
H	-4.09396200	1.54817600	2.03567100
C	0.56852100	-0.92959300	2.20949200
C	0.69526000	-2.32922800	2.24752900
C	1.52382500	-0.06186200	2.73650000
C	1.87248700	-2.84511800	2.77540600
C	2.68264700	-0.63753600	3.26450800

C	2.88281300	-2.01523200	3.27253600
H	2.00229900	-3.92363500	2.81229800
H	3.44682900	0.01902000	3.67329100
C	1.35410100	1.43221200	2.73794100
H	0.30474900	1.72189200	2.66947100
H	1.89401400	1.88281100	1.89484400
H	1.77492100	1.85376100	3.65328900
C	4.15097600	-2.61759500	3.81613600
H	4.83156300	-1.84762000	4.18468700
H	4.66582300	-3.18724600	3.03619400
H	3.93414200	-3.30780900	4.63626100
C	-0.41432300	-3.23911700	1.78192800
H	-0.49841300	-3.25515200	0.69052400
H	-1.37882600	-2.92095200	2.19236800
H	-0.22453000	-4.25870700	2.11960300
C	0.10842400	-0.90613000	-0.71840400
O	0.27376100	-2.02767800	-1.11954700
C	0.92576700	0.29597600	-1.07626200
C	2.07233100	-0.01967400	-2.02767100
H	1.28167000	0.77200100	-0.15045900
H	1.63103900	-0.57315600	-2.86603100
C	3.20618200	-0.83803500	-1.46238300
C	3.85253100	-1.77268000	-2.27553600
C	3.66018900	-0.67450000	-0.14985400
C	4.92425800	-2.52255500	-1.79740000
H	3.50567600	-1.91394600	-3.29636900
C	4.72784500	-1.42487200	0.33482700
H	3.19314700	0.05773900	0.50431500
C	5.36521900	-2.35191800	-0.48685700
H	5.41039700	-3.24389900	-2.44691800

H	5.06467800	-1.27582600	1.35699300
H	6.19826600	-2.93669400	-0.10936900
H	1.04125800	3.10544200	-2.66391600
C	-2.85604100	2.89134600	-0.51073400
C	-2.01912400	3.29827200	0.57451900
C	-2.59528700	3.97471700	1.66494900
C	-3.95969000	4.22039300	1.66035300
C	-4.77241200	3.80591500	0.58311200
C	-4.23392800	3.14480700	-0.50878600
C	-0.79782100	2.20320500	-0.95764700
C	-0.69281300	2.84261300	0.26129100
H	-1.97922900	4.29641600	2.50037500
H	-4.41560100	4.73985300	2.49776500
H	-5.83879000	4.00646600	0.61387300
H	-4.85807900	2.81817000	-1.33499700
H	0.19122400	2.97434200	0.86556000
N	-2.06834100	2.26004300	-1.43416800
H	-1.97384600	1.45202600	-2.24408500
C	0.01377700	1.28155600	-1.87746700
O	-0.93182600	0.56898900	-2.60165800
C	1.03778500	2.02201400	-2.80773900
C	2.43086600	1.39833800	-2.58191800
H	0.69717700	1.81735000	-3.82519100
H	2.96838700	1.27688700	-3.52808700
C	3.33014800	2.16335200	-1.63276300
C	4.71442700	1.96472900	-1.68964600
C	2.82833300	3.02300200	-0.65129100
C	5.56907000	2.58823100	-0.78668600
H	5.12133200	1.29593500	-2.44448300
C	3.67999400	3.64534500	0.26191500

H	1.76194400	3.22541900	-0.60307100
C	5.05310100	3.42668400	0.20047100
H	6.63918600	2.41734600	-0.85110300
H	3.26533500	4.30868100	1.01552900
H	5.71747400	3.91223600	0.90813700

TS6RS

C	4.92354700	-0.49692600	2.17633600
C	3.54232900	-0.58297900	2.01538500
C	2.74292800	-1.23419600	2.95108500
C	3.35582100	-1.80722900	4.06236000
C	4.74007200	-1.72146000	4.23172900
C	5.53190500	-1.06466600	3.29313800
C	5.56383700	0.25642900	1.04058500
C	4.45071300	0.43506600	-0.01507300
C	3.10619900	0.10203400	0.73703900
H	1.66652700	-1.28313800	2.82086100
H	2.75360700	-2.32190200	4.80368200
H	5.20263900	-2.17364600	5.10314300
H	6.60777900	-1.00188300	3.42550400
H	6.41915700	-0.26672700	0.60176500
H	4.41284900	1.45253200	-0.39781800
H	5.92016900	1.23684400	1.37341400
H	2.51632600	1.00711800	0.90566500
N	2.28312100	-0.80324800	-0.08193600
O	4.66604200	-0.36524800	-1.17017100
C	0.95503100	-0.94256400	-0.19621400
C	2.85166300	-1.77038300	-0.85686600
N	0.76370300	-1.98773700	-1.00106900
N	1.94387200	-2.51395700	-1.42483600

C	4.33630300	-1.73080800	-1.01520900
H	4.83311900	-2.18624200	-0.14758900
H	4.63304700	-2.26231200	-1.91892300
C	-0.47319700	-2.63681400	-1.36149000
C	-0.81932600	-2.66548400	-2.71784600
C	-1.24786700	-3.21753400	-0.35229800
C	-2.01204000	-3.30362000	-3.04904000
C	-2.42766100	-3.84747200	-0.74772200
C	-2.82539800	-3.89950500	-2.08278700
H	-2.31586900	-3.32867300	-4.09223400
H	-3.05267200	-4.30163400	0.01670800
C	-0.88149800	-3.15430100	1.10776700
H	-1.23987300	-2.22191200	1.56266300
H	0.19810700	-3.22715500	1.27035100
H	-1.36086000	-3.97423200	1.64520500
C	-4.09712200	-4.60486100	-2.47413000
H	-4.49858200	-4.20538400	-3.40769000
H	-4.85798400	-4.50453000	-1.69645100
H	-3.91312000	-5.67398800	-2.62106700
C	0.03728100	-2.00409200	-3.76103300
H	0.23476200	-0.97153200	-3.45700800
H	-0.48448700	-1.99216900	-4.71920100
H	0.98627200	-2.53132100	-3.88743800
C	-0.06821800	-0.09229600	0.53325100
O	0.21342300	0.23504500	1.66800300
C	-1.25623600	0.32181800	-0.23528900
C	-2.38831300	0.89942800	0.60621700
H	-1.62160600	-0.50726300	-0.84761600
H	-1.96167500	1.61617600	1.32092600
C	-3.14326900	-0.15693400	1.37519700

C	-3.04953900	-0.21708800	2.76804100
C	-3.89546700	-1.13257000	0.71179100
C	-3.68948900	-1.22648600	3.48471500
H	-2.46028300	0.53159700	3.29069400
C	-4.53984200	-2.13930400	1.42533000
H	-3.97009000	-1.11698500	-0.37357700
C	-4.43747200	-2.19126900	2.81465000
H	-3.60342700	-1.25785300	4.56635200
H	-5.12135200	-2.88699200	0.89366100
H	-4.93896800	-2.97781400	3.36934100
H	-1.74680300	3.29886900	-0.61594300
C	2.48808800	2.50642700	-1.88080600
C	2.37548500	3.20360100	-0.63416900
C	3.47757800	3.94643300	-0.17014200
C	4.63146800	3.99520600	-0.93698000
C	4.71989400	3.31122700	-2.16876900
C	3.65817000	2.56293300	-2.65118800
C	0.46877100	2.11381600	-1.06932000
C	1.05847000	2.93231900	-0.12755700
H	3.42259400	4.47792600	0.77609600
H	5.48474800	4.56886100	-0.58801200
H	5.63853500	3.36868600	-2.74423700
H	3.72664200	2.02676600	-3.59252300
H	0.61933300	3.30318300	0.78889600
N	1.31239300	1.84588600	-2.09724500
H	0.59205300	1.26692400	-2.77217900
C	-0.87511300	1.42771200	-1.35756600
O	-0.75370500	0.84163800	-2.57698000
C	-2.06443900	2.42886100	-1.20196700
C	-3.18258000	1.69136000	-0.45480200

H	-2.36164100	2.77326100	-2.19472500
H	-3.63578200	0.96837900	-1.14599800
C	-4.28037300	2.55095700	0.12126900
C	-5.61890500	2.27333800	-0.16480600
C	-3.99003200	3.62072200	0.97550800
C	-6.64366800	3.04631000	0.37720600
H	-5.85827900	1.43989000	-0.82053500
C	-5.00965500	4.39524300	1.51965000
H	-2.95553400	3.85310100	1.21740900
C	-6.34181700	4.11157400	1.22078600
H	-7.67751500	2.81482300	0.14006100
H	-4.76465900	5.22346800	2.17734200
H	-7.13699700	4.71695900	1.64401300

TS6SR

C	-5.23764000	-0.32814500	0.16379000
C	-3.93957900	-0.46683300	-0.32467000
C	-3.67270000	-0.56002600	-1.68407200
C	-4.74649700	-0.46602700	-2.56913800
C	-6.04760400	-0.29030000	-2.09151700
C	-6.30467000	-0.22730200	-0.72135500
C	-5.23185900	-0.33439600	1.67264900
C	-3.88268900	-0.98693000	2.01611100
C	-2.96655500	-0.55131100	0.83660200
H	-2.65394200	-0.69721500	-2.04025700
H	-4.56985300	-0.53372200	-3.63744700
H	-6.87071900	-0.22071500	-2.79548600
H	-7.32028100	-0.11820200	-0.35352700
H	-6.05904700	-0.88781300	2.12267200
H	-3.48242900	-0.65939100	2.97662100

H	-5.25244500	0.69267400	2.05843900
H	-2.46333700	0.40089000	1.03968300
N	-1.95778700	-1.58139100	0.60583000
O	-3.98423800	-2.40945000	2.12090800
C	-0.64931600	-1.53710700	0.33947200
C	-2.34582900	-2.88943700	0.51711900
N	-0.29462700	-2.78896400	0.06855000
N	-1.34282200	-3.65458900	0.18775700
C	-3.74307900	-3.19513000	0.96320700
H	-4.46249500	-2.99912000	0.16078100
H	-3.81144900	-4.24101800	1.26238200
C	1.02742400	-3.26649100	-0.24974800
C	1.85763500	-3.65670800	0.80035500
C	1.38686900	-3.33078600	-1.60053300
C	3.12067300	-4.13949600	0.45714700
C	2.66587300	-3.80237500	-1.88422100
C	3.54065700	-4.21124400	-0.87089200
H	3.79451700	-4.45195200	1.25049600
H	2.98598800	-3.85961700	-2.92151200
C	0.42679400	-2.89783000	-2.67574000
H	0.15684100	-1.83699900	-2.57409000
H	-0.49955800	-3.47911600	-2.61941200
H	0.86814300	-3.05318300	-3.66121200
C	4.92181400	-4.70061700	-1.21966500
H	5.45306200	-5.05408800	-0.33371700
H	5.50974000	-3.89665400	-1.67388300
H	4.87515900	-5.51835100	-1.94398400
C	1.41384500	-3.53788500	2.23364600
H	1.33311600	-2.48656700	2.53143200
H	2.13378500	-4.01825400	2.89695100

H	0.43610300	-4.00328400	2.38799300
C	0.30020900	-0.39420900	0.68165400
O	0.21522600	-0.00258300	1.82338800
C	1.16248800	0.15142700	-0.38414800
C	2.28617000	1.05751800	0.09121600
H	1.52141300	-0.65598000	-1.03243300
H	1.85141600	1.78872400	0.78223300
C	3.44854900	0.38972800	0.78378700
C	4.08167700	1.02906500	1.85397300
C	3.95696800	-0.83574500	0.34151600
C	5.19372900	0.46023700	2.46948000
H	3.69719800	1.98479200	2.20135700
C	5.06815700	-1.40741900	0.95599200
H	3.48703300	-1.35850200	-0.48982800
C	5.69092900	-0.76172300	2.02174500
H	5.67116000	0.97089400	3.29985500
H	5.44489500	-2.36248800	0.60047300
H	6.55625000	-1.20845200	2.50074600
H	1.08967000	2.86898900	-2.30698500
C	-2.75335900	2.62181600	-0.32305200
C	-2.00929300	3.25289800	0.72172700
C	-2.69230200	4.07068900	1.64223000
C	-4.06239600	4.22728200	1.51874500
C	-4.78320400	3.58516700	0.48730000
C	-4.14171800	2.78392900	-0.44225200
C	-0.64136400	1.99268900	-0.53398800
C	-0.64409600	2.83505300	0.56390100
H	-2.15209200	4.56748700	2.44372100
H	-4.59751700	4.85265400	2.22713200
H	-5.85826200	3.72487700	0.42219400

H	-4.68787000	2.27917300	-1.23497900
H	0.18673200	3.10885200	1.19859500
N	-1.88594300	1.87397600	-1.06445900
H	-1.64383900	1.04770700	-1.85739500
C	0.28873100	1.06224200	-1.34160900
O	-0.53263400	0.32996000	-2.15964600
C	1.41214300	1.84958600	-2.08102700
C	2.69697300	1.80470000	-1.21690500
H	1.57384500	1.33373600	-3.03088800
H	3.43668200	1.16981600	-1.71876500
C	3.35714600	3.12737700	-0.90900100
C	4.74869300	3.24461400	-0.93087700
C	2.59790500	4.24068000	-0.53108000
C	5.37088200	4.44531400	-0.59383700
H	5.34896900	2.38318700	-1.21332200
C	3.21565400	5.44111300	-0.19354400
H	1.51301000	4.16250300	-0.49940600
C	4.60546600	5.54851900	-0.22583400
H	6.45373700	4.51814300	-0.62083200
H	2.61102600	6.29599500	0.09324400
H	5.08725300	6.48591800	0.03345400

TS6SS

C	-0.08582000	-0.25930200	-1.24623100
O	-0.23672800	-0.84659000	-2.29599600
C	0.95146100	-0.53132700	-0.22631200
C	2.24857800	-1.18279900	-0.74902000
H	1.17115900	0.37133900	0.35040500
H	2.06071400	-1.59043400	-1.74682400
C	3.38057600	-0.18366000	-0.85493900

C	3.95949200	0.10470800	-2.09228400
C	3.90017600	0.44618100	0.28253000
C	5.03002900	0.99292000	-2.19753100
H	3.57484400	-0.38423700	-2.98475000
C	4.97911500	1.31710700	0.18700700
H	3.46677300	0.23982300	1.25857600
C	5.54897600	1.59566600	-1.05542200
H	5.46551400	1.19951000	-3.17041400
H	5.37829600	1.78098900	1.08415500
H	6.39267600	2.27514000	-1.12921400
H	2.05068100	-1.29100100	2.09589200
C	-2.83418900	-0.69010500	2.13922300
C	-2.13588800	0.32385700	2.87266000
C	-2.87359300	1.21458700	3.67516000
C	-4.25237600	1.09386400	3.73273900
C	-4.92390300	0.08295000	3.01433100
C	-4.22790700	-0.81900900	2.22417500
C	-0.68327900	-0.89465400	1.69161700
C	-0.74152200	0.16759000	2.56663000
H	-2.36511200	1.99042600	4.24247700
H	-4.82795000	1.78043600	4.34624700
H	-6.00416100	0.00205400	3.09167900
H	-4.73888500	-1.61296500	1.68920100
H	0.08501900	0.76241800	2.93271500
N	-1.91134500	-1.41071100	1.43446100
H	-1.59269300	-2.24438800	0.69051700
C	0.32411300	-1.60826000	0.80189200
O	-0.34108000	-2.60229800	0.16091700
C	1.62866400	-2.08083700	1.46019100
C	2.51210400	-2.38018600	0.24832900

