

ELECTRONIC SUPPORTING INFORMATION FOR

Prediction on the origin of selectivities of NHC-catalyzed asymmetric dearomatization (CADA) reactions

Yang Wang^a, Qiu-Yu Wu^a, Tian-Hua Lai^a, Kai-Jun Zheng^a, Ling-Bo Qu^{b,*}, and Donghui Wei^{b,*}

^a Department of Material and Chemical Engineering, Zhengzhou University of Light Industry, Zhengzhou, Henan Province, 450002, P.R. China

^b College of Chemistry and Molecular Engineering, Center of Computational Chemistry, Zhengzhou University, Zhengzhou, Henan Province, 450001, P.R. China

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* Corresponding Authors: gulingbo@cqu.edu.cn (Y. Wang) and donghuiwei@zzu.edu.cn (D. H. Wei)

1. Computational Details

All the calculations involved in the reaction were performed by using density functional theory (DFT) method with the Gaussian 09 suite of programs, which has been identified to be a powerful and widely used method for exploring the mechanisms of organocatalyst, enzyme as well as transition metal-catalyzed reactions. The solution-phase structure optimization of all the stationary points was carried out at M06-2X/6-31G(d, p) level in DCM solvent using the integral equation formalism polarizable continuum model (IEF-PCM). The M06-2X/6-31G(d, p) harmonic frequencies were performed at 298.15 K and 1 atm to provide the thermal corrections for Gibbs free energies and make sure that the local minima had no imaginary frequencies, while the transition states had one and only one imaginary frequency. The intrinsic reaction coordinate (IRC) was calculated to ensure the transition state connected the correct reactant and product along with the reaction coordinates. Non-covalent interaction (NCI) analysis was plotted by using Multiwfn (version 3.3.8) and the computed 3D-structures were rendered using the CYLView software. In addition, we further refined the energy by employing the single-point energy calculations at the M06-2X-D3/6-31++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 the thermal correction at the M06-2X/6-31G(d, p)//IEF-PCM_{DCM} level to the corresponding single-point energy at the M06-2X-D3/6-31++G (2df, 2pd)//IEF-PCM_{DCM} level. In addition, 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 $\Delta G^{\ddagger}$ is the Gibbs free energy difference between the two diastereomeric transition states.

2. Global reactivity index (GRI)

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

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. Energy profile of direct [1,2]-proton transfer process