H	1.43937900	-2.96301500	2.07861400
H	2.05679700	-3.25428600	-0.22994800
C	3.96605500	-2.70119200	0.50413300
C	4.79560700	-3.01690000	-0.57971500
C	4.52195100	-2.70783300	1.78399100
C	6.13892100	-3.31840900	-0.39357300
H	4.37684500	-3.01616900	-1.58382700
C	5.86992100	-3.01366700	1.97718100
H	3.90170000	-2.47331500	2.64390000
C	6.68356400	-3.31675800	0.89110200
H	6.76282900	-3.55741900	-1.24933800
H	6.28145500	-3.01324700	2.98198800
H	7.73234700	-3.55216700	1.04157800
C	-4.68029500	-1.77888100	-1.02117800
C	-3.38676500	-1.64870000	-1.54124600
C	-2.54423600	-2.75253900	-1.62948900
C	-2.99578800	-3.97569100	-1.13483600
C	-4.27438100	-4.10045300	-0.59351900
C	-5.13364900	-3.00341300	-0.54710600
C	-5.43323600	-0.48183900	-1.11217500
C	-4.66347200	0.22815200	-2.24000700
C	-3.18714700	-0.25750500	-2.10239700
H	-1.54532800	-2.66902100	-2.03394500
H	-2.33929600	-4.83834600	-1.17427300
H	-4.61063500	-5.06282900	-0.22078000
H	-6.14084500	-3.10308600	-0.15327200
H	-5.36195300	0.05494200	-0.15799700
H	-5.01223200	-0.16524200	-3.19766500
H	-6.49088600	-0.60011800	-1.35600000
H	-2.65458400	-0.25470900	-3.05413200

N	-2.44348400	0.73921500	-1.25118200
O	-4.83105300	1.62398600	-2.32989000
C	-1.12961500	0.80491800	-0.94425900
C	-2.96373300	1.96786200	-0.93311500
N	-0.91064600	2.03861300	-0.48764000
N	-2.04850000	2.77427600	-0.47771500
C	-4.39388800	2.31406700	-1.18235500
H	-4.99935800	2.08194200	-0.29818900
H	-4.46765700	3.38289800	-1.38401500
C	0.34736800	2.69040100	-0.21908400
C	0.52344300	3.31387700	1.02419200
C	1.30705900	2.73848000	-1.23965600
C	1.76058600	3.90727300	1.26309400
C	2.51996400	3.35806400	-0.94238500
C	2.77339900	3.92665700	0.30290900
H	1.92891600	4.38097800	2.22736200
H	3.28866400	3.38764600	-1.71027800
C	1.08155700	2.20148000	-2.63098400
H	1.45158200	1.17745000	-2.73475200
H	1.63582200	2.81449600	-3.34415000
H	0.02801300	2.21781300	-2.92299700
C	4.09226600	4.58896200	0.59982100
H	4.82434100	4.37552400	-0.18151300
H	4.49556500	4.23984000	1.55445200
H	3.97122500	5.67434000	0.67237800
C	-0.57393500	3.43032900	2.04808700
H	-1.13142200	4.35780500	1.88277000
H	-0.14678500	3.46783800	3.05315100
H	-1.28062300	2.60360500	2.00141800

M6RR

C	-3.92104500	-2.85572500	-0.61687800
C	-3.10122700	-1.99680100	-1.36069500
C	-2.33809900	-2.46067500	-2.42452800
C	-2.37837600	-3.82311500	-2.71903000
C	-3.17207600	-4.68904800	-1.96546800
C	-3.95610900	-4.21251800	-0.91371200
C	-4.71291200	-2.08162500	0.40919700
C	-4.64393600	-0.65514400	-0.17968500
C	-3.25156700	-0.58501400	-0.85111600
H	-1.71759500	-1.77585400	-2.99456300
H	-1.78962900	-4.21285600	-3.54280700
H	-3.19127900	-5.74627100	-2.21062600
H	-4.59183000	-4.88698500	-0.34832500
H	-4.23410900	-2.12781300	1.39682600
H	-5.37638300	-0.57312800	-0.98636200
H	-5.74051200	-2.43176200	0.52420900
H	-3.15195500	0.22572700	-1.57164300
N	-2.28211200	-0.31453200	0.25532500
O	-4.91883900	0.41680400	0.68315100
C	-0.97466700	-0.59534000	0.35108700
C	-2.67039100	0.10582700	1.50220000
N	-0.63723700	-0.41227900	1.62214400
N	-1.69062700	0.02394700	2.36144100
C	-4.06835900	0.55291200	1.79836500
H	-4.43969100	-0.01302500	2.66204200
H	-4.04249200	1.61961100	2.04833900
C	0.57344900	-0.91709200	2.22336100
C	0.70711200	-2.31651500	2.25625000
C	1.52165100	-0.04642100	2.75965600

C	1.88523300	-2.82862200	2.78574000
C	2.68057200	-0.61923500	3.29056300
C	2.88773500	-1.99600100	3.29360600
H	2.02043100	-3.90661900	2.81847600
H	3.43909600	0.03901800	3.70702500
C	1.34785700	1.44779300	2.76985500
H	0.29965000	1.73895000	2.69077100
H	1.89911500	1.90481200	1.93777600
H	1.75772200	1.86261300	3.69319800
C	4.15344900	-2.59484700	3.84690400
H	4.84688600	-1.82094700	4.18188000
H	4.65373100	-3.20050800	3.08492800
H	3.93442700	-3.25062700	4.69443900
C	-0.39801300	-3.23166800	1.78909900
H	-0.47144200	-3.26312900	0.69741200
H	-1.36731600	-2.90872400	2.18439000
H	-0.21184100	-4.24667800	2.14222400
C	0.07964600	-0.90242100	-0.71860100
O	0.23640200	-2.02102900	-1.13068100
C	0.88150300	0.30057400	-1.12642600
C	2.04399600	-0.02373200	-2.05757100
H	1.22402700	0.81702500	-0.21805500
H	1.62035600	-0.57177500	-2.90806300
C	3.15762000	-0.85378300	-1.46943000
C	3.80586400	-1.79754200	-2.26996600
C	3.59291300	-0.68781400	-0.15101900
C	4.86476300	-2.55385700	-1.77386200
H	3.47245500	-1.93993000	-3.29505900
C	4.64957800	-1.44282400	0.34983700
H	3.12454200	0.05226800	0.49369000

C	5.29035400	-2.37869200	-0.45907000
H	5.35374900	-3.28212000	-2.41330800
H	4.97696700	-1.28889500	1.37403500
H	6.11482500	-2.96648200	-0.06781600
H	1.07781400	3.13654500	-2.50207400
C	-2.84851500	2.92414200	-0.52006500
C	-1.95791700	3.21780100	0.56610300
C	-2.44530800	3.88231700	1.70942700
C	-3.78321600	4.23549600	1.76364600
C	-4.65923900	3.93860500	0.69234800
C	-4.20435700	3.29148800	-0.44294200
C	-0.92708300	2.11413200	-1.08175700
C	-0.70024700	2.67808000	0.17313900
H	-1.78154200	4.11233500	2.53993400
H	-4.17094400	4.74690000	2.64020000
H	-5.70499100	4.22208300	0.76802300
H	-4.87864400	3.05342900	-1.26174700
H	0.22189000	2.70106100	0.73300400
N	-2.19925600	2.26034000	-1.52494300
H	-1.62854100	0.99376200	-2.88572200
C	0.00432100	1.28808300	-1.94281700
O	-0.79667700	0.48519600	-2.80898400
C	1.05462500	2.08098500	-2.77969200
C	2.43040800	1.39770600	-2.59067600
H	0.73766100	2.01877500	-3.82296700
H	2.94354300	1.27809300	-3.54959100
C	3.37455800	2.11749700	-1.64828000
C	4.75159600	1.89558400	-1.76248400
C	2.92425900	2.94948500	-0.61951600
C	5.65007100	2.47237100	-0.87102500

H	5.11799600	1.24580600	-2.55373800
C	3.82059600	3.52551400	0.28164200
H	1.86428700	3.16683700	-0.51935600
C	5.18609900	3.28623000	0.16126900
H	6.71361500	2.28470700	-0.98072800
H	3.44583100	4.16863800	1.07250100
H	5.88465200	3.73573200	0.85966500

M6RS

C	4.74287000	1.52363500	2.10767900
C	3.38380300	1.25650900	1.95415200
C	2.47631600	1.50080600	2.98038800
C	2.95593100	2.02886300	4.17714500
C	4.31565200	2.30720900	4.33467000
C	5.21758100	2.05813500	3.30213400
C	5.51104200	1.16087800	0.86280400
C	4.53612000	0.30840900	0.02311300
C	3.11213500	0.67227900	0.58256700
H	1.42035100	1.28641900	2.84828100
H	2.26781800	2.22396500	4.99303200
H	4.67427000	2.71530400	5.27422900
H	6.27539100	2.26626100	3.43140300
H	6.42597800	0.59682200	1.06419000
H	4.58490000	0.53920900	-1.04057500
H	5.79555100	2.06049400	0.30659000
H	2.60054300	1.36441100	-0.09342200
N	2.28196100	-0.53169600	0.67999900
O	4.85091100	-1.07841000	0.09614100
C	0.97424000	-0.72895900	0.47492500
C	2.81922900	-1.73960000	1.01391400

N	0.75501200	-2.01761400	0.72051800
N	1.90683500	-2.67030600	1.04613900
C	4.30187400	-1.79333400	1.18295000
H	4.58915800	-1.36770200	2.15427600
H	4.65325500	-2.82304000	1.12387600
C	-0.49700700	-2.72743200	0.70054300
C	-0.69598300	-3.65196600	-0.33178000
C	-1.44029900	-2.45869500	1.69342800
C	-1.90450500	-4.34097500	-0.33278200
C	-2.63451500	-3.17921200	1.64242100
C	-2.87740700	-4.12509100	0.64853900
H	-2.09300900	-5.06390700	-1.12262900
H	-3.39531800	-2.98588300	2.39350900
C	-1.20729100	-1.42102400	2.76110900
H	-1.45953000	-0.41679400	2.39761500
H	-0.16808200	-1.40747100	3.10227700
H	-1.84897900	-1.61629800	3.62186600
C	-4.15750600	-4.91760000	0.63179700
H	-4.59925000	-4.92467400	-0.36847600
H	-4.88793800	-4.50021100	1.32742900
H	-3.96724200	-5.95802200	0.91398700
C	0.34304400	-3.85362400	-1.40211100
H	1.24249900	-4.32223100	-0.99095100
H	0.63597900	-2.88858200	-1.83473200
H	-0.04887300	-4.49667700	-2.19172600
C	-0.02515000	0.37220500	0.22292600
O	0.22878800	1.44496800	0.73148600
C	-1.21220700	0.12111400	-0.65328500
C	-2.47727500	0.84380900	-0.12383600
H	-1.35947100	-0.94877500	-0.80072600

H	-2.19417600	1.41762300	0.76595300
C	-3.61432700	-0.07901200	0.23953400
C	-4.24044400	0.01732800	1.48285300
C	-4.08943800	-1.01423600	-0.68733200
C	-5.31869900	-0.80697800	1.80298700
H	-3.88380700	0.74986800	2.20326100
C	-5.16652000	-1.83478000	-0.37204300
H	-3.60629000	-1.08509500	-1.66085400
C	-5.78431900	-1.73476000	0.87534500
H	-5.79618200	-0.71827500	2.77398400
H	-5.52945900	-2.55383500	-1.10044200
H	-6.62749000	-2.37400800	1.11879400
H	-0.88138700	2.77815000	-1.33481300
C	2.43843400	-0.32006300	-2.67221700
C	2.66879200	1.05669600	-3.01496900
C	3.94111200	1.45653400	-3.46790900
C	4.94779000	0.50986400	-3.57773800
C	4.71844600	-0.84108300	-3.23059900
C	3.47965900	-1.26043300	-2.77591300
C	0.55920200	0.70509800	-2.38481000
C	1.41733100	1.71058000	-2.80603700
H	4.13107200	2.49267400	-3.73803800
H	5.93050300	0.80783200	-3.93184200
H	5.53083500	-1.55687600	-3.31533900
H	3.30394700	-2.29825800	-2.50091100
H	1.17539400	2.75219200	-2.97121500
N	1.14332800	-0.52498500	-2.28167800
H	-1.09951500	-0.74227000	-3.23402800
C	-0.90519800	0.76364900	-2.06255300
O	-1.65032100	0.02781700	-3.02561600

C	-1.53259800	2.14488900	-1.94707800
C	-2.86072400	1.87690100	-1.22859100
H	-1.65833200	2.61060800	-2.92770100
H	-3.53265500	1.37965000	-1.93686400
C	-3.55891900	3.09122400	-0.66680500
C	-4.89585200	3.35159300	-0.97172600
C	-2.88703900	3.96417500	0.19714900
C	-5.54714600	4.46253900	-0.43772700
H	-5.43055900	2.67544400	-1.63390200
C	-3.53247100	5.07457100	0.73084900
H	-1.84905400	3.76709600	0.45776400
C	-4.86666600	5.32840000	0.41317400
H	-6.58698100	4.65002000	-0.68698000
H	-2.99468000	5.74299000	1.39613900
H	-5.37072100	6.19486200	0.82925600

M6SR

C	-4.89450700	-1.35689200	1.07544400
C	-3.65442900	-1.03383300	0.52710200
C	-3.53686900	-0.43328300	-0.71913200
C	-4.70718200	-0.15117500	-1.42165400
C	-5.95469800	-0.46612800	-0.88054300
C	-6.05933800	-1.07190000	0.37166900
C	-4.73425000	-1.99669100	2.43184700
C	-3.24695900	-2.39234700	2.49587200
C	-2.54431100	-1.42556200	1.47898100
H	-2.56478900	-0.17809200	-1.13429800
H	-4.64043600	0.33537400	-2.38894600
H	-6.85497900	-0.23692900	-1.44181400
H	-7.03130600	-1.32083400	0.78668200

H	-5.36359400	-2.87767200	2.58353800
H	-2.82391200	-2.27735000	3.49397100
H	-4.96588700	-1.28211100	3.22911100
H	-2.09555400	-0.56519700	1.98023200
N	-1.47059900	-2.14900600	0.78830400
O	-3.04808700	-3.76761100	2.17872700
C	-0.23852900	-1.79459300	0.40320300
C	-1.67846600	-3.42261900	0.34077300
N	0.25559400	-2.84506400	-0.25003100
N	-0.62993200	-3.87675300	-0.28750200
C	-2.93168900	-4.09339800	0.80402200
H	-3.79792500	-3.76507000	0.21771300
H	-2.82763500	-5.17505000	0.72490100
C	1.57064500	-2.98862300	-0.82061600
C	2.68279800	-2.96410500	0.02733800
C	1.65856900	-3.13792500	-2.21028700
C	3.93750200	-3.04983500	-0.57793700
C	2.93682100	-3.21868300	-2.75491700
C	4.08443900	-3.16333300	-1.95911500
H	4.82016200	-3.02859000	0.05602900
H	3.03895600	-3.32446000	-3.83185000
C	0.43229400	-3.22361500	-3.07765200
H	-0.31414600	-2.48975300	-2.76732600
H	-0.01642000	-4.21906200	-3.01116300
H	0.69558800	-3.03292900	-4.11908400
C	5.45361400	-3.20592800	-2.58406200
H	5.76903900	-2.19922200	-2.87708100
H	5.45918100	-3.82737400	-3.48207400
H	6.19499500	-3.59654800	-1.88406000
C	2.58251500	-2.82459500	1.52513400

H	2.66947200	-1.77485500	1.83310000
H	3.40655900	-3.36157200	1.99862800
H	1.64594600	-3.22504600	1.92137500
C	0.48458100	-0.54229100	0.87047100
O	0.33803100	-0.27178300	2.04032600
C	1.32031000	0.20835600	-0.11295500
C	2.11358200	1.36839100	0.49640600
H	2.00738500	-0.50850900	-0.58369300
H	1.45362400	1.91370600	1.17752500
C	3.31147500	0.87900500	1.27654900
C	3.36438700	1.02651700	2.66408500
C	4.35673400	0.20472600	0.63291900
C	4.43281200	0.51055300	3.39565800
H	2.55259600	1.53912700	3.17261900
C	5.42453900	-0.31183800	1.36009600
H	4.32977800	0.06914100	-0.44725500
C	5.46439500	-0.16208700	2.74612800
H	4.45661500	0.63295600	4.47386800
H	6.22689100	-0.83126800	0.84460900
H	6.29606800	-0.56623000	3.31429100
H	1.13440900	2.50717200	-2.52544800
C	-2.56821900	2.57352600	-1.37595500
C	-2.46456100	2.59296500	0.05385200
C	-3.48328200	3.19280800	0.81882100
C	-4.57074700	3.75481000	0.17326000
C	-4.66751000	3.73757800	-1.23764700
C	-3.68070400	3.15593900	-2.01304900
C	-0.72857400	1.55800300	-0.89250300
C	-1.24877300	1.91276400	0.35278900
H	-3.41963400	3.21318200	1.90464300

H	-5.36225700	4.22062100	0.75367600
H	-5.53167000	4.19098000	-1.71542600
H	-3.75461300	3.13893600	-3.09787100
H	-0.81103600	1.76582500	1.33038400
N	-1.50099300	1.93624300	-1.94476900
H	-0.59331700	0.14165300	-2.66983100
C	0.52361200	0.81209500	-1.28321100
O	0.15297000	-0.23552200	-2.17093000
C	1.59233000	1.73724400	-1.90117800
C	2.43288500	2.29637500	-0.73201200
H	2.22339400	1.11030100	-2.54001600
H	3.49436500	2.18285300	-0.97365500
C	2.21393500	3.75145000	-0.37005700
C	3.24231700	4.43921100	0.28331600
C	1.00581600	4.41697100	-0.60388200
C	3.07555800	5.75819100	0.69531500
H	4.18548100	3.92962000	0.46880800
C	0.83936700	5.73869300	-0.19407200
H	0.18622400	3.90401200	-1.10091200
C	1.86957100	6.41373300	0.45659700
H	3.88778200	6.27427500	1.19801200
H	-0.10463700	6.24047500	-0.38341300
H	1.73461300	7.44316400	0.77324800

M6SS

C	-0.21845800	-0.15176300	-1.27983200
O	-0.34894600	-0.57016800	-2.41103800
C	0.84972100	-0.61074200	-0.33015100
C	2.17175700	-1.00912300	-1.03566600
H	1.03724800	0.15856100	0.42329100

H	1.95297400	-1.21861100	-2.08603900
C	3.19985400	0.09907300	-0.98381300
C	3.60958200	0.73741800	-2.15561200
C	3.79246300	0.48191600	0.22533100
C	4.59604700	1.72335500	-2.12856600
H	3.16074300	0.44728700	-3.10317900
C	4.79467300	1.44388600	0.25452500
H	3.48520600	0.00116600	1.15125500
C	5.20178100	2.06853400	-0.92434300
H	4.90143700	2.20646700	-3.05173700
H	5.25565400	1.71363900	1.20034700
H	5.98538900	2.82016900	-0.90127500
H	2.11841300	-1.78099300	1.72547900
C	-2.50516800	-0.64969700	2.08214000
C	-1.93041600	-1.22710600	3.26494700
C	-2.60384900	-1.09758100	4.49464100
C	-3.80139300	-0.40366700	4.54398100
C	-4.35109600	0.18279200	3.38192400
C	-3.71305800	0.06550000	2.15949900
C	-0.62964700	-1.53345100	1.48106100
C	-0.69515000	-1.80352000	2.84106000
H	-2.18583400	-1.53077800	5.40053400
H	-4.32451700	-0.29872000	5.49012400
H	-5.28488400	0.73325500	3.45322500
H	-4.12066100	0.53111800	1.26503100
H	0.02752100	-2.34546500	3.43694000
N	-1.70305500	-0.85110900	0.99646400
H	-1.10379700	-2.71628200	-0.42552300
C	0.39450500	-1.89873600	0.45637400
O	-0.14387500	-2.84586900	-0.45524400

C	1.73762500	-2.43374300	0.93090700
C	2.59780900	-2.35997900	-0.33563800
H	1.64162500	-3.44778500	1.32837400
H	2.23297600	-3.15416500	-0.99644700
C	4.08507200	-2.57172900	-0.16924100
C	4.90588300	-2.55443600	-1.30433900
C	4.67903800	-2.79167000	1.07364000
C	6.27917600	-2.73650700	-1.19920700
H	4.45644800	-2.38651200	-2.28073500
C	6.05758400	-2.97798300	1.18420400
H	4.06738500	-2.81890300	1.97042000
C	6.86255500	-2.94684200	0.05088900
H	6.89680900	-2.71527800	-2.09173100
H	6.49988000	-3.14598300	2.16137300
H	7.93514700	-3.08867500	0.13681500
C	-4.74864100	-1.33733600	-1.22319900
C	-3.49347900	-1.25567500	-1.83210200
C	-2.72675500	-2.39835500	-2.03770500
C	-3.19146000	-3.61277900	-1.53339400
C	-4.41212300	-3.68170300	-0.85858600
C	-5.20924800	-2.54848400	-0.71903300
C	-5.47344700	-0.02010000	-1.28944700
C	-4.68418300	0.71371900	-2.39422600
C	-3.23508000	0.15603600	-2.30633900
H	-1.78400900	-2.34847000	-2.57031100
H	-2.60097200	-4.51271400	-1.67430900
H	-4.75742800	-4.63376500	-0.46898900
H	-6.18175500	-2.61278100	-0.24089200
H	-5.42839100	0.50230800	-0.32845100
H	-5.06887900	0.39856200	-3.36671500

H	-6.52863300	-0.12358300	-1.55115200
H	-2.69773300	0.21582500	-3.25293400
N	-2.47805900	1.01599800	-1.34452900
O	-4.76645500	2.12062800	-2.39635400
C	-1.22220700	0.89976000	-0.86274900
C	-2.95935800	2.20528800	-0.85979700
N	-0.98177700	2.00800300	-0.17114000
N	-2.06769000	2.82846600	-0.14620400
C	-4.32509500	2.71418200	-1.19831200
H	-5.01473700	2.53039600	-0.36558300
H	-4.26859600	3.79092300	-1.36262600
C	0.27166500	2.52452600	0.32319500
C	0.50839100	2.52634800	1.69822700
C	1.14445100	3.08612200	-0.61661700
C	1.69208100	3.12737400	2.12920600
C	2.30282600	3.68143900	-0.12934800
C	2.58919700	3.71413500	1.23714100
H	1.91116700	3.14027700	3.19403300
H	3.00581000	4.11596300	-0.83470500
C	0.84718000	3.04627300	-2.09293500
H	-0.17737200	3.36697800	-2.30707800
H	0.97832400	2.03626200	-2.49763300
H	1.53167000	3.70223900	-2.63276700
C	3.84018500	4.38838200	1.73438600
H	3.65223500	5.44842300	1.93363800
H	4.63791000	4.32390500	0.99021500
H	4.19255100	3.93350700	2.66322600
C	-0.43536400	1.86846100	2.66546700
H	-0.24890500	0.78810500	2.70982900
H	-1.48010400	1.99718200	2.37309600

H	-0.29760000	2.27984700	3.66724600
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TS7RR

C	-5.06611800	-2.37886300	-0.47697700
C	-3.73068400	-2.02782700	-0.65343800
C	-2.74820600	-2.98869700	-0.87887800
C	-3.13000500	-4.32687400	-0.91841100
C	-4.46893400	-4.68760200	-0.74318900
C	-5.44539800	-3.71838300	-0.52559900
C	-5.93154600	-1.16517300	-0.25811600
C	-4.94733700	0.01342300	-0.07385800
C	-3.54479400	-0.53018600	-0.54413200
H	-1.71502700	-2.69384100	-1.03797600
H	-2.38207400	-5.09418900	-1.08962900
H	-4.75066300	-5.73522500	-0.77582200
H	-6.48429700	-4.00272100	-0.38823800
H	-6.58150100	-1.24890800	0.61867100
H	-5.22488000	0.87342900	-0.68345800
H	-6.57863800	-0.98435000	-1.12177400
H	-3.23304100	-0.07668800	-1.48316400
N	-2.50461100	-0.21777900	0.45395700
O	-4.95021200	0.51638400	1.25489800
C	-1.18413900	0.01468800	0.33087400
C	-2.80481900	-0.18704600	1.78680300
N	-0.73707200	0.16304600	1.58585100
N	-1.74799800	0.05027900	2.50170600
C	-4.24144100	-0.28748700	2.17867600
H	-4.58239300	-1.33132700	2.16195700
H	-4.38912700	0.12443800	3.17628900
C	0.59615900	0.32855100	2.12343400

S200

C	1.18099600	-0.78977800	2.72888800
C	1.16593000	1.60740200	2.17758500
C	2.43740800	-0.61957900	3.31496300
C	2.41846200	1.71817600	2.77839300
C	3.06729000	0.62362200	3.35171500
H	2.91151100	-1.47552700	3.78859200
H	2.88098600	2.70061000	2.83411100
C	0.46516600	2.83651800	1.66950500
H	-0.62135200	2.73280500	1.70411000
H	0.74005100	3.06201200	0.63371200
H	0.74835400	3.69424900	2.28305500
C	4.38229600	0.81490600	4.06227000
H	4.22741400	1.34497900	5.00710300
H	5.07061600	1.41224300	3.45853500
H	4.85758700	-0.14216500	4.28908000
C	0.45459200	-2.09981800	2.88949400
H	1.16503100	-2.92765400	2.91476900
H	-0.27255000	-2.29154700	2.09741500
H	-0.09578900	-2.09210200	3.83589800
C	-0.52820000	0.09266500	-1.05608100
O	-1.12421000	-0.52919500	-1.95425800
C	0.96203300	0.34892400	-1.20619400
C	1.87085000	-0.70332000	-1.86374000
H	1.38730000	0.71248700	-0.26618800
H	1.37651800	-0.93992100	-2.81079600
C	2.11271600	-2.04206400	-1.20871100
C	1.21250200	-2.58408800	-0.29245700
C	3.18533500	-2.84281400	-1.62396800
C	1.36126000	-3.88417400	0.19068300
H	0.36698400	-1.99112100	0.04073500

C	3.34880100	-4.13395000	-1.13527300
H	3.90308400	-2.44780300	-2.33724800
C	2.43321500	-4.66465000	-0.22677200
H	0.63340200	-4.28462300	0.89020400
H	4.19184600	-4.73116700	-1.46841700
H	2.55494700	-5.67520200	0.14900600
H	2.97994800	2.19513000	-1.44532100
C	-1.69028900	3.07698300	-0.73849700
C	-1.07412600	4.30473900	-1.14620800
C	-1.70795200	5.52553400	-0.85439800
C	-2.90962700	5.51915100	-0.16727900
C	-3.49803600	4.30667800	0.24711700
C	-2.90407300	3.08642000	-0.02974000
C	0.20625400	2.57558500	-1.74063600
C	0.15165500	3.94934000	-1.79632200
H	-1.25567600	6.46378600	-1.16536600
H	-3.40585000	6.45720000	0.06184800
H	-4.43498600	4.32773300	0.79562300
H	-3.37168800	2.16950200	0.31420100
H	0.87831200	4.61340600	-2.24353900
N	-0.88632700	2.03338600	-1.12206800
H	-0.19065200	0.67413600	-3.42823800
C	1.11070100	1.49959600	-2.24434600
O	0.68340100	1.08401800	-3.53960100
C	2.62084200	1.63430400	-2.31382200
C	3.13157800	0.15287400	-2.25609200
H	2.94361500	2.15014300	-3.22073100
H	3.45065000	-0.14814300	-3.25825900
C	4.33309100	0.03215500	-1.34237100
C	5.61546800	0.14720900	-1.88560500

C	4.21173100	-0.16096800	0.03836600
C	6.74986700	0.06963500	-1.08039600
H	5.72498100	0.29359000	-2.95770100
C	5.34348300	-0.26050400	0.84214200
H	3.23037200	-0.27372900	0.49545700
C	6.61728200	-0.14189200	0.28884100
H	7.73536200	0.16280200	-1.52614200
H	5.22689500	-0.44902600	1.90430000
H	7.49717400	-0.21991800	0.91945400

TS7RS

C	-4.45055000	2.43598500	-1.76146100
C	-3.16099000	2.06018300	-1.39310500
C	-2.04333400	2.72487800	-1.89064300
C	-2.24079300	3.78541500	-2.77097400
C	-3.53226500	4.17128600	-3.13981300
C	-4.64469000	3.50125500	-2.63731700
C	-5.48818900	1.56801300	-1.10023600
C	-4.69804100	0.41193200	-0.44785000
C	-3.19191600	0.87831200	-0.44611500
H	-1.04640000	2.42310600	-1.58653000
H	-1.38482500	4.31726800	-3.17330500
H	-3.66901300	4.99827000	-3.82921700
H	-5.64730700	3.79815900	-2.92987300
H	-6.22756600	1.16816800	-1.80103800
H	-5.01867400	0.22132300	0.57628000
H	-6.03747900	2.12672800	-0.33602200
H	-2.85402000	1.12794800	0.56065000
N	-2.32053100	-0.20106900	-0.93478000
O	-4.90872800	-0.82725900	-1.11307600