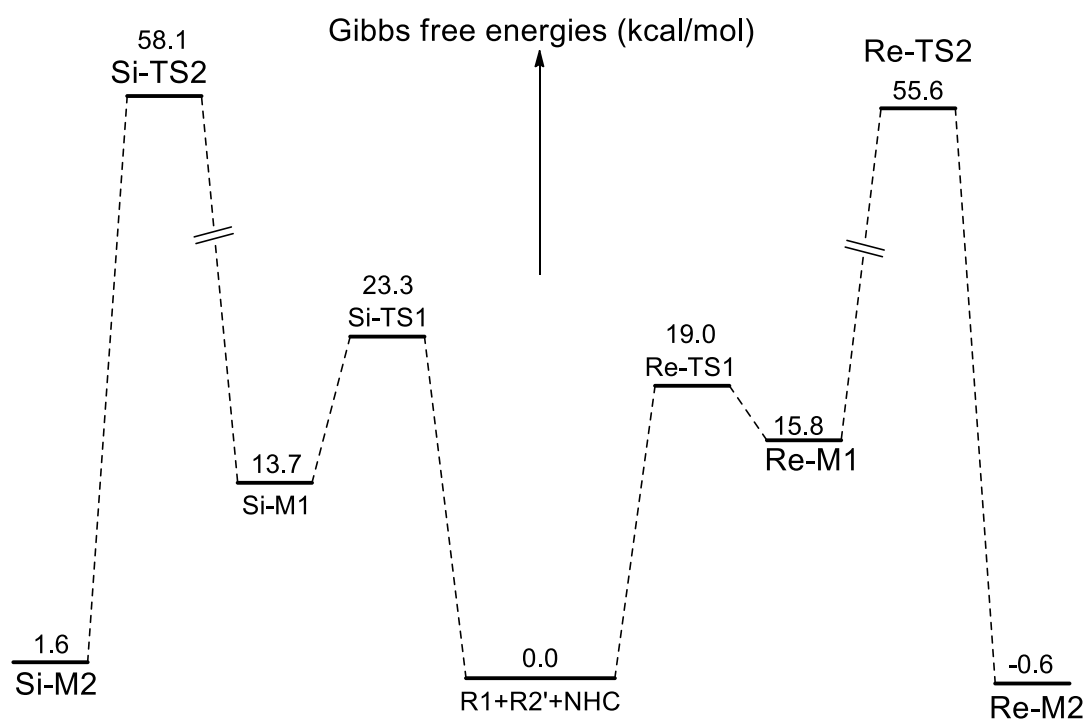


Fig. S1 The energy profile of the direct [1,2]-proton transfer process

5. The whole energy profile involved in Stages 2 and 3

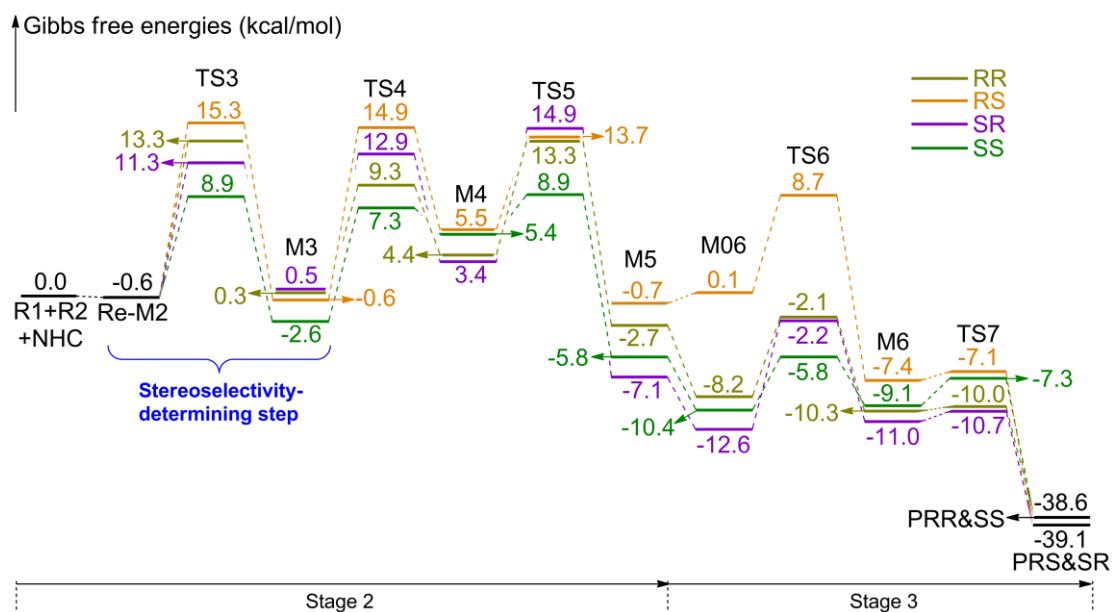


Fig.S2 The whole energy profile involved in **Stages 2 and 3**

6. Benchmark calculations involved in Mannich-type transformations

Table S1. Comparison of the single-point energies of the transition states involved in

Mannich-type transformations				
	G-correction	M06-2X-D3	B3LYP-D3	ω B97X-D
R1	0.1102444	-422.93864	-423.140572	-422.96827
R2	0.2223425	-672.65742	-672.97580	-672.70566
NHC	0.2003973	-11228.58283	-11228.86490	-11228.62595
R1+R2 +NHC	-	-12324.17889 (0.0)	-12324.98127 (0.0)	-12324.29988 (0.0)
Re-M2	0.3416699	-11651.55352 (-0.6)	-11652.03304 (2.2)	-11651.62130 (2.5)
TS3RR	0.5913713	-12323.62478 (13.3)	-12325.00949 (20.8)	-12324.33069 (14.8)
TS3RS	0.5913694	-12323.62148 (15.3)	-12325.01052 (19.0)	-12324.32787 (16.6)
TS3SR	0.5901078	-12323.62784 (11.3)	-12325.00746 (20.4)	-12324.33332 (12.4)
TS3SS	0.5907595	-12323.63174 (8.9)	-12325.01349 (15.4)	-12324.33678 (10.6)
M3RR	0.5921327	-12323.64547 (0.3)	-12325.02277 (8.9)	-12324.35532 (-0.5)
M3RS	0.5954745	-12323.64682 (0.6)	-12325.02762 (8.0)	-12324.36133 (-1.8)
M3SR	0.5968357	-12323.64516 (-0.6)	-12325.02792 (8.6)	-12324.36068 (-0.6)
M3SS	0.5914050	-12323.65013 (-2.6)	-12325.02701 (5.8)	-12324.35903 (-2.9)
TS5RR	0.5944253	-12323.62468 (13.3)	-12325.01373 (14.1)	-12324.34208 (12.1)
TS5RS	0.5959237	-12323.62415 (13.7)	-12325.01014 (16.3)	-12324.34321 (9.8)
TS5SR	0.5950645	-12323.62223 (14.9)	-12325.01666 (11.5)	-12324.33915 (11.8)
TS5SS	0.5932285	-12323.63172 (8.9)	-12325.01839 (10.8)	-12324.34637 (6.1)