C	-1.05207000	-0.53055500	-0.63441000
C	-2.74063400	-1.06111200	-1.91022500
N	-0.74741500	-1.54177600	-1.44306100
N	-1.80188300	-1.89814700	-2.24000600
C	-4.17654500	-0.98812400	-2.31385300
H	-4.34609800	-0.15999300	-3.01502100
H	-4.48661500	-1.92285300	-2.77979700
C	0.50813200	-2.22466200	-1.61505100
C	1.44633000	-1.66127500	-2.47870700
C	0.69791800	-3.43075000	-0.93650100
C	2.63014100	-2.37004300	-2.67488800
C	1.90266900	-4.09211700	-1.15703500
C	2.87091700	-3.58144000	-2.02805400
H	3.38780300	-1.95478400	-3.33323100
H	2.09036800	-5.02954900	-0.63926800
C	-0.35398500	-3.94909300	0.00756400
H	-0.02029600	-4.87077500	0.48604600
H	-1.28936600	-4.15406500	-0.52296300
H	-0.57700800	-3.20688200	0.78460900
C	4.14904500	-4.34012100	-2.26922900
H	4.89935200	-3.70380400	-2.74299200
H	3.96752900	-5.20090500	-2.92099100
H	4.56146100	-4.71952300	-1.33049500
C	1.18773300	-0.34000200	-3.15164500
H	1.14016300	0.47271900	-2.41662100
H	0.23908800	-0.34915700	-3.69765400
H	1.99184700	-0.10416300	-3.85021100
C	-0.24237800	0.21725600	0.40971200
O	-0.52579500	1.41736800	0.49599800
C	1.11760100	-0.29659500	0.88419300

C	2.25250400	0.67125500	0.44890400
H	1.28323600	-1.32424500	0.55528300
H	1.82396800	1.43574400	-0.20756300
C	3.41604900	0.02436100	-0.26663700
C	3.95895300	0.60473200	-1.41508600
C	4.01907500	-1.12707600	0.25212300
C	5.07344400	0.04490200	-2.03940500
H	3.50833700	1.50836200	-1.81962200
C	5.13031400	-1.68738500	-0.36767200
H	3.61634000	-1.56738300	1.16137000
C	5.66123800	-1.10466000	-1.51812800
H	5.48256300	0.50965700	-2.93144500
H	5.58636000	-2.58142000	0.04767800
H	6.52998000	-1.54195600	-2.00089200
H	0.74611000	1.85296100	2.56126900
C	-2.32057700	-1.25716800	2.46162100
C	-2.16507100	-1.25685400	3.88615500
C	-3.25723500	-1.62028800	4.69628700
C	-4.45516300	-1.97543800	4.10049100
C	-4.58784400	-2.00280600	2.69545500
C	-3.52948400	-1.66044900	1.86988500
C	-0.25530500	-0.66580400	2.89263200
C	-0.81079200	-0.87455700	4.13875100
H	-3.15828700	-1.62677100	5.77876900
H	-5.30290800	-2.25447100	4.71898900
H	-5.53038600	-2.31299900	2.25324300
H	-3.63474100	-1.72619400	0.79017200
H	-0.31952400	-0.76719800	5.09614800
N	-1.13263800	-0.90053200	1.87585100
H	1.77013500	-2.02321300	2.93428300

C	1.11288300	-0.26141600	2.44325200
O	2.11842000	-1.12228300	2.96929600
C	1.56865800	1.16142500	2.75800300
C	2.71947100	1.38675300	1.76545700
H	1.88089000	1.25761000	3.80130200
H	3.59415100	0.84380300	2.13966000
C	3.10713000	2.82823100	1.54492900
C	4.41710100	3.25741200	1.76184000
C	2.16039000	3.75937900	1.09829900
C	4.77870800	4.58707900	1.54824900
H	5.16031300	2.54122800	2.10300900
C	2.51790600	5.08661400	0.88486200
H	1.13907300	3.43070600	0.91306800
C	3.82936000	5.50558700	1.11070500
H	5.80253100	4.90297800	1.72361100
H	1.77307200	5.79733100	0.53977900
H	4.10700900	6.54156200	0.94380900

TS7SR

C	-5.15324300	-0.20873500	0.80914000
C	-3.85406600	0.24182200	1.05583000
C	-3.48865300	0.75349300	2.29497800
C	-4.44452600	0.77002600	3.31230400
C	-5.73276300	0.28777600	3.08324900
C	-6.09831300	-0.19903500	1.82706600
C	-5.30620500	-0.60356500	-0.64139000
C	-4.12813100	0.10947700	-1.32307500
C	-3.04006900	0.10891900	-0.22039700
H	-2.49066800	1.14798700	2.46291400
H	-4.18350600	1.16976700	4.28662700

H	-6.46469000	0.31187600	3.88414100
H	-7.11160700	-0.54283700	1.64264700
H	-6.25825800	-0.30198600	-1.08374000
H	-3.78148800	-0.40743700	-2.22055600
H	-5.19298500	-1.68750500	-0.77165600
H	-2.47713600	-0.81816400	-0.24165300
N	-2.12887200	1.23394500	-0.43213000
O	-4.46937800	1.43455900	-1.74059100
C	-0.79767900	1.41450500	-0.41798800
C	-2.70425800	2.47092500	-0.58151400
N	-0.63125900	2.74014900	-0.47702100
N	-1.80764600	3.41380800	-0.59054800
C	-4.17683800	2.50791100	-0.86068500
H	-4.75609300	2.46347100	0.06796300
H	-4.41760500	3.43183100	-1.38728600
C	0.60553500	3.44163900	-0.23779900
C	1.34343400	3.92152900	-1.31921000
C	0.98463700	3.60583900	1.09950500
C	2.55084700	4.55406900	-1.02305700
C	2.19717800	4.24941300	1.33861800
C	2.99269900	4.72104300	0.29064400
H	3.16007200	4.92615900	-1.84258600
H	2.52478400	4.39100300	2.36540300
C	0.09893800	3.13916500	2.22728800
H	-0.02947000	2.05046000	2.23848900
H	-0.89898100	3.58190800	2.13889000
H	0.52087600	3.43851800	3.18746100
C	4.29108600	5.42703000	0.58432600
H	4.92277600	5.48071600	-0.30497100
H	4.84478800	4.91453400	1.37525500

H	4.10320700	6.45007900	0.92511600
C	0.84526000	3.76687200	-2.72919400
H	0.70721800	2.70938600	-2.96750600
H	1.55415400	4.20093500	-3.43530100
H	-0.11937900	4.26850000	-2.85294700
C	0.46590800	0.53022900	-0.64730600
O	1.02370400	0.77140100	-1.69150800
C	1.10796100	-0.15112100	0.52823800
C	2.33168400	-0.98690900	0.16573600
H	1.38234600	0.65137500	1.23350800
H	2.01381100	-1.67266600	-0.62918900
C	3.56746200	-0.25300000	-0.30295000
C	4.57419300	-0.98265100	-0.94688300
C	3.76776700	1.11463100	-0.09568000
C	5.75513700	-0.36953000	-1.35431300
H	4.42217100	-2.04268500	-1.13324300
C	4.94764700	1.73139800	-0.50746600
H	2.99777400	1.72516600	0.37018700
C	5.94838000	0.99240200	-1.13209400
H	6.52175900	-0.95425700	-1.85328700
H	5.07690800	2.79774500	-0.34529200
H	6.86586600	1.47500000	-1.45374300
H	0.86849900	-2.91525100	2.36427600
C	-1.50323200	-2.39887700	-1.57321300
C	-2.04700000	-3.33486500	-0.63195100
C	-3.03693900	-4.24619300	-1.05547600
C	-3.47358000	-4.20521000	-2.36716100
C	-2.93634100	-3.27540400	-3.28907500
C	-1.95467400	-2.37908200	-2.90677700
C	-0.54969900	-1.98158000	0.32653500

C	-1.39864900	-3.04979600	0.60656800
H	-3.45746800	-4.96660600	-0.35821900
H	-4.23976400	-4.89863900	-2.70156000
H	-3.30108300	-3.27094200	-4.31195300
H	-1.53835500	-1.66315600	-3.61076700
H	-1.53605100	-3.54952900	1.55736800
N	-0.59526600	-1.57346800	-0.96665500
H	-1.47866600	-0.89212300	2.25523800
C	0.20865500	-1.11848700	1.30010800
O	-0.71581500	-0.33020500	2.05716900
C	1.20049100	-1.88877300	2.18849200
C	2.57775700	-1.82509900	1.46729800
H	1.25710800	-1.38059500	3.15490900
H	3.27314100	-1.25382600	2.09189200
C	3.20657500	-3.16553200	1.17042400
C	4.53825100	-3.42053400	1.50087300
C	2.47418200	-4.15998200	0.51056900
C	5.13204900	-4.64076300	1.18088800
H	5.11686200	-2.65050400	2.00493800
C	3.06355000	-5.37871200	0.19076400
H	1.43365100	-3.97078900	0.24713700
C	4.39587800	-5.62292800	0.52485700
H	6.16962800	-4.82217100	1.44384100
H	2.48392800	-6.14039700	-0.32147000
H	4.85543300	-6.57391400	0.27480400

TS7SS

C	0.50147300	-0.03874900	-1.02487700
O	1.09022800	-0.50117500	-2.03299400
C	-0.89810700	0.54386900	-1.22098800

S209

C	-1.92101800	-0.14754000	-2.12430100
H	-1.35074600	0.80456300	-0.25844600
H	-1.40017500	-0.30324500	-3.07221600
C	-2.42985400	-1.51087500	-1.70342000
C	-1.87581300	-2.62484200	-2.35140800
C	-3.38740900	-1.74715300	-0.70791000
C	-2.27425700	-3.92273100	-2.04311400
H	-1.11519200	-2.46230000	-3.11070400
C	-3.80475600	-3.04412000	-0.41402000
H	-3.81285600	-0.92673600	-0.14309600
C	-3.25670400	-4.13687200	-1.07925000
H	-1.82504000	-4.76278300	-2.56377800
H	-4.56020100	-3.19711900	0.35168400
H	-3.58468200	-5.14448400	-0.84362300
H	-2.44017900	2.96710500	-1.44088800
C	1.99018100	2.38937900	0.29130100
C	1.67505000	3.78050700	0.17414600
C	2.39388700	4.71653700	0.93708300
C	3.38472000	4.27356200	1.79674100
C	3.68154400	2.90027700	1.91062400
C	2.99874400	1.95301100	1.16561800
C	0.30319600	2.58792500	-1.12548800
C	0.58354800	3.87943200	-0.75099400
H	2.16867700	5.77657100	0.85444200
H	3.94326500	4.98930400	2.39194200
H	4.46428000	2.57865500	2.59079100
H	3.25302800	0.90062600	1.25077400
H	0.08109400	4.77714400	-1.08342700
N	1.13798900	1.68269600	-0.52081300
H	0.59141300	0.94404600	-3.16471300

C	-0.66786800	1.86624400	-2.00552600
O	-0.09964600	1.62021200	-3.28850100
C	-2.08543800	2.34665800	-2.26631100
C	-2.93562800	1.03992400	-2.40890700
H	-2.11584200	2.94954700	-3.17572400
H	-3.27485300	0.92760800	-3.44238000
C	-4.17445900	1.06002400	-1.53831100
C	-5.36457200	0.50681400	-2.02033000
C	-4.16760000	1.57217900	-0.23592600
C	-6.50739900	0.44771500	-1.22685100
H	-5.38860200	0.10385000	-3.02968400
C	-5.30771300	1.51823000	0.56130200
H	-3.26169700	2.00206200	0.18402800
C	-6.48279200	0.95179500	0.07148200
H	-7.41819300	0.01089600	-1.62441600
H	-5.27505000	1.92382000	1.56832300
H	-7.37229800	0.91410100	0.69259000
C	5.42816900	-1.46889800	-0.67160300
C	4.18004600	-0.90387700	-0.92654400
C	4.06370700	0.37753700	-1.46184200
C	5.22688600	1.10471200	-1.69746900
C	6.48032300	0.55085900	-1.42477300
C	6.59004800	-0.74196900	-0.91976100
C	5.31476500	-2.88266200	-0.17170300
C	3.79770900	-3.15862200	-0.04868300
C	3.06314600	-1.86814400	-0.59828600
H	3.08557100	0.79552700	-1.67807300
H	5.15681400	2.11058200	-2.09842000
H	7.37743200	1.13091800	-1.61712700
H	7.56500100	-1.17862800	-0.72452300

H	5.80442800	-3.03329000	0.79639200
H	3.49954700	-4.00674000	-0.66453600
H	5.77532700	-3.58765400	-0.86946600
H	2.45806800	-2.10051100	-1.46997200
N	2.11000500	-1.34396400	0.41598100
O	3.42846900	-3.53542800	1.26698500
C	0.94361600	-0.67502000	0.29440500
C	2.28511100	-1.59278800	1.75138900
N	0.44899800	-0.58379500	1.53447800
N	1.28556100	-1.15377800	2.45301800
C	3.43078300	-2.44808200	2.17032600
H	4.37624500	-1.88949200	2.14322900
H	3.26615000	-2.83052800	3.17696300
C	-0.91428700	-0.36372900	1.97561100
C	-1.70913900	-1.51695000	2.04637300
C	-1.33497100	0.88640800	2.42802900
C	-2.98807200	-1.37833400	2.57449400
C	-2.63517200	0.96885300	2.93571300
C	-3.46949200	-0.14451800	3.01965300
H	-3.62448400	-2.25746600	2.64242400
H	-2.99108300	1.93207000	3.29376000
C	-0.45305800	2.10119000	2.37192700
H	0.59295900	1.85109700	2.56403400
H	-0.77983900	2.83642500	3.10974100
H	-0.49643900	2.57207600	1.38226600
C	-4.86067000	-0.04387900	3.58762900
H	-5.60477600	-0.27744100	2.81913100
H	-5.06524400	0.95970200	3.96695600
H	-4.99702800	-0.75594300	4.40629300
C	-1.19718300	-2.85167500	1.57303200

H	-0.29317600	-3.14527100	2.11500600
H	-0.96541900	-2.82495900	0.50090300
H	-1.95581500	-3.62036000	1.72126700

M7RR

C	-4.61642800	-2.87539800	-0.30116200
C	-3.39194200	-2.27064600	-0.56910800
C	-2.26288000	-3.01652600	-0.89480000
C	-2.37412100	-4.40413200	-0.91759700
C	-3.59663000	-5.02195700	-0.63655900
C	-4.72672500	-4.26398000	-0.33646700
C	-5.68753900	-1.85166500	-0.02641600
C	-4.94652400	-0.49464800	0.06408700
C	-3.48130400	-0.76811900	-0.44748200
H	-1.33724800	-2.50739900	-1.14648400
H	-1.50483600	-5.00739100	-1.16062300
H	-3.66843000	-6.10483300	-0.65915400
H	-5.67646800	-4.74842600	-0.13006600
H	-6.24138700	-2.03959800	0.89934500
H	-5.41263800	0.26024700	-0.57012300
H	-6.42210000	-1.82717000	-0.83694100
H	-3.26030600	-0.26568200	-1.38681500
N	-2.48308100	-0.27645800	0.53108900
O	-5.00227900	0.06470200	1.36845900
C	-1.21792900	0.17270400	0.38002600
C	-2.76680500	-0.28767100	1.86876000
N	-0.79325700	0.39466700	1.63704500
N	-1.75497000	0.12091400	2.57039300
C	-4.16224800	-0.59842900	2.29351400
H	-4.34150700	-1.68183000	2.30800800

H	-4.35068300	-0.19002600	3.28597600
C	0.51325500	0.74523400	2.14303700
C	1.25616400	-0.27099700	2.75892900
C	0.93711200	2.07916200	2.11747300
C	2.52104100	0.06211000	3.24469300
C	2.21716000	2.35038700	2.60046700
C	3.03027400	1.35718400	3.14720400
H	3.11350600	-0.71334600	3.72486800
H	2.57152800	3.37831500	2.57850600
C	0.05474100	3.21104300	1.66594600
H	-0.99398100	2.91700800	1.60083900
H	0.36119900	3.59086200	0.68731900
H	0.13525800	4.03270300	2.38189900
C	4.41445500	1.69167900	3.63610300
H	4.41764900	2.63287400	4.19141600
H	5.09852800	1.80433000	2.78850500
H	4.80833800	0.90466900	4.28325500
C	0.71029600	-1.65249500	3.01482600
H	1.50168000	-2.39767200	2.91402700
H	-0.10724000	-1.92583900	2.34604500
H	0.32096100	-1.70213700	4.03669400
C	-0.62848900	0.44478000	-1.09068200
O	-1.26133000	-0.24635600	-1.95813100
C	0.92686800	0.47474700	-1.18168200
C	1.80043800	-0.59911900	-1.83502100
H	1.33660500	0.74895300	-0.20267100
H	1.34825100	-0.78330700	-2.81399300
C	1.95661900	-1.95465100	-1.19589200
C	1.14630000	-2.37799600	-0.14750100
C	2.87723100	-2.86880100	-1.72828200

C	1.22942600	-3.67841200	0.35422400
H	0.42316600	-1.68540800	0.27110400
C	2.97800900	-4.15922700	-1.22474000
H	3.52041100	-2.55981400	-2.54851900
C	2.14843500	-4.57316600	-0.18085700
H	0.57108800	-3.98846500	1.16071800
H	3.70013200	-4.84915300	-1.65023400
H	2.22007700	-5.58379200	0.20786500
H	3.05557800	2.10747900	-0.99001200
C	-1.84296900	2.92916400	-0.95788800
C	-1.35502600	4.20546800	-1.37392900
C	-2.18133300	5.33452700	-1.25386900
C	-3.45483300	5.18838300	-0.73298700
C	-3.91967800	3.92713200	-0.31298500
C	-3.13092100	2.79287200	-0.41395000
C	0.25656700	2.68663700	-1.68394800
C	-0.00977100	4.02010900	-1.84315000
H	-1.81948600	6.30905400	-1.56886400
H	-4.10370900	6.05327300	-0.63972200
H	-4.91839800	3.83704500	0.10268800
H	-3.51437400	1.84261200	-0.06206600
H	0.65332400	4.77283900	-2.24492900
N	-0.82447400	2.02392300	-1.14957500
H	0.85717100	2.12508900	-3.95386200
C	1.25578300	1.66425400	-2.10770800
O	0.94854300	1.30040700	-3.46089300
C	2.76730900	1.72365100	-1.97432400
C	3.14806100	0.20622700	-2.10916800
H	3.24406500	2.33476700	-2.74462800
H	3.44461600	0.01786400	-3.14466000

C	4.31790700	-0.14917900	-1.22126400
C	5.57569400	-0.39402500	-1.77375400
C	4.17716600	-0.22137000	0.16945300
C	6.66959900	-0.69996400	-0.96425000
H	5.69955400	-0.34750300	-2.85309400
C	5.26134500	-0.53743900	0.98022900
H	3.20300200	-0.05548700	0.62437900
C	6.51556900	-0.77480000	0.41626000
H	7.63956500	-0.88433000	-1.41575200
H	5.12407700	-0.60690100	2.05583400
H	7.36211300	-1.02168100	1.04893200

M7RS

C	-2.32287600	4.54611500	-0.07130500
C	-1.56009400	3.38694700	0.03007400
C	-0.24379300	3.33426600	-0.41705200
C	0.30524400	4.47944700	-0.98701700
C	-0.45168300	5.65069300	-1.09000200
C	-1.76627500	5.69458500	-0.63050300
C	-3.70868200	4.33699600	0.48454800
C	-3.82820900	2.81130500	0.72388200
C	-2.36105400	2.25509800	0.62792100
H	0.32916200	2.41571600	-0.31082300
H	1.32596300	4.46413400	-1.35673100
H	-0.01027400	6.53582100	-1.53681900
H	-2.34967800	6.60645700	-0.71638000
H	-4.50271800	4.67451100	-0.18909400
H	-4.24062300	2.59116300	1.70873600
H	-3.83685100	4.87681500	1.42786500
H	-1.96234600	1.92352900	1.58506700

N	-2.30373500	1.08860300	-0.27452100
O	-4.73290400	2.18816800	-0.17765900
C	-1.44005300	0.05740700	-0.34275500
C	-3.11280800	1.02672000	-1.37652000
N	-1.77087100	-0.58114700	-1.47320800
N	-2.81390400	0.00993700	-2.12773200
C	-4.21954100	2.02281900	-1.48471100
H	-3.85278000	2.96877000	-1.90625500
H	-5.01559900	1.63467300	-2.11958000
C	-1.08020100	-1.68105400	-2.09303400
C	-0.10555600	-1.34909500	-3.04863700
C	-1.35296500	-2.98684800	-1.69744000
C	0.66574200	-2.38430700	-3.55966000
C	-0.53695900	-3.99233800	-2.23517800
C	0.48050500	-3.70999400	-3.14403300
H	1.44353600	-2.15362900	-4.28362100
H	-0.71838300	-5.02228400	-1.93698300
C	-2.47210000	-3.34871800	-0.76054400
H	-3.12212800	-4.08646500	-1.23880200
H	-3.08015500	-2.48689200	-0.48123200
H	-2.07381800	-3.79426600	0.15562100
C	1.37689600	-4.79915500	-3.67187800
H	1.49220200	-4.71913400	-4.75574300
H	0.98159800	-5.78875000	-3.43580700
H	2.37476300	-4.71792500	-3.22905200
C	0.12762700	0.08444400	-3.44327900
H	0.46075700	0.67871000	-2.58223500
H	-0.78851800	0.54030000	-3.82922800
H	0.90616500	0.15038800	-4.20428400
C	-0.37242100	-0.26418600	0.77987300

O	-0.24616700	0.74166900	1.58485500
C	0.96876800	-0.85430600	0.16006500
C	2.16611100	0.10061300	0.30028300
H	0.82697500	-1.15552200	-0.87570000
H	1.79891500	0.99307400	0.81819000
C	2.78485600	0.49937500	-1.01704100
C	3.00518700	1.84065900	-1.33485900
C	3.15020400	-0.47958600	-1.95009500
C	3.55083700	2.20309600	-2.56688700
H	2.74993100	2.60593200	-0.60457000
C	3.69889400	-0.12308600	-3.17720700
H	2.98820200	-1.52836000	-1.70304600
C	3.89368100	1.22254600	-3.49314500
H	3.71038700	3.25176000	-2.79948700
H	3.97390900	-0.89425800	-3.89127400
H	4.31623000	1.50227800	-4.45299000
H	1.74111100	-1.07901100	2.79480700
C	-2.06199000	-1.83735200	2.11210000
C	-1.86136800	-3.12588000	2.68821400
C	-2.90447700	-3.70658400	3.42831000
C	-4.09090300	-3.00998200	3.58357300
C	-4.26926900	-1.73711100	3.00538100
C	-3.26527600	-1.13673100	2.26273900
C	-0.00930900	-2.54306300	1.56888600
C	-0.53493700	-3.55483000	2.32857000
H	-2.77758800	-4.68873600	3.87443200
H	-4.90069800	-3.44886700	4.15770700
H	-5.21135300	-1.21679700	3.14511800
H	-3.41231400	-0.15781900	1.81675300
H	-0.04052600	-4.47036600	2.61887900

N	-0.92195200	-1.53501000	1.40868200
H	1.32423500	-3.41575300	-0.47420500
C	1.30380200	-2.12728000	0.97994500
O	1.94785800	-3.12746200	0.20986600
C	2.30040600	-1.61574900	2.02091000
C	3.17759900	-0.62687300	1.24114500
H	2.86060100	-2.43008700	2.48833100
H	3.87682000	-1.20103900	0.62173600
C	3.96306300	0.32391300	2.11241900
C	5.35756800	0.35141900	2.08143900
C	3.29251900	1.20375700	2.97228100
C	6.07312000	1.23137600	2.89319200
H	5.88798700	-0.32296500	1.41380700
C	4.00323600	2.08136500	3.78368700
H	2.20378900	1.20128200	2.99081800
C	5.39794900	2.09728200	3.74779600
H	7.15810200	1.23937300	2.85519700
H	3.46891900	2.75696400	4.44471600
H	5.95295900	2.78280200	4.38043100

M7SR

C	-5.38358700	0.39116100	-0.98260200
C	-4.04349300	0.03920600	-1.14158900
C	-3.55616600	-0.44815900	-2.34747700
C	-4.44089300	-0.55573600	-3.42093700
C	-5.77795900	-0.18168200	-3.27811700
C	-6.26033000	0.29086600	-2.05698000
C	-5.65490000	0.81600600	0.44089600
C	-4.44746100	0.26761000	1.22314400
C	-3.30266300	0.24421700	0.16725700

H	-2.51545100	-0.74400500	-2.44275500
H	-4.08740800	-0.93899200	-4.37251000
H	-6.45415700	-0.27433600	-4.12188800
H	-7.30678200	0.55714900	-1.94299600
H	-6.58889600	0.42162500	0.84846000
H	-4.17579400	0.88905500	2.07877800
H	-5.68579200	1.90857400	0.52520800
H	-2.76241000	1.18868200	0.16785800
N	-2.38326700	-0.85893700	0.45859300
O	-4.70684500	-1.02534700	1.76705000
C	-1.04310500	-1.01845100	0.40530800
C	-2.94249600	-2.09715200	0.65969700
N	-0.86401400	-2.33817900	0.51309200
N	-2.03490000	-3.02428500	0.68712800
C	-4.41169100	-2.14351500	0.94452800
H	-4.99750700	-2.14792000	0.01814300
H	-4.64596400	-3.04029500	1.51828200
C	0.36299200	-3.06896600	0.33128200
C	1.10193000	-3.46354300	1.44927700
C	0.70691300	-3.40964700	-0.97981000
C	2.27258900	-4.17910100	1.20913800
C	1.88506300	-4.13279600	-1.16368100
C	2.67923900	-4.51808400	-0.08336500
H	2.88167300	-4.48458900	2.05653200
H	2.18273100	-4.40609200	-2.17300300
C	-0.18068700	-3.03818100	-2.14112800
H	-0.26848000	-1.95228100	-2.26635200
H	-1.19243300	-3.43122800	-1.99436600
H	0.21504700	-3.45416800	-3.06901600
C	3.93812300	-5.31740100	-0.29356200

S220

H	4.73929500	-4.95303200	0.35498700
H	4.27735500	-5.25878500	-1.33030100
H	3.77059500	-6.37244400	-0.05381000
C	0.62709100	-3.14639200	2.83858900
H	0.51193000	-2.06328800	2.93453100
H	1.33834500	-3.51430200	3.58018200
H	-0.34310100	-3.61827100	3.02676800
C	0.14877700	0.02515900	0.63828100
O	0.71629600	-0.27723800	1.75393400
C	1.01392900	0.17001500	-0.66320100
C	2.37026700	0.79278100	-0.31331100
H	1.14483300	-0.77749200	-1.19364900
H	2.20311900	1.48825300	0.51833700
C	3.42013200	-0.20502000	0.12107500
C	3.90023900	-0.20888400	1.43238200
C	3.93647200	-1.14385900	-0.77783600
C	4.88554500	-1.10795600	1.83149800
H	3.47782100	0.49178500	2.14576700
C	4.92454700	-2.04262800	-0.38546200
H	3.55960000	-1.18144300	-1.79797100
C	5.40706500	-2.02532700	0.92114400
H	5.24708100	-1.09135200	2.85515300
H	5.31483600	-2.76091700	-1.10089200
H	6.18046200	-2.72308500	1.22852100
H	1.26288500	3.01917900	-2.39240200
C	-1.14793000	2.13897500	1.55292600
C	-1.51225300	3.35640500	0.90902700
C	-2.24090800	4.30872700	1.64522400
C	-2.57879700	4.02743200	2.95764100
C	-2.20462200	2.81120100	3.57076000

C	-1.48637700	1.84938000	2.88116500
C	-0.40360600	2.06621900	-0.55774400
C	-1.01574900	3.29127400	-0.44335400
H	-2.53689200	5.24828900	1.18780100
H	-3.14178800	4.75584500	3.53257100
H	-2.48296800	2.63054700	4.60423500
H	-1.17457700	0.91151000	3.32728600
H	-1.08965300	4.05811700	-1.20155800
N	-0.50127100	1.38023900	0.61709600
H	-1.16046800	1.20354200	-2.83709700
C	0.33136400	1.21528400	-1.56745600
O	-0.58907300	0.54235300	-2.42352400
C	1.45445500	1.94468800	-2.32114100
C	2.77534700	1.62649200	-1.56917900
H	1.49360300	1.54769700	-3.33895800
H	3.38739400	0.99018100	-2.21545800
C	3.61317700	2.82410100	-1.18488100
C	4.99206300	2.82564900	-1.40079600
C	3.03351000	3.92889000	-0.55016300
C	5.77674800	3.90772300	-1.00432900
H	5.45470000	1.96753600	-1.88209700
C	3.81253800	5.01131100	-0.15436800
H	1.96088200	3.93585500	-0.36019700
C	5.18852400	5.00531900	-0.38263600
H	6.84743100	3.89182200	-1.18302500
H	3.34607500	5.86075000	0.33494400
H	5.79617800	5.85063800	-0.07589700

M7SS

C	0.51872800	0.32439700	-0.89034100
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S222