7. NCI pictures of the transition states with different substrates

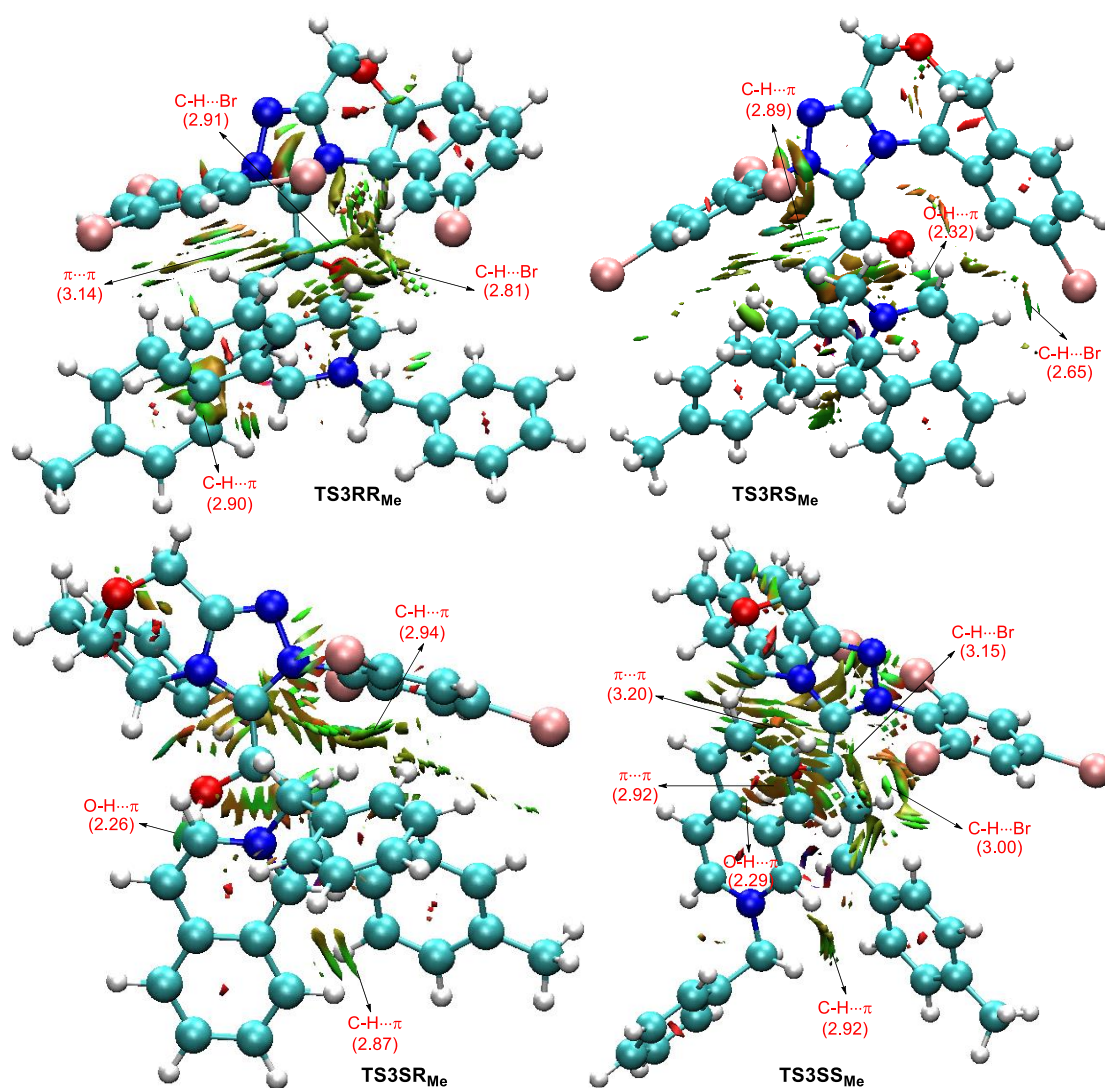


Fig. S3 The NCI pictures of the transition states with R=4-MePh

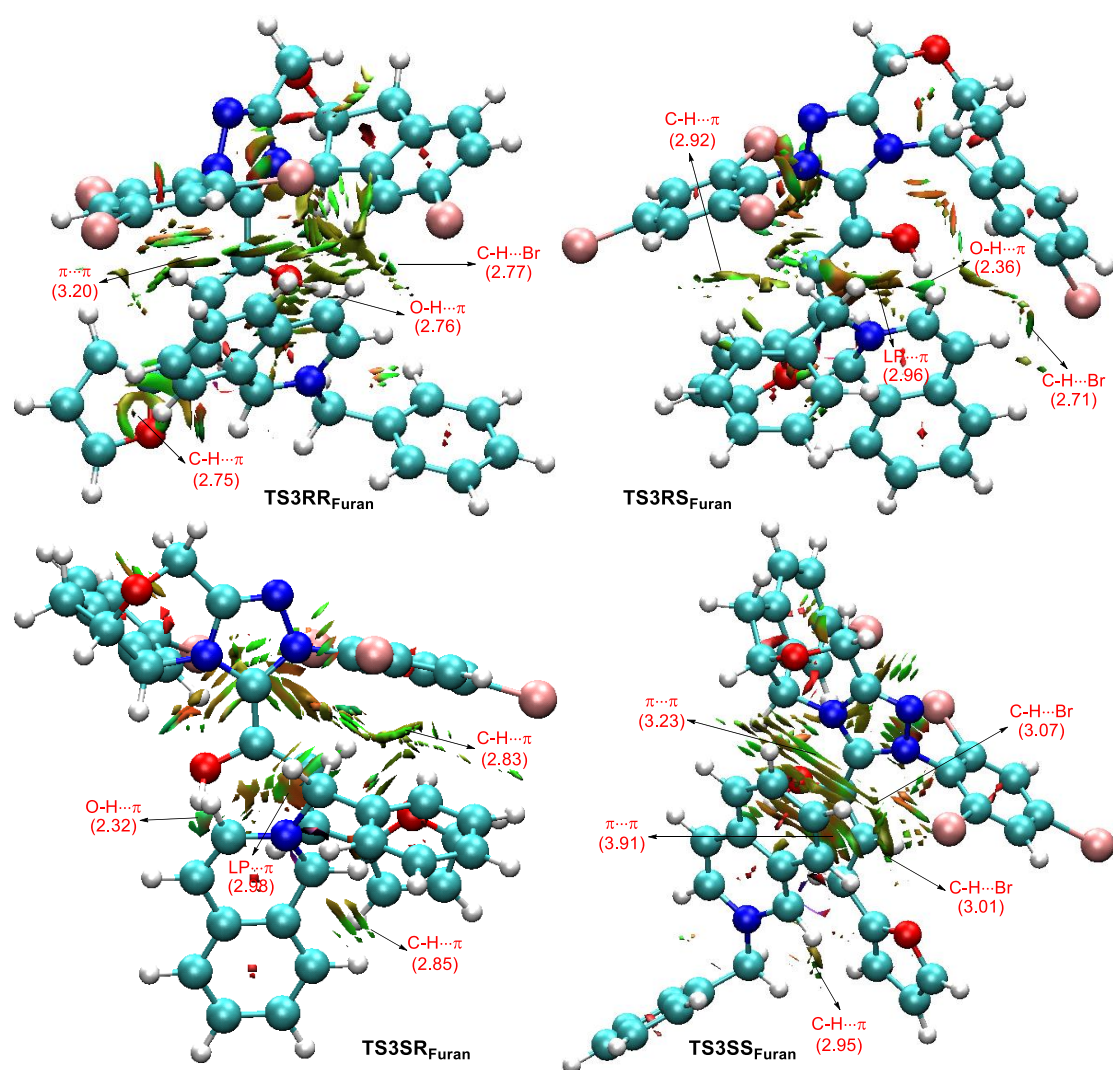


Fig. S4 The NCI pictures of the transition states with R=Furan

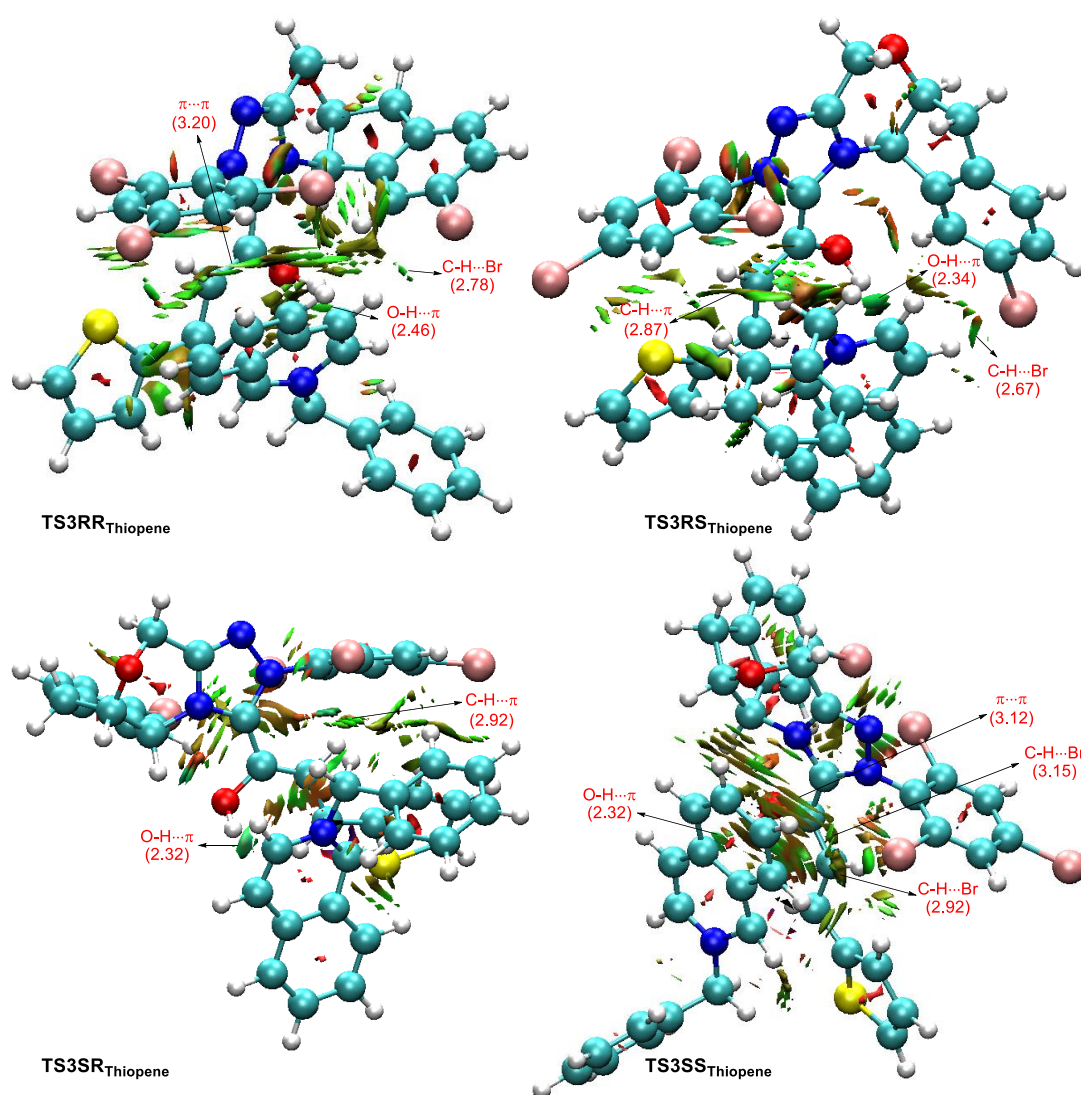


Fig. S5 The NCI pictures of the transition states with R=Thiophene

8. Graphic data of Parr functional analysis

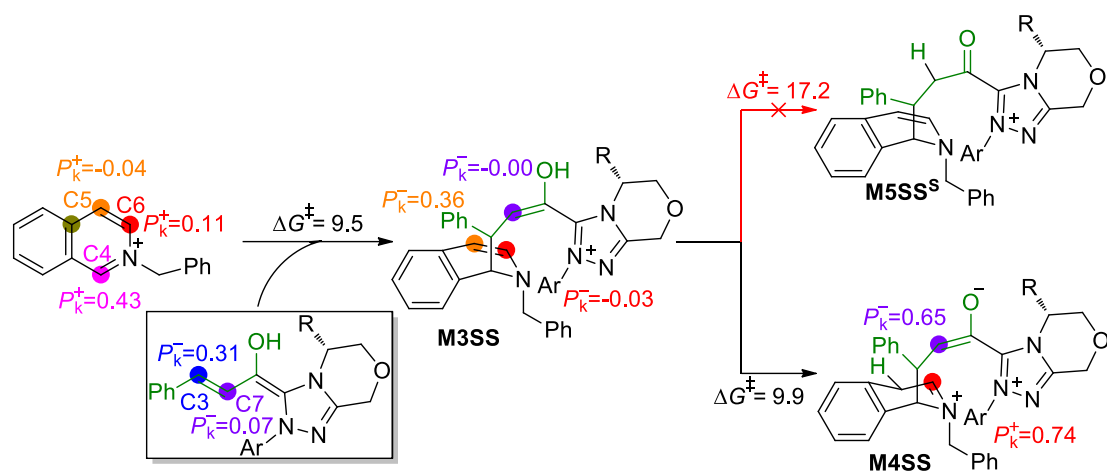


Fig. S6 Possible active sites of isoquinoline and Breslow intermediate by Parr functional analysis

9. Cartesian Coordinates and Energies of the Optimized Structures

R1

C	-0.93650000	-0.58746900	-0.00013900
C	-1.98369100	0.25368100	-0.00010300
H	-1.15195300	-1.65715300	-0.00023300
H	-1.88598100	1.33542400	0.00001100
C	0.48696500	-0.24074800	-0.00007200
C	1.43166500	-1.27524300	0.00007200
C	0.93930800	1.08740900	-0.00014600
C	2.79437700	-0.99490900	0.00016600
H	1.08901200	-2.30642900	0.00011700
C	2.29905500	1.36682400	-0.00005300
H	0.22653600	1.90576600	-0.00029400
C	3.23047800	0.32725400	0.00010500
H	3.51347500	-1.80733700	0.00028200
H	2.63679200	2.39789400	-0.00011700
H	4.29249400	0.54993600	0.00016900
C	-3.34438300	-0.29057000	-0.00027600
O	-4.35235500	0.38788200	0.00047300
H	-3.40517700	-1.39853300	-0.00104300