O	1.20752600	-0.18386500	-1.88580500
C	-1.01151400	0.44213000	-1.15639100
C	-1.83172200	-0.56491200	-1.95871200
H	-1.54084500	0.70662000	-0.23432700
H	-1.24939800	-0.74252300	-2.86627300
C	-1.98282500	-1.94129300	-1.32614600
C	-0.81297200	-2.72373500	-1.36418700
C	-3.11982800	-2.50717000	-0.74088300
C	-0.77213200	-4.00800600	-0.83513900
H	0.06887600	-2.28835700	-1.83042600
C	-3.08452000	-3.80747200	-0.22972100
H	-4.04972800	-1.96034800	-0.67634600
C	-1.91855700	-4.56216200	-0.26527000
H	0.14753300	-4.58409300	-0.88197700
H	-3.98654700	-4.22478000	0.20842900
H	-1.90118400	-5.56924400	0.13899100
H	-3.01935000	2.32946300	-1.47462800
C	1.80672400	2.61750900	-0.24194100
C	1.50643700	3.95382900	-0.63462400
C	2.37976600	4.98775700	-0.25895600
C	3.51245000	4.68302700	0.47663100
C	3.78947500	3.35722100	0.86392900
C	2.94226300	2.31594400	0.52170100
C	-0.14173800	2.61835900	-1.36468400
C	0.26102400	3.92428500	-1.35599000
H	2.16440900	6.01357000	-0.54378800
H	4.19621300	5.47460200	0.76596500
H	4.68259600	3.14444600	1.44273300
H	3.16494300	1.29995400	0.83298800
H	-0.23749300	4.75845500	-1.82777000

N	0.75835700	1.83161100	-0.66383700
H	0.32268400	0.83879000	-3.14605200
C	-1.06015500	1.67302100	-2.08794100
O	-0.47618400	1.37477100	-3.35275600
C	-2.54908900	1.82257400	-2.32148400
C	-3.05108300	0.33721800	-2.43629900
H	-2.76486400	2.39196700	-3.22786900
H	-3.22164700	0.10325900	-3.49045700
C	-4.36708800	0.13615800	-1.72040200
C	-5.42787800	-0.49234800	-2.37729500
C	-4.54485200	0.51580700	-0.38473100
C	-6.62393000	-0.76558600	-1.71685000
H	-5.30485300	-0.79046000	-3.41521000
C	-5.73226000	0.23278600	0.28299700
H	-3.73988800	1.01004500	0.15538900
C	-6.77639300	-0.41249300	-0.37905900
H	-7.43259600	-1.26010100	-2.24590800
H	-5.84359300	0.51250300	1.32592200
H	-7.70201600	-0.63134000	0.14346000
C	5.22438800	-1.90278200	-0.41765900
C	4.09548200	-1.14372100	-0.72124900
C	4.20915300	0.09167500	-1.35577500
C	5.48266500	0.58768900	-1.62112600
C	6.61868500	-0.15330100	-1.28549400
C	6.49684700	-1.40905500	-0.69576900
C	4.86105200	-3.24827800	0.14654000
C	3.31837800	-3.24610600	0.26471100
C	2.82242800	-1.87458200	-0.35456400
H	3.31084800	0.62628800	-1.64588300
H	5.59180800	1.55563300	-2.09969900

H	7.60481800	0.24652700	-1.50041500
H	7.37884000	-1.99706800	-0.46000000
H	5.31362800	-3.43976000	1.12553900
H	2.87592600	-4.05898100	-0.31102100
H	5.19230800	-4.05401700	-0.51470000
H	2.18942300	-2.02459200	-1.22556200
N	1.97142400	-1.14542700	0.62612500
O	2.89170000	-3.48599900	1.59554800
C	0.91788500	-0.31623700	0.46569800
C	2.11243500	-1.35230700	1.97364100
N	0.46404200	-0.07413300	1.70602900
N	1.20338900	-0.72194300	2.65232500
C	3.09417700	-2.37003700	2.43924100
H	4.12298000	-1.99084600	2.38323900
H	2.87229500	-2.66213200	3.46502900
C	-0.82603200	0.43834300	2.12950100
C	-1.81748200	-0.53366700	2.33664700
C	-1.02405500	1.79144400	2.41073700
C	-3.07153800	-0.09780100	2.75910000
C	-2.30074700	2.17103300	2.83098300
C	-3.33357400	1.25208100	3.00329900
H	-3.85458600	-0.83519600	2.91667000
H	-2.47789000	3.21999000	3.05716100
C	0.05818000	2.82801100	2.32518800
H	1.05470600	2.38613500	2.35481200
H	-0.03778900	3.52433200	3.16150900
H	-0.02933200	3.40202700	1.39777000
C	-4.68770500	1.71756500	3.47244400
H	-5.33858200	0.87351500	3.71087700
H	-5.17740900	2.32358200	2.70325500

H	-4.59500300	2.34136300	4.36557500
C	-1.52189300	-2.00177900	2.19216100
H	-0.87276300	-2.33429400	3.00842500
H	-1.01927100	-2.23609300	1.24812800
H	-2.44538600	-2.57904100	2.22724600

TS8RR

C	4.11543400	3.29395100	-0.14246900
C	2.99374200	2.50275000	-0.37344300
C	1.74999400	3.06165100	-0.65381200
C	1.64518500	4.45026700	-0.69016500
C	2.76581600	5.25246400	-0.45534100
C	4.00741700	4.68233600	-0.18352600
C	5.33934800	2.45291100	0.11533600
C	4.82892200	0.99225000	0.19780200
C	3.32723200	1.03291500	-0.27392400
H	0.88732600	2.42776900	-0.84913100
H	0.68397100	4.90664800	-0.90379300
H	2.66692300	6.33308100	-0.48641200
H	4.87527400	5.30976600	-0.00217700
H	5.85845700	2.72098600	1.04170400
H	5.39814700	0.33715900	-0.46279200
H	6.06590300	2.55591100	-0.69638400
H	3.18885200	0.52779300	-1.22900400
N	2.44721900	0.36603700	0.69656500
O	5.00952500	0.42449200	1.48638800
C	1.22427400	-0.19950900	0.51846700
C	2.74554100	0.38786800	2.03309500
N	0.86450700	-0.49349100	1.78161500
N	1.79349800	-0.14418800	2.73384700

C	4.08465000	0.89776300	2.44729500
H	4.08428500	1.99561900	2.50292800
H	4.36481800	0.49333700	3.41980300
C	-0.40197800	-0.99777200	2.23369200
C	-1.26369300	-0.09281400	2.87052700
C	-0.71033800	-2.35249700	2.09319100
C	-2.51022200	-0.56096200	3.27892400
C	-1.98348400	-2.76620000	2.49608300
C	-2.89830300	-1.88804200	3.07405100
H	-3.19168100	0.12759400	3.77271300
H	-2.24903800	-3.81480100	2.38032300
C	0.28611000	-3.36928100	1.60866300
H	1.26936800	-2.93387200	1.42742800
H	-0.05339900	-3.83967800	0.68287400
H	0.39277000	-4.15548900	2.36153800
C	-4.27577500	-2.36143900	3.45880400
H	-4.24391900	-3.36966900	3.87876700
H	-4.92744400	-2.39203200	2.57838100
H	-4.73514200	-1.69391400	4.19159300
C	-0.83765500	1.32278900	3.15908600
H	-1.70815200	1.93946000	3.39186800
H	-0.30477800	1.77007100	2.31439200
H	-0.15981800	1.34593800	4.01742400
C	0.64176000	-0.60328800	-1.38645700
O	1.35434700	0.09910000	-2.10540600
C	-0.89027200	-0.56697000	-1.36174900
C	-1.76291000	0.49410900	-2.00940500
H	-1.22151900	-0.76286100	-0.33398200
H	-1.40015500	0.62871800	-3.02999100
C	-1.83595100	1.85880000	-1.37959200

C	-1.86314800	2.05322900	0.00424200
C	-1.91216400	2.98142100	-2.20975000
C	-1.97271800	3.33411500	0.54068400
H	-1.81507700	1.19207100	0.66541400
C	-2.02740200	4.26377800	-1.67852800
H	-1.88253700	2.84357700	-3.28766700
C	-2.06117700	4.44338800	-0.29780600
H	-1.99358200	3.46941000	1.61729900
H	-2.08616000	5.12077800	-2.34250700
H	-2.14974000	5.44000500	0.12319000
H	-3.04578400	-2.21083700	-0.98811300
C	1.92072000	-2.92486400	-1.18509900
C	1.45601400	-4.23599200	-1.48861700
C	2.34536900	-5.31574000	-1.37051700
C	3.64825200	-5.07383400	-0.96830100
C	4.08649000	-3.76926400	-0.66796200
C	3.23449500	-2.68127600	-0.76654900
C	-0.25556400	-2.80708200	-1.73782300
C	0.06499100	-4.13098200	-1.85382400
H	2.01283900	-6.32546100	-1.59260400
H	4.34555500	-5.90034300	-0.87718100
H	5.11242200	-3.61240000	-0.35059200
H	3.57354800	-1.68083600	-0.52078200
H	-0.58787500	-4.93284500	-2.16704300
N	0.84814100	-2.07987800	-1.32390500
H	-1.03434700	-2.36733400	-4.02812700
C	-1.28592700	-1.80967600	-2.18034800
O	-1.01741700	-1.52336100	-3.55975400
C	-2.79254100	-1.82474200	-1.97937500
C	-3.15302800	-0.30434900	-2.12054100

H	-3.30935700	-2.43185700	-2.72618200
H	-3.53652000	-0.12468100	-3.12828600
C	-4.19934900	0.18162800	-1.14418600
C	-5.15321100	1.10856600	-1.57452300
C	-4.20299100	-0.19088700	0.20438500
C	-6.08767400	1.64657200	-0.69383600
H	-5.15553700	1.41709400	-2.61703900
C	-5.13242200	0.34868900	1.09077400
H	-3.46233300	-0.89140700	0.58619900
C	-6.08073000	1.26661600	0.64584800
H	-6.81969700	2.36221900	-1.05499900
H	-5.11263800	0.05184300	2.13553800
H	-6.80619500	1.68208300	1.33785500

TS8RS

C	2.77169200	4.32051700	-0.61517700
C	1.95062200	3.19998900	-0.53690800
C	0.66890900	3.26957300	0.00211000
C	0.22076000	4.49684000	0.48299100
C	1.04074100	5.62731400	0.41164000
C	2.31686100	5.54979400	-0.14123000
C	4.09706600	3.98488300	-1.25025800
C	4.11477500	2.44067000	-1.37708300
C	2.64632700	1.96804200	-1.06787000
H	0.03483500	2.38503800	0.03338200
H	-0.77062700	4.57396100	0.91832100
H	0.67756900	6.57653100	0.79274700
H	2.94932300	6.43108100	-0.19285300
H	4.95604000	4.32235900	-0.66109100
H	4.39632400	2.12737000	-2.38278800

H	4.18674800	4.44752100	-2.23804200
H	2.14316300	1.57107300	-1.94982400
N	2.64120900	0.91036800	-0.05413400
O	5.09342500	1.83819300	-0.54212700
C	1.67670300	-0.00363500	0.20638700
C	3.57122100	0.88806600	0.95194800
N	2.10130200	-0.54055100	1.35954200
N	3.27538100	-0.00853600	1.84330100
C	4.74564400	1.80160200	0.82935700
H	4.49878800	2.80177000	1.21344300
H	5.59866500	1.41160200	1.38476100
C	1.36038100	-1.48593300	2.14298500
C	0.48314100	-0.97367400	3.11011500
C	1.50527900	-2.85013300	1.89513200
C	-0.30834700	-1.88101700	3.80846500
C	0.68951600	-3.72374200	2.62384800
C	-0.22469300	-3.25875700	3.57148600
H	-1.00972000	-1.50696800	4.55077800
H	0.77523900	-4.79227100	2.44328100
C	2.53696600	-3.36321900	0.92956000
H	3.52497600	-3.35084800	1.40212700
H	2.59294800	-2.74504300	0.03106100
H	2.31041800	-4.38702300	0.62772900
C	-1.13257000	-4.21120300	4.30496000
H	-1.19820100	-3.95230200	5.36456400
H	-0.77985500	-5.24055300	4.21905500
H	-2.14545500	-4.16535400	3.89170600
C	0.40218800	0.50962400	3.35596800
H	0.10605200	1.04934500	2.44757500
H	1.37546900	0.90163300	3.66603500

H	-0.33407700	0.73284400	4.12906400
C	0.09130100	-0.34783300	-1.07860800
O	0.13878000	0.58332500	-1.88817300
C	-1.07406100	-0.58938100	-0.07326200
C	-2.27854100	0.34671200	-0.27751500
H	-0.69361700	-0.53619300	0.94580000
H	-2.04571300	1.01565500	-1.11395700
C	-2.62256500	1.17791800	0.93612100
C	-2.81460400	2.55657200	0.83929200
C	-2.79083100	0.56129000	2.18284000
C	-3.15558600	3.30913100	1.96431100
H	-2.69310400	3.04348100	-0.12587900
C	-3.13009500	1.30841600	3.30562000
H	-2.64459700	-0.51589800	2.26504400
C	-3.31107200	2.68785000	3.20009200
H	-3.30247400	4.38127500	1.87137500
H	-3.25206300	0.81571800	4.26595300
H	-3.57505800	3.27224000	4.07555400
H	-2.39504800	-1.60048100	-2.28911700
C	1.47954900	-2.24991200	-2.21230900
C	1.25949600	-3.65515200	-2.20758800
C	2.18822600	-4.48041800	-2.85928900
C	3.28555900	-3.90089800	-3.47739800
C	3.48408600	-2.50671200	-3.46041200
C	2.58592400	-1.66025100	-2.82847500
C	-0.38290200	-2.68219300	-1.02882200
C	0.05651600	-3.90507100	-1.44935100
H	2.04947400	-5.55732000	-2.87496900
H	4.00937700	-4.53116500	-3.98409900
H	4.35506100	-2.08703200	-3.95319900

H	2.72399600	-0.58436000	-2.81692000
H	-0.41449300	-4.85985600	-1.26695800
N	0.46440700	-1.69299900	-1.47298200
H	-1.25552400	-2.86640400	1.37691000
C	-1.56005600	-2.04083300	-0.35221600
O	-2.01887100	-2.71400500	0.79977800
C	-2.76075100	-1.82308000	-1.27998100
C	-3.45772500	-0.59289500	-0.68313300
H	-3.39921400	-2.70873200	-1.32835800
H	-3.95967100	-0.91224500	0.23748700
C	-4.47371200	0.07224100	-1.57880000
C	-5.80208600	0.21077600	-1.17387100
C	-4.10065000	0.57543800	-2.83097200
C	-6.74102500	0.82846800	-1.99867800
H	-6.10341600	-0.16976300	-0.20131700
C	-5.03438100	1.19048800	-3.65801100
H	-3.06662300	0.48950700	-3.15876900
C	-6.36035100	1.31789600	-3.24463000
H	-7.76954500	0.92636900	-1.66538400
H	-4.72695400	1.57276100	-4.62640800
H	-7.08927100	1.79759500	-3.89000500

TS8SR

C	-5.26566400	-0.65821000	1.55979100
C	-3.91296800	-0.32392900	1.54930300
C	-3.24089900	0.04053100	2.71003200
C	-3.95527700	0.06024700	3.90728600
C	-5.31003000	-0.27965100	3.92893500
C	-5.97476800	-0.64136100	2.75724400
C	-5.74209000	-0.99719000	0.16748900