R2

C	-3.33652700	-2.20238900	-0.04843600
C	-2.02045400	-1.82613400	-0.11804600
C	-1.68954200	-0.44750500	-0.06857700
C	-2.71222000	0.53232300	0.05330200
C	-4.05972000	0.11340700	0.12556200
C	-4.35773700	-1.22688600	0.07385300
H	0.46595200	-0.72587700	-0.23762200
H	-3.60445600	-3.25211500	-0.08589900
H	-1.22892000	-2.56269400	-0.21133100
C	-0.35163800	-0.02065700	-0.14161700
C	-2.32045300	1.89642100	0.09500600
H	-4.84339900	0.85721700	0.22043200
H	-5.39182800	-1.55000200	0.12666500
C	-1.00588900	2.23341700	0.01951400

H	-3.06440300	2.67893800	0.18912800
H	-0.64688200	3.25399400	0.04402000
N	-0.03657900	1.26423900	-0.09747200
C	1.38077800	1.74732000	-0.21125200
H	1.49799400	2.49763000	0.57300000
H	1.45339000	2.24108800	-1.18297500
C	2.40051300	0.65489000	-0.07373900
C	2.94322300	0.05292800	-1.21060400
C	2.79723000	0.22445600	1.19547200
C	3.87781900	-0.97121200	-1.08015900
H	2.63556500	0.39013200	-2.19665700
C	3.72917100	-0.79990300	1.32457700
H	2.37710600	0.69521100	2.08038200
C	4.26966500	-1.39737500	0.18668100
H	4.30132800	-1.43157100	-1.96626300
H	4.03858800	-1.12779900	2.31112800
H	5.00071300	-2.19242700	0.28906700
NHC			
C	4.19260600	0.83676600	0.87515300
C	3.48832000	0.66545200	-0.31822300
C	3.52707200	-0.53023800	-1.02334200
C	4.30832500	-1.55496300	-0.50096900
C	5.02756800	-1.40697800	0.68335100
C	4.96916800	-0.20110600	1.37902800
C	3.94685800	2.20795300	1.45140600
C	3.40444500	2.98148500	0.22844700
C	2.71318000	1.91503100	-0.65922000
H	2.96538700	-0.66510200	-1.94070000
H	5.52651500	-0.08295700	2.30295300
H	3.20119600	2.14563000	2.25277400
H	4.25199700	3.37456800	-0.33794800
H	4.84020700	2.67664800	1.86919600
H	2.74232200	2.17359500	-1.71968500
N	1.30908400	1.79515200	-0.25393300
O	2.58794800	4.10129500	0.49615300
C	0.45548700	0.80986700	-0.66905400
C	0.68792300	2.65473900	0.61905500

N	-0.64658000	1.17193900	0.02126400
N	-0.54094900	2.29348200	0.82108100
C	1.41128300	3.81774800	1.22660900
H	1.63100400	3.61058900	2.28144400
H	0.78534500	4.71024800	1.18182900
C	-1.84762600	0.42768600	0.05860300
C	-1.93889300	-0.71869100	0.85027800
C	-2.96470300	0.82260000	-0.67570700
C	-3.10319100	-1.47416800	0.89569300
C	-4.14493500	0.09065600	-0.64396000
C	-4.19198200	-1.05452300	0.14109100
H	-3.15789200	-2.36601600	1.50676900
H	-5.00396800	0.40439400	-1.22294700
Br	-0.45622900	-1.24332500	1.88236800
Br	-5.77957000	-2.07257600	0.17773700
Br	-2.87139600	2.37334100	-1.73429200
H	5.62879600	-2.22962300	1.05370200
Br	4.40402900	-3.20379000	-1.43509700

AcOH

C	-0.09176700	0.12097200	0.00006400
O	-0.63762400	1.19873300	-0.00004800
O	-0.77833300	-1.03469700	-0.00003800
H	-1.72252100	-0.81045500	-0.00011400
C	1.39156400	-0.11339400	0.00004700
H	1.66997300	-0.69456200	0.88163100
H	1.66994400	-0.69466300	-0.88148100
H	1.91147600	0.84192200	-0.00001500

AcO⁻

C	-0.20126400	-0.00012000	-0.01376000
O	-0.75211200	-1.12720100	0.00313100
O	-0.75568900	1.12536800	0.00284400
C	1.34690900	0.00130300	-0.00445300
H	1.74455400	0.90177700	-0.47789300
H	1.69606900	-0.00614400	1.03477800
H	1.74792100	-0.88806700	-0.49541300

EtOH

C	-1.21842100	-0.22107800	-0.00000900
C	0.08741600	0.54820100	0.00000800
H	-1.28151200	-0.85752600	0.88626200
H	-2.07037900	0.46290300	0.00004100
H	-1.28154500	-0.85744400	-0.88633400
H	0.14165300	1.19627300	-0.88582800
H	0.14163400	1.19626900	0.88584900
O	1.14464500	-0.39839800	0.00001800
H	1.97902300	0.08397100	-0.00013000

Re-TS1

C	-4.08003000	0.57516700	0.45633900
C	-5.29177900	0.76742200	-0.19709700
C	-6.01714200	-0.33650300	-0.64289900
C	-5.49964700	-1.61506800	-0.44779900
C	-4.28366400	-1.76928100	0.21819400
C	-3.56324100	-0.69004900	0.70726900
C	-3.37777500	1.88470700	0.73473000
C	-4.29784100	2.96902400	0.05946200
C	-5.60924900	2.23535400	-0.32103700
H	-6.96422900	-0.21026200	-1.15791000
H	-6.02901100	-2.48735700	-0.81437100
H	-2.63476700	-0.80719500	1.26096800
H	-3.21620800	2.05795200	1.79958000
H	-4.48225900	3.78522400	0.75738600
H	-6.41292600	2.51795800	0.36593400
C	-1.93409300	2.06785000	-1.26637300
C	-3.08523400	2.70357400	-1.97555200
C	-0.92431000	1.30707800	0.55852600
H	-3.79088500	1.93703400	-2.32545300
H	-5.92780200	2.52918000	-1.32595000
N	-2.06335500	1.84829900	0.08264600
N	-0.76071100	1.71436000	-1.68745400
N	-0.15488900	1.24406500	-0.53738300
O	-3.68833500	3.59714000	-1.05915400
H	-2.73970400	3.28077300	-2.83299600
C	1.06818500	0.53648400	-0.69518200

C	2.28489600	1.20703200	-0.77500800
C	1.05207500	-0.85267900	-0.84260900
C	3.46374300	0.53250700	-1.06716100
C	2.21831700	-1.55344000	-1.11663800
C	3.40616700	-0.84197800	-1.25095400
H	4.40429700	1.06585900	-1.12372600
H	2.20141100	-2.63032600	-1.22875900
Br	-3.54515700	-3.50670800	0.42750700
Br	-0.56623300	-1.79177500	-0.60887200
Br	4.98597500	-1.78022300	-1.66102600
Br	2.33348800	3.04200800	-0.39348900
C	1.75886700	0.88837200	2.53371800
C	0.61046900	0.22237800	2.38336700
H	1.70466000	1.95330200	2.76835100
H	0.56977600	-0.83141400	2.10834600
C	3.11096100	0.35957900	2.30219800
C	4.17049600	1.26141400	2.14277300
C	3.36765500	-1.01077400	2.14967600
C	5.44421300	0.81271200	1.80343100
H	3.98069400	2.32606000	2.25257000
C	4.63997100	-1.45927100	1.81941000
H	2.56506700	-1.72944000	2.28802900
C	5.68122000	-0.54874200	1.63249600
H	6.24961000	1.52797800	1.66889700
H	4.82059700	-2.52212300	1.69022100
H	6.66940800	-0.90180200	1.35537600
C	-0.71461800	0.91740900	2.48368000
O	-1.73811400	0.32213100	2.89862100
H	-0.57768800	2.00010800	2.70717700

Si-TS1

C	2.75516300	-1.46223200	0.55790500
C	3.66088400	-2.27246700	1.23494100
C	3.78158100	-3.61523800	0.88325400
C	2.96391700	-4.13179000	-0.11922900
C	2.05066500	-3.29650300	-0.76159100
C	1.93228400	-1.94716800	-0.45442400
C	2.69493400	-0.07707400	1.16572700

C	3.56530300	-0.18258400	2.46852200
C	4.35991900	-1.50505600	2.32857900
H	4.47937200	-4.26633100	1.40040600
H	3.01670000	-5.18035000	-0.38936900
H	1.19753300	-1.32548100	-0.97109900
H	3.05966300	0.70780900	0.49915900
H	4.22996500	0.67751100	2.54490600
H	5.39884000	-1.29218100	2.05760400
C	0.70891700	-0.34010700	2.59687300
C	1.61165300	-0.91231700	3.64254700
C	0.34375400	0.67477200	0.65489200
H	1.82518400	-1.96832500	3.42469500
H	4.37805500	-2.03729300	3.28444600
N	1.30092600	0.21939700	1.48861900
N	-0.58226400	-0.24339900	2.53613400
N	-0.77712700	0.38823800	1.32619700
O	2.78900000	-0.12715400	3.65653600
H	1.15203000	-0.84400200	4.62848000
C	-2.07606200	0.44505600	0.76262400
C	-2.81471700	1.62402500	0.74927800
C	-2.60885400	-0.70547000	0.17688500
C	-4.09303700	1.65845300	0.20674800
C	-3.88664800	-0.69849100	-0.36369200
C	-4.61458100	0.48614300	-0.32638800
H	-4.66567200	2.57706200	0.20220700
H	-4.30165200	-1.59296000	-0.81064400
Br	0.86686300	-4.02759400	-2.05035900
Br	-1.55600700	-2.25775400	0.08347900
Br	-6.36300000	0.50947700	-1.03193300
Br	-2.04887100	3.20093100	1.42678800
C	2.00187400	2.79144500	-1.36727700
C	1.59690400	1.53234900	-1.55851000
H	1.27270600	3.50177300	-0.97144400
H	2.24787800	0.76405200	-1.97563300
C	3.34181600	3.34365100	-1.62264300
C	3.53179600	4.72842200	-1.53473000
C	4.44502100	2.53744600	-1.94089000
C	4.77971400	5.29712700	-1.77059800

H	2.68636500	5.36240600	-1.28123100
C	5.69165100	3.10425600	-2.17648600
H	4.32855200	1.45907200	-2.00049700
C	5.86441800	4.48626600	-2.09403200
H	4.90502500	6.37288400	-1.69974100
H	6.53454200	2.46616100	-2.42225100
H	6.83993500	4.92563800	-2.27547000
C	0.19369700	1.08436600	-1.25020700
O	-0.27161800	0.05567400	-1.80182800
H	-0.47109900	1.95397400	-1.04643200

Re-M1

C	4.10307600	0.57343900	-0.49241300
C	5.32444300	0.76185200	0.14430200
C	6.05322800	-0.34542800	0.57577400
C	5.52819700	-1.62192300	0.38400300
C	4.30352100	-1.76985200	-0.26769000
C	3.58027400	-0.68852900	-0.74691200
C	3.40399900	1.88851200	-0.75793600
C	4.31203600	2.95700700	-0.04494700
C	5.64409600	2.22990400	0.26465500
H	7.00798100	-0.22372500	1.07749800
H	6.05966800	-2.49678500	0.74143000
H	2.64681000	-0.77343400	-1.30264300
H	3.23925300	2.06876300	-1.81918700
H	4.46037100	3.81802400	-0.69617500
H	6.40846400	2.51943500	-0.46346300
C	1.96833600	1.96602600	1.25066300
C	3.13527200	2.54146800	1.98552900
C	0.91047700	1.37692000	-0.58081900
H	3.84466700	1.75027900	2.26444900
H	6.01179100	2.52175000	1.25292100
N	2.08079100	1.83444900	-0.10880800
N	0.79118000	1.61669700	1.66542900
N	0.14251500	1.24515700	0.51107000
O	3.71792700	3.50142700	1.12639900
H	2.80037300	3.05163500	2.88848100
C	-1.08271900	0.53329100	0.67919200