C	-4.62594800	-0.47650400	-0.76336100
C	-3.35471900	-0.41257000	0.14407700
H	-2.18495500	0.29680900	2.67545800
H	-3.45709000	0.34482800	4.82840400
H	-5.85372800	-0.25508200	4.86797800
H	-7.03073600	-0.89400700	2.77859200
H	-6.70000800	-0.53872200	-0.09328500
H	-4.45273400	-1.13456100	-1.61824500
H	-5.85111100	-2.08113900	0.04866100
H	-2.74536300	-1.30714100	0.02519400
N	-2.55352600	0.75760000	-0.18880100
O	-4.95172300	0.78684200	-1.33562000
C	-1.21396700	0.95761800	-0.18086300
C	-3.18780300	1.96233500	-0.35098500
N	-1.12045400	2.28669100	-0.31120000
N	-2.33014700	2.93317700	-0.42955600
C	-4.67234300	1.92359500	-0.53281800
H	-5.19010900	1.88185300	0.43415400
H	-5.00991800	2.80455000	-1.07901600
C	0.08485100	3.05933600	-0.22617700
C	0.62204800	3.61243400	-1.39218500
C	0.63123200	3.27230600	1.04111900
C	1.77509000	4.38044400	-1.26046500
C	1.78627400	4.05304700	1.12053800
C	2.37085500	4.60791100	-0.01651100
H	2.21985300	4.81694100	-2.15174900
H	2.23378300	4.23338800	2.09547600
C	-0.02383000	2.71314000	2.27960000
H	0.06336900	1.62193300	2.33761300
H	-1.09321600	2.94869400	2.29344800

H	0.43322700	3.13664200	3.17561200
C	3.62176400	5.44187800	0.07746800
H	4.43998800	4.96555100	-0.47197600
H	3.93766400	5.57027400	1.11533300
H	3.46623500	6.43281700	-0.35885800
C	-0.04287300	3.39065600	-2.72227600
H	-0.15087500	2.31773700	-2.90133800
H	0.54936500	3.83228700	-3.52575600
H	-1.03911900	3.84359300	-2.73663300
C	0.21097200	-0.16888400	-0.88203700
O	0.63477800	0.43996100	-1.87481000
C	1.05838100	-0.50064500	0.36197200
C	2.47910200	-0.95756500	0.00743000
H	1.09251000	0.34860600	1.04611200
H	2.43290100	-1.59832300	-0.88456700
C	3.48141300	0.14272800	-0.23911200
C	4.33093800	0.09560800	-1.34670700
C	3.63848200	1.18738000	0.67651700
C	5.30892400	1.06840800	-1.54064300
H	4.22158500	-0.71387100	-2.06365500
C	4.61690700	2.15880100	0.48964900
H	2.99244900	1.25151400	1.54953100
C	5.45603800	2.10424600	-0.62114500
H	5.95651400	1.01622600	-2.41028700
H	4.71923100	2.96367400	1.21217500
H	6.21987300	2.86198700	-0.76704800
H	1.55599200	-3.56685900	0.88012800
C	-1.44199700	-1.86494200	-2.00941300
C	-1.93218900	-3.11099800	-1.52618600
C	-2.90168100	-3.78983000	-2.28379600

C	-3.34910000	-3.22069200	-3.46493900
C	-2.84947800	-1.98144300	-3.91844800
C	-1.89015600	-1.28482700	-3.20107700
C	-0.48393300	-2.28336200	-0.02134900
C	-1.29499000	-3.36284200	-0.25545200
H	-3.29736300	-4.74187000	-1.94284300
H	-4.10074400	-3.73483300	-4.05532800
H	-3.22677300	-1.56572200	-4.84714900
H	-1.49451300	-0.33167400	-3.53283100
H	-1.43206900	-4.22547400	0.38108000
N	-0.55778700	-1.40267100	-1.06710400
H	-0.93011900	-1.95611300	2.46972900
C	0.40649400	-1.71980100	1.06126100
O	-0.36167800	-1.23865200	2.15897900
C	1.56539900	-2.65481800	1.48382900
C	2.84963700	-1.84714000	1.22332700
H	1.46438900	-2.94446600	2.53288600
H	3.00618900	-1.17050300	2.07417800
C	4.11256700	-2.64636900	1.01730900
C	5.26793500	-2.34027500	1.73938300
C	4.17322700	-3.66981200	0.06468700
C	6.45291500	-3.04202200	1.52754500
H	5.23665900	-1.53823900	2.47262100
C	5.35426800	-4.37340400	-0.15041900
H	3.29043400	-3.91853000	-0.51983500
C	6.49901800	-4.06302200	0.58269700
H	7.33958300	-2.78825000	2.10003600
H	5.38274300	-5.16501800	-0.89287900
H	7.42023000	-4.61155600	0.41436700

TS8SS

C	0.46926200	0.44397900	-1.39192200
O	1.13451300	-0.16560300	-2.22658800
C	-1.06503500	0.35819300	-1.27534000
C	-1.99775100	-0.66129600	-1.94415600
H	-1.34352500	0.48326600	-0.22230000
H	-1.60708400	-0.82751900	-2.95399800
C	-2.00553300	-2.01984000	-1.25298400
C	-0.74369500	-2.56213900	-0.96444100
C	-3.12525900	-2.78488200	-0.91283500
C	-0.59431700	-3.76693600	-0.28727000
H	0.13239800	-2.01969200	-1.30184200
C	-2.98165000	-3.99763300	-0.23460900
H	-4.12393100	-2.45402800	-1.16093000
C	-1.72442600	-4.48493100	0.10301600
H	0.40228800	-4.14607800	-0.06971500
H	-3.87104200	-4.56083200	0.03135300
H	-1.62352100	-5.42216000	0.64113500
H	-3.20511000	1.96819400	-0.82331300
C	1.70323600	2.69946700	-0.73603000
C	1.17414700	4.01971200	-0.73719700
C	2.00474600	5.08231800	-0.34726000
C	3.31475500	4.81481800	0.01739900
C	3.81599600	3.49874500	0.01041400
C	3.01958000	2.42668900	-0.35865500
C	-0.45507600	2.62598000	-1.38607400
C	-0.20098400	3.94548200	-1.16869800
H	1.62271800	6.09877000	-0.33543400
H	3.96624000	5.63046600	0.31446200
H	4.84490600	3.31631400	0.30495000

H	3.38951600	1.41012800	-0.33229700
H	-0.88377800	4.76913600	-1.31582700
N	0.67646600	1.86401100	-1.11114000
H	-0.28229700	1.29156400	-3.53971400
C	-1.44142400	1.67539000	-1.99835100
O	-1.19936900	1.57275200	-3.40092400
C	-2.94072900	1.68879900	-1.84699500
C	-3.33205200	0.20263400	-2.14606300
H	-3.42810500	2.38064800	-2.53708400
H	-3.58297500	0.12830800	-3.20691800
C	-4.57236100	-0.16975800	-1.36654200
C	-5.71910700	-0.61402200	-2.02692900
C	-4.60399400	-0.06966600	0.02750400
C	-6.85950700	-0.98118800	-1.31293600
H	-5.71322500	-0.68950900	-3.11123200
C	-5.73536600	-0.43982500	0.74572900
H	-3.72316300	0.28632000	0.55663500
C	-6.86847500	-0.90320800	0.07679800
H	-7.73979300	-1.32873200	-1.84471100
H	-5.73657700	-0.36912300	1.83007800
H	-7.75257700	-1.19237800	0.63562500
C	5.12237200	-1.73494400	-0.05478100
C	4.01389600	-1.30481400	-0.79434600
C	4.15410400	-0.33538900	-1.78221800
C	5.40919200	0.24352700	-1.97776000
C	6.50461300	-0.15551800	-1.21255600
C	6.37086100	-1.15814600	-0.25189700
C	4.75042600	-2.87612100	0.85281000
C	3.46257000	-3.38994900	0.17537100
C	2.79069900	-2.12683300	-0.43486900

H	3.29322200	-0.02685600	-2.36513200
H	5.53214600	1.01047700	-2.73564200
H	7.47425500	0.30315500	-1.37915800
H	7.23082000	-1.49386100	0.31984900
H	4.56024200	-2.51161300	1.86891000
H	3.74214800	-4.03096900	-0.66386800
H	5.51608500	-3.65199300	0.91784100
H	2.17075400	-2.35774300	-1.30397500
N	1.90804400	-1.52915900	0.59785500
O	2.60807100	-4.17280400	0.97851500
C	1.16334500	-0.38247200	0.52241700
C	1.63452600	-2.15834300	1.79087000
N	0.54313500	-0.37602100	1.71459300
N	0.81102600	-1.46066200	2.50899400
C	2.17035300	-3.51016800	2.14543700
H	2.97037700	-3.43270300	2.89128300
H	1.36262500	-4.10748100	2.57260000
C	-0.39546700	0.60313800	2.18474400
C	-1.72394200	0.19173500	2.39279800
C	0.02914100	1.90816500	2.44764300
C	-2.64580000	1.15939300	2.78137700
C	-0.94586300	2.84519000	2.80676900
C	-2.28335100	2.49814900	2.96082800
H	-3.67968600	0.86164600	2.94588500
H	-0.63380800	3.87065400	2.99146400
C	1.47804800	2.31630600	2.48678500
H	2.13519200	1.59186700	2.00968400
H	1.78502900	2.42090200	3.53312100
H	1.62817300	3.28177100	1.99649600
C	-3.32294400	3.52844300	3.31541500

H	-4.02806300	3.13849500	4.05385400
H	-3.90031900	3.81111200	2.42920800
H	-2.86371700	4.43340500	3.71814600
C	-2.14106600	-1.24785400	2.23565200
H	-1.78819800	-1.83826400	3.08604400
H	-1.72017100	-1.70021300	1.33304800
H	-3.22906300	-1.32906700	2.18490100

PRR

C	-1.51198200	1.08032600	0.46473600
O	-1.61394000	2.27676100	0.58856100
C	-0.29309800	0.17329800	0.37463800
C	1.06194200	0.26800200	1.05671000
H	-0.12828200	0.09011800	-0.71109700
H	0.90027100	0.43982200	2.12436800
C	1.99816500	1.33655200	0.54305900
C	1.62828100	2.23332600	-0.45906500
C	3.28007800	1.44571100	1.09631800
C	2.52189000	3.20365800	-0.91398100
H	0.62957200	2.19678300	-0.88341100
C	4.17361400	2.40887300	0.64431400
H	3.57992600	0.75754900	1.88315900
C	3.79791200	3.29062700	-0.36962200
H	2.21318300	3.89247900	-1.69409700
H	5.16459400	2.47424300	1.08261100
H	4.49461800	4.04283900	-0.72539500
H	0.36705000	-2.26450400	-0.63100000
C	-3.90251400	0.31851900	-0.14657200
C	-4.36874900	-0.99549000	-0.39074800
C	-5.69320900	-1.17157500	-0.80835100

C	-6.49688700	-0.05138100	-0.96962100
C	-6.00512000	1.24227400	-0.72531900
C	-4.69670800	1.45074000	-0.30926800
C	-2.21344600	-1.16031300	0.24380500
C	-3.27379800	-1.91662100	-0.12857300
H	-6.08254100	-2.16621300	-1.00154700
H	-7.52571500	-0.17374500	-1.29188900
H	-6.66147400	2.09526500	-0.86255000
H	-4.30103300	2.44042300	-0.11382200
H	-3.30768800	-2.99358900	-0.20492500
N	-2.57576000	0.19620700	0.23688100
H	-1.36922900	-1.93623200	2.53902400
C	-0.82315500	-1.19281600	0.81951300
O	-0.93824500	-1.12418200	2.24261000
C	0.33904100	-2.09575600	0.44938300
C	1.57537800	-1.24818800	0.91616800
H	0.30402800	-3.06614900	0.94978900
H	1.85544200	-1.58092900	1.91839700
C	2.77095600	-1.44416600	0.01355100
C	3.96385400	-1.95859300	0.52315200
C	2.71887000	-1.10565000	-1.34362400
C	5.07873800	-2.13288200	-0.29575500
H	4.02085600	-2.22211700	1.57646900
C	3.82882500	-1.27089400	-2.16397600
H	1.80384100	-0.69328400	-1.76320600
C	5.01470600	-1.78740200	-1.64168900
H	5.99660200	-2.53596800	0.12061500
H	3.77096400	-0.99466600	-3.21210800
H	5.88131200	-1.91727700	-2.28202800

PRS

C	-1.36776700	-0.98309100	-0.70383800
O	-1.32790600	-1.45199800	-1.81718200
C	-0.26999700	-0.95304900	0.35514400
C	1.10025700	-0.45641200	-0.16253200
H	-0.20743200	-1.96070200	0.78186000
H	0.96675500	-0.06468800	-1.17835000
C	2.19287000	-1.49709300	-0.19316300
C	2.96002800	-1.69265100	-1.34096800
C	2.48617400	-2.24759100	0.95099300
C	3.99579600	-2.62563300	-1.35336000
H	2.74234400	-1.10948000	-2.23186600
C	3.51838700	-3.17951100	0.94227600
H	1.90033600	-2.09357300	1.85610000
C	4.27616900	-3.37210000	-0.21268200
H	4.58161100	-2.76868700	-2.25592000
H	3.73445100	-3.75523200	1.83675800
H	5.08161000	-4.09948700	-0.22079500
H	-0.35972800	1.84240600	0.28263600
C	-3.80016400	-0.16923100	-0.48525200
C	-4.40369100	0.49710400	0.60749400
C	-5.76785800	0.80373200	0.53346700
C	-6.47223200	0.44199900	-0.60689000
C	-5.84566100	-0.22228800	-1.67542300
C	-4.49452000	-0.54097700	-1.63317200
C	-2.23149800	0.20000300	1.12040100
C	-3.38025100	0.72172100	1.61564000
H	-6.26314100	1.31596600	1.35210500
H	-7.52953100	0.67559400	-0.67746400
H	-6.42787000	-0.49027500	-2.55069800

H	-3.99256100	-1.05123100	-2.44654600
H	-3.50759700	1.21741800	2.56672800
N	-2.46728100	-0.34914900	-0.13952900
H	-0.98611200	-1.13045800	2.95571800
C	-0.76551900	0.05943300	1.43347900
O	-0.48253100	-0.33015600	2.75703300
C	0.07143000	1.31162900	1.13885100
C	1.44523900	0.73423600	0.77915200
H	0.08697100	1.98772500	1.99651600
H	1.87482300	0.31480200	1.69652800
C	2.44214200	1.69551600	0.18067400
C	3.72807900	1.80053000	0.71431500
C	2.11587400	2.47273200	-0.93639200
C	4.66559400	2.66720800	0.15567600
H	3.99555500	1.19516700	1.57651200
C	3.04853900	3.33977800	-1.49693100
H	1.12408700	2.40012700	-1.37669900
C	4.32730900	3.44116500	-0.95078600
H	5.65959100	2.73735300	0.58617500
H	2.77749600	3.93679800	-2.36195400
H	5.05444500	4.11877700	-1.38650400
PSR			
C	-1.40240700	1.19466600	-0.31968500
O	-1.37413000	1.99821600	-1.22225500
C	-0.29334000	0.83090400	0.65778700
C	1.03193100	0.42309800	-0.02476500
H	-0.15787700	1.67294300	1.34404900
H	0.81455300	0.12364600	-1.05847100
C	2.10416400	1.48368400	-0.05635500