C	-2.29997300	1.19803900	0.78198500
C	-1.04688900	-0.85488700	0.82858800
C	-3.47017800	0.50722000	1.07054300
C	-2.20468000	-1.56826400	1.10321300
C	-3.40025300	-0.86915600	1.23826100
H	-4.41556500	1.03103600	1.13585200
H	-2.17644200	-2.64540400	1.21040000
Br	3.55726600	-3.50546300	-0.47409900
Br	0.58442200	-1.76451800	0.57811000
Br	-4.97235600	-1.82490500	1.63405700
Br	-2.36328900	3.03590200	0.42838100
C	-1.82711100	1.00768700	-2.45298800
C	-0.66892000	0.39131100	-2.20498200
H	-1.80823700	2.07853600	-2.66163300
H	-0.62051200	-0.67095000	-1.96314500
C	-3.16402200	0.41218600	-2.29899800
C	-4.25959600	1.26424600	-2.11210800
C	-3.36693900	-0.97214700	-2.19946800
C	-5.51542500	0.75303100	-1.79415000
H	-4.11128600	2.33919000	-2.17800500
C	-4.62042700	-1.48246900	-1.88747700
H	-2.53532800	-1.65244100	-2.35936200
C	-5.69767900	-0.62158800	-1.67058200
H	-6.34913400	1.43023100	-1.63635400
H	-4.75889800	-2.55582800	-1.79906200
H	-6.67102700	-1.02334300	-1.40743200
C	0.65642600	1.12303700	-2.10917800
O	1.70911500	0.53604000	-2.65883400
H	0.44642800	2.17805700	-2.44099800

Si-M1

C	3.97420300	0.94271600	-0.61382800
C	5.18867000	1.23452300	-0.00433000
C	6.08431000	0.20229500	0.27254900
C	5.73025500	-1.10863700	-0.03839200
C	4.50489500	-1.36346100	-0.65566600
C	3.61787900	-0.34926500	-0.98277200
C	3.07309100	2.15277000	-0.67740400

C	3.88931300	3.28900900	0.03810400
C	5.30994800	2.71126200	0.27352700
H	7.03803500	0.40370500	0.75004800
H	6.39505500	-1.93105600	0.20036500
H	2.68593200	-0.53137500	-1.51043600
H	2.73411100	2.38893000	-1.68477300
H	3.91842600	4.17133200	-0.59990000
H	6.02348100	3.17699900	-0.41281300
C	1.82965400	1.93344100	1.46778900
C	2.91580600	2.71810700	2.12845000
C	0.80133700	1.08739100	-0.27215400
H	3.76248700	2.06009300	2.37000800
H	5.64991600	2.93756800	1.28892700
N	1.85779300	1.82502300	0.09892500
N	0.80273600	1.32237700	1.97598100
N	0.18437800	0.79457400	0.87581700
O	3.28414600	3.74958600	1.23824700
H	2.55042500	3.17322400	3.04904700
C	-0.94951000	-0.04521700	0.99996500
C	-2.21615400	0.51535500	1.15476900
C	-0.80822600	-1.42744100	0.88225700
C	-3.34527400	-0.28727900	1.18400600
C	-1.92958300	-2.24940900	0.88924400
C	-3.18106400	-1.66003300	1.03262800
H	-4.33157600	0.15141100	1.26940900
H	-1.82937100	-3.32094600	0.77027400
Br	3.99636900	-3.15608300	-1.01847800
Br	0.90391300	-2.17369200	0.62116000
Br	-4.72225700	-2.73919100	0.95622800
Br	-2.39269900	2.37776700	1.17763600
C	-2.09788000	0.50700500	-1.92273100
C	-1.00016700	1.26912700	-1.91523300
H	-1.96301800	-0.57203300	-1.81023800
H	-1.04143100	2.35229700	-2.02594900
C	-3.50280900	0.94297700	-1.97254200
C	-4.50917900	-0.02109300	-1.82088000
C	-3.88271500	2.28697700	-2.09655800
C	-5.85259700	0.34033800	-1.78517200

H	-4.22986900	-1.06578800	-1.69906900
C	-5.22403300	2.64870700	-2.07146500
H	-3.12295500	3.05472800	-2.20826400
C	-6.21494000	1.67869500	-1.91313900
H	-6.61252300	-0.42367400	-1.65363900
H	-5.50004500	3.69392200	-2.16963800
H	-7.26071500	1.96749200	-1.88688900
C	0.40412100	0.68314300	-1.73498900
O	1.31935800	1.06838600	-2.60419600
H	0.24873600	-0.42445100	-1.61919400

Re-M02^A

C	3.59981200	0.82953400	-0.05860300
C	4.76577900	1.22947000	-0.70114200
C	4.96256200	2.57995900	-0.98564600
C	3.96896100	3.50149500	-0.65704700
C	2.80287500	3.06117200	-0.03149100
C	2.60635100	1.72952800	0.29929400
C	3.52110700	-0.67446700	0.05827300
C	4.70138100	-1.19421600	-0.83160900
C	5.62882800	0.03369400	-1.02304000
H	5.86358700	2.91716000	-1.48820300
H	4.08924900	4.55090900	-0.90099500
H	1.69689900	1.39671900	0.78621300
H	3.60015400	-1.04519300	1.07527700
H	5.20452100	-2.01813100	-0.32643200
H	6.47894100	-0.02871600	-0.33631000
C	2.04228700	-1.08730300	-1.85403000
C	3.25795000	-1.01882500	-2.72082400
C	1.01197700	-1.18119000	0.07284100
H	3.54280600	0.02822200	-2.89506000
H	6.03151500	0.04825700	-2.03997900
N	2.22062700	-1.08544500	-0.49539100
N	0.78829700	-1.19035800	-2.16968300
N	0.15676000	-1.24021000	-0.95888400
O	4.27374500	-1.74861800	-2.06705800
H	3.05999300	-1.49528800	-3.68086900
C	-1.25672000	-1.06732200	-0.94606800