C	2.75628800	1.79347100	-1.25024300
C	2.50194700	2.13420000	1.11643700
C	3.77932800	2.73934600	-1.27838800
H	2.45859900	1.28781400	-2.16514700
C	3.52251500	3.07904200	1.09229100
H	2.00904400	1.89892100	2.05783300
C	4.16409700	3.38543100	-0.10732500
H	4.27430000	2.97029400	-2.21635900
H	3.81808500	3.57761900	2.01004400
H	4.95954500	4.12353500	-0.12720900
H	-0.27972300	-1.97385500	0.06390900
C	-3.80048300	0.27237600	-0.42779600
C	-4.38487900	-0.74478000	0.36270600
C	-5.72614400	-1.07883700	0.13854000
C	-6.42726800	-0.39807100	-0.84772500
C	-5.81961200	0.61003200	-1.61565300
C	-4.49151500	0.96432900	-1.41897500
C	-2.24619300	-0.51679000	1.03415500
C	-3.37035600	-1.23317000	1.28231800
H	-6.20679600	-1.85541500	0.72499000
H	-7.46722000	-0.64724100	-1.03191900
H	-6.39859600	1.12144200	-2.37735600
H	-4.00487200	1.73881900	-1.99976800
H	-3.49261600	-2.01762500	2.01506500
N	-2.48897500	0.39598400	0.00963500
H	-0.94701700	-0.88110400	3.34037600
C	-0.80296500	-0.39763100	1.46078300
O	-0.63573500	-0.11765400	2.83663900
C	0.10529800	-1.55045000	0.99854100
C	1.44994100	-0.85381800	0.75440800

H	0.15503300	-2.35331000	1.73963800
H	1.83886200	-0.53281100	1.72912100
C	2.51311400	-1.66080300	0.05267100
C	3.80313300	-1.73530700	0.58168500
C	2.24722200	-2.31223300	-1.15671900
C	4.80405600	-2.45046600	-0.07257600
H	4.02361300	-1.22277900	1.51450900
C	3.24375600	-3.02795100	-1.81327000
H	1.25293200	-2.25993900	-1.59407000
C	4.52630900	-3.10048300	-1.27178900
H	5.80066600	-2.49833600	0.35492800
H	3.01963500	-3.52955100	-2.74942800
H	5.30396900	-3.65816800	-1.78360100

PSS

C	1.50465700	1.08253300	0.44646700
O	1.60485600	2.28245600	0.53637100
C	0.29327500	0.16616300	0.38319600
C	-1.06145700	0.26042200	1.06278900
H	0.12738800	0.07132800	-0.70201400
H	-0.90143700	0.42221700	2.13258500
C	-1.99985200	1.32988100	0.55607700
C	-1.64177800	2.21874800	-0.45739800
C	-3.27494100	1.44372300	1.12398500
C	-2.53975700	3.18714200	-0.90751000
H	-0.64912500	2.17623100	-0.89521100
C	-4.17288300	2.40516600	0.67681600
H	-3.56585400	0.76067900	1.91867400
C	-3.80861100	3.27974900	-0.34737800
H	-2.24052900	3.86969300	-1.69675600

H	-5.15842400	2.47450800	1.12661000
H	-4.50868200	4.03057300	-0.69947400
H	-0.34828600	-2.25453300	-0.63120700
C	3.89909600	0.32349300	-0.14346100
C	4.37255900	-0.98909100	-0.37753500
C	5.69580700	-1.16027100	-0.80151200
C	6.48954200	-0.03587900	-0.98007200
C	5.98971500	1.25689500	-0.74676100
C	4.68301500	1.46026000	-0.32322000
C	2.21982900	-1.16712200	0.26730900
C	3.28652300	-1.91570300	-0.10011100
H	6.09102800	-2.15399700	-0.98680200
H	7.51695800	-0.15385300	-1.30831900
H	6.63829600	2.11315200	-0.89950300
H	4.28044000	2.44889600	-0.13687700
H	3.32882900	-2.99313900	-0.16328100
N	2.57545200	0.19613600	0.25339400
H	1.62042500	-0.72896100	2.57777300
C	0.82784800	-1.20607400	0.83910200
O	0.90113900	-1.29084300	2.25961800
C	-0.33399700	-2.09953500	0.45070700
C	-1.57379300	-1.25513300	0.91189800
H	-0.29844100	-3.07111500	0.94605300
H	-1.86162200	-1.59334900	1.91013900
C	-2.76387700	-1.44383600	0.00046000
C	-3.96370600	-1.94913400	0.50314700
C	-2.70098200	-1.10721800	-1.35669100
C	-5.07479100	-2.11616100	-0.32228200
H	-4.02878100	-2.21162500	1.55622700
C	-3.80727500	-1.26509500	-2.18359000

H	-1.78051600	-0.70232900	-1.77168300
C	-5.00005500	-1.77236700	-1.66811900
H	-5.99792100	-2.51251200	0.08889700
H	-3.74097300	-0.99050600	-3.23164900
H	-5.86357000	-1.89653900	-2.31372700

TS6RS'

C	-5.85366200	-1.34134300	-0.94488200
C	-4.59825900	-1.50159500	-0.36312500
C	-4.35028100	-2.50594100	0.56743600
C	-5.39591000	-3.35929900	0.91249500
C	-6.65740200	-3.20674000	0.33103100
C	-6.89493200	-2.19906800	-0.60171400
C	-5.85966200	-0.19334300	-1.92173000
C	-4.53442800	0.55829300	-1.66718000
C	-3.62937600	-0.46468000	-0.88590400
H	-3.36161400	-2.61650600	1.00299600
H	-5.23049400	-4.14838400	1.63861500
H	-7.46233000	-3.87826600	0.61226400
H	-7.87771900	-2.08028300	-1.04794900
H	-6.70625700	0.48695100	-1.79095200
H	-4.04003300	0.85344400	-2.59278900
H	-5.89291300	-0.56125800	-2.95245400
H	-2.84494800	-0.86814200	-1.53183800
N	-2.93413300	0.22205100	0.19781600
O	-4.74285900	1.78524500	-0.97463700
C	-1.66599700	0.11492000	0.60599900
C	-3.50156700	1.24497700	0.90063800
N	-1.52262300	1.02250200	1.56987600
N	-2.66145100	1.76041100	1.75256900

C	-4.84939500	1.68862900	0.43569300
H	-5.62892900	0.98070900	0.74573300
H	-5.08228800	2.67895400	0.82517000
C	-0.31311500	1.26934200	2.30567000
C	0.40748300	2.42793000	1.99192500
C	0.15229200	0.27816100	3.17149800
C	1.67447600	2.55154000	2.55414700
C	1.42939600	0.45339100	3.70648300
C	2.20801700	1.56631800	3.39182200
H	2.27226200	3.42492400	2.30331800
H	1.83368200	-0.31604900	4.35888600
C	-0.66031600	-0.95043800	3.49161100
H	-0.55282400	-1.71596000	2.71599600
H	-1.72399200	-0.71452200	3.58637300
H	-0.31710900	-1.38905300	4.43023900
C	3.60335400	1.71153000	3.93974300
H	3.88775500	0.83701300	4.52830600
H	3.68420800	2.59984700	4.57337400
H	4.32573700	1.82183100	3.12520700
C	-0.15193400	3.46641400	1.05859700
H	-1.00348500	3.98034700	1.51383900
H	-0.49930200	3.00677200	0.12655000
H	0.61346500	4.20144600	0.80468000
C	-0.69921400	-0.95542100	0.15853600
O	-1.12549600	-2.09508700	0.14308700
C	0.73645500	-0.54051800	-0.10656000
C	1.71165700	-1.71448800	-0.26773600
H	1.09166100	0.15930400	0.65419400
H	1.11802100	-2.61674000	-0.46107800
C	2.52623800	-1.95045300	0.98237800

C	2.02219500	-2.81495500	1.95975400
C	3.71433800	-1.26417900	1.25096200
C	2.67656600	-2.98573500	3.17638700
H	1.10043900	-3.35574400	1.75578900
C	4.37689100	-1.43736900	2.46490500
H	4.13332000	-0.58792500	0.51067300
C	3.85938600	-2.29455400	3.43378500
H	2.26642000	-3.66216200	3.92027300
H	5.30108800	-0.89959000	2.65460900
H	4.37628900	-2.42731400	4.37909400
H	1.67658500	-0.31501500	-3.35355600
C	1.05394700	3.68148800	-2.16007300
C	2.21723300	3.49035100	-1.36545000
C	3.03609200	4.59754000	-1.08898500
C	2.68441400	5.83974500	-1.59355500
C	1.52592100	6.00556700	-2.37741800
C	0.69786200	4.93270200	-2.67127200
C	1.11798700	1.52549600	-1.53065800
C	2.23204000	2.10817800	-0.97656200
H	3.93002600	4.48025600	-0.48242200
H	3.30924500	6.70195100	-1.38225100
H	1.27607500	6.99118600	-2.75720700
H	-0.19811700	5.05767900	-3.27134400
H	2.95165400	1.62558100	-0.32859900
N	0.42714400	2.46358800	-2.25395500
H	-0.49127200	2.23622400	-2.61256600
C	0.52509700	0.13216100	-1.49880900
O	-0.83555400	0.17517300	-1.72185500
C	1.32204200	-0.81280600	-2.44646200
C	2.45775600	-1.37016900	-1.57781700

H	0.63572900	-1.61797900	-2.73578700
H	3.15710800	-0.54566000	-1.38676600
C	3.23973100	-2.52379600	-2.15692400
C	4.62678700	-2.44370400	-2.29794700
C	2.59868300	-3.70422300	-2.55045500
C	5.35844400	-3.50869700	-2.82012000
H	5.13902400	-1.53330400	-1.99612400
C	3.32437100	-4.77054000	-3.07141100
H	1.51927300	-3.79028000	-2.45046500
C	4.70893400	-4.67670400	-3.20865000
H	6.43603300	-3.42424500	-2.92215900
H	2.80850900	-5.67744800	-3.37165300
H	5.27491300	-5.50859900	-3.61569400

M6RS'

C	5.24231100	-1.16343400	1.89083300
C	3.85619300	-1.08191700	1.80115400
C	3.01648500	-1.76452500	2.67767900
C	3.60721400	-2.54235500	3.67105900
C	4.99888600	-2.62733200	3.77549800
C	5.82571500	-1.94102000	2.88893600
C	5.91415700	-0.33545200	0.82540000
C	4.77119000	0.16727700	-0.09283100
C	3.43488400	-0.19172100	0.65642500
H	1.93228300	-1.69367200	2.57762400
H	2.98239400	-3.08919300	4.36985900
H	5.44084900	-3.24018300	4.55489500
H	6.90592900	-2.01644400	2.97146400
H	6.64272800	-0.90350000	0.23742900
H	4.82111300	1.24629500	-0.24068100

H	6.45019600	0.51234100	1.26269900
H	2.90522500	0.69811200	0.99388900
N	2.51176700	-0.91021500	-0.23321000
O	4.85230900	-0.36446500	-1.40736400
C	1.17664900	-1.05991200	-0.17604800
C	2.97403900	-1.73368200	-1.22516700
N	0.88810200	-1.94212900	-1.13357000
N	2.00086300	-2.36808000	-1.80639100
C	4.43840500	-1.71224400	-1.51385900
H	4.97838900	-2.36364300	-0.81202400
H	4.63103600	-2.05029800	-2.53181700
C	-0.39795800	-2.51107700	-1.44429700
C	-1.15011200	-1.97473400	-2.48829900
C	-0.79877200	-3.63123500	-0.70320000
C	-2.38002300	-2.57780100	-2.76366600
C	-2.03046100	-4.19272200	-1.01911900
C	-2.83386400	-3.67783300	-2.04201900
H	-2.99857900	-2.16577700	-3.55682900
H	-2.36987200	-5.06070600	-0.45887200
C	0.08903400	-4.20441500	0.36627900
H	0.23336100	-3.45801200	1.15354700
H	1.06926200	-4.46933000	-0.04450000
H	-0.35860600	-5.10350900	0.79318400
C	-4.14544400	-4.33737200	-2.37839400
H	-4.70198900	-4.58514200	-1.47073500
H	-3.97644400	-5.27010200	-2.92660300
H	-4.76738500	-3.68519700	-2.99492800
C	-0.66898900	-0.82169800	-3.32981600
H	-0.29858800	-1.18397800	-4.29374800
H	0.14115500	-0.26218200	-2.85579500

H	-1.49673800	-0.13412600	-3.52723100
C	0.15105100	-0.49891000	0.84994800
O	-0.17726200	-1.37580400	1.71708800
C	-0.91603800	0.39317600	0.10009100
C	-2.31912200	0.36853300	0.70029600
H	-0.91285100	0.31681100	-0.98819800
H	-2.27885700	-0.27247700	1.59098200
C	-3.40188300	-0.13611200	-0.22119100
C	-4.22910600	-1.19401200	0.15663700
C	-3.61730600	0.46710000	-1.46647000
C	-5.24944400	-1.63783200	-0.68311600
H	-4.07048800	-1.67267100	1.11934300
C	-4.63229600	0.02690300	-2.30962700
H	-2.98336500	1.29581700	-1.77845800
C	-5.45510800	-1.02901300	-1.91792600
H	-5.88507400	-2.46126100	-0.37121600
H	-4.78348000	0.50778900	-3.27159700
H	-6.25062200	-1.37345000	-2.57179500
H	-1.04872100	3.35958800	1.71342300
C	2.03372700	4.04749700	-0.88020000
C	1.24384800	3.73386900	-2.01489800
C	1.51954400	4.37861600	-3.23160200
C	2.55262500	5.29913900	-3.28526000
C	3.32483400	5.59420400	-2.14389300
C	3.07945500	4.97467900	-0.92916000
C	0.51456700	2.50510600	-0.26527400
C	0.28729500	2.74649400	-1.59517000
H	0.93007000	4.15494500	-4.11576400
H	2.77464400	5.80447100	-4.21961700
H	4.12670400	6.32174800	-2.21799700

H	3.67089500	5.20219200	-0.04800900
H	-0.47471100	2.27919400	-2.20346200
N	1.56316500	3.28934700	0.16648200
H	1.93408200	3.27829100	1.10471500
C	-0.16728400	1.58985600	0.69726600
O	0.78831600	0.75993200	1.38515200
C	-1.15772500	2.27277600	1.66625100
C	-2.54042800	1.83978200	1.15158500
H	-0.97424100	1.85997400	2.66329300
H	-2.76178200	2.42991000	0.25142100
C	-3.68497200	2.00667500	2.12024200
C	-4.82753300	2.72354900	1.75977300
C	-3.64285300	1.41062200	3.38583700
C	-5.89910300	2.85427500	2.64169900
H	-4.87760400	3.18183200	0.77516900
C	-4.70964900	1.53823100	4.26926600
H	-2.76785500	0.83711700	3.68241300
C	-5.84265100	2.26302400	3.90031300
H	-6.77789700	3.41751400	2.34325400
H	-4.65791000	1.07005900	5.24741600
H	-6.67476100	2.36293000	4.58987600