C	-2.11876800	-2.14416900	-0.77331600
C	-1.77376000	0.22266700	-1.08517400
C	-3.49440000	-1.94950700	-0.74720200
C	-3.14300300	0.43996800	-1.06356500
C	-3.98327600	-0.65628600	-0.89770100
H	-4.16597500	-2.78536300	-0.59639000
H	-3.54401300	1.44452100	-1.12956300
Br	1.39409700	4.28302100	0.32891900
Br	-0.59462700	1.68186100	-1.15671600
Br	-5.83978600	-0.36406700	-0.82414500
Br	-1.39026400	-3.84242200	-0.44767000
C	-0.87384000	0.63727300	2.08126200
C	-0.66996600	-0.65482500	1.81825900
H	-0.01356700	1.29516700	2.20186200
H	-1.50944500	-1.32996900	1.67267200
C	-2.20401000	1.26975000	2.08507800
C	-2.30773300	2.61423400	1.70749400
C	-3.37700800	0.54247600	2.32900100
C	-3.55695200	3.20493400	1.53415400
H	-1.39930500	3.18094100	1.51559500
C	-4.62300000	1.13482100	2.16304400
H	-3.31112900	-0.49336900	2.65001400
C	-4.71720200	2.46484500	1.75127700
H	-3.62358400	4.24371000	1.22661000
H	-5.52371800	0.55815600	2.34793000
H	-5.69085800	2.92387100	1.61296800
C	0.70681600	-1.22869400	1.57658000
O	1.69351500	-0.54261600	2.25523300
H	0.72076900	-2.30668100	1.80326700
C	3.38208400	-3.24444300	2.27106200
O	2.81395700	-3.32869100	1.16731500
O	3.27569900	-2.25981200	3.08283600
H	2.36476900	-1.25943100	2.64088100
C	4.30382400	-4.36606400	2.73312100
H	5.31397600	-3.97086500	2.86976300
H	3.96942400	-4.73979200	3.70398100
H	4.32241000	-5.17965500	2.00856700

Re-M02^E

C	3.03113000	-1.30440700	-0.28765600
C	4.12077600	-1.93315500	-0.88318700
C	5.02952400	-1.17934500	-1.62208300
C	4.80379900	0.18606000	-1.80027900
C	3.68403300	0.77806400	-1.21902100
C	2.79824600	0.05590300	-0.43216500
C	2.09867000	-2.31864900	0.34316000
C	2.57624200	-3.67783200	-0.26060700
C	4.04844400	-3.42482900	-0.65773300
H	5.88392700	-1.64952300	-2.09846700
H	5.47412300	0.78061700	-2.41037300
H	1.93253500	0.53251900	0.01278700
H	2.08539200	-2.31196500	1.43497300
H	2.44484800	-4.47199700	0.47175000
H	4.71106100	-3.72882100	0.15983500
C	0.40431300	-2.19992200	-1.42290400
C	1.32066600	-3.06221900	-2.23354600
C	-0.24108000	-1.33128600	0.48010900
H	2.13831100	-2.46504800	-2.65811200
H	4.31579900	-4.01369300	-1.53874200
N	0.74001900	-2.01858000	-0.10670300
N	-0.73641800	-1.64379400	-1.70185800
N	-1.12205300	-1.10470100	-0.50078800
O	1.78481300	-4.08569700	-1.37433700
H	0.76750600	-3.53515200	-3.04509200
C	-2.19769800	-0.17899800	-0.45603900
C	-3.45487400	-0.55290500	0.01334300
C	-1.98467600	1.12687300	-0.90606500
C	-4.50443600	0.35556100	0.01658300
C	-3.02190700	2.04827300	-0.91449900
C	-4.27275000	1.64107300	-0.46017800
H	-5.48113000	0.06580000	0.38296200
H	-2.85830200	3.06031700	-1.26300800
Br	3.27904000	2.59827300	-1.57124000
Br	-0.25813200	1.64960200	-1.45636000
Br	-5.69846000	2.86974200	-0.47799900
Br	-3.69960100	-2.28536000	0.69069000

C	1.36180300	0.74812600	2.68037900
C	0.24247100	0.48442200	2.00425700
H	1.78447800	-0.07395400	3.25608800
H	-0.27875600	1.25267100	1.43238300
C	2.07997400	2.03255100	2.69754800
C	3.00276100	2.29110000	3.71947300
C	1.91056200	2.99251500	1.68988400
C	3.71811200	3.48343900	3.75042100
H	3.15407800	1.54548600	4.49529400
C	2.63362400	4.17996000	1.71419400
H	1.22481300	2.79926700	0.86824800
C	3.53609500	4.43254800	2.74613300
H	4.42544500	3.66839400	4.55264100
H	2.50430900	4.90274400	0.91435400
H	4.10276900	5.35790000	2.76096700
C	-0.32375600	-0.93417000	1.96807500
O	0.32095800	-1.82207600	2.73704700
H	-1.42334000	-0.86029000	2.14499400
C	-1.29361100	-4.84781900	0.21421200
C	-0.95590400	-4.62762200	1.68389500
H	-0.55529700	-5.51108700	-0.24476500
H	-2.28818800	-5.29171100	0.09809700
H	-1.28692500	-3.90323500	-0.33881000
H	-1.66145100	-3.89691800	2.11220000
H	-1.11288600	-5.57054500	2.23048400
O	0.36809800	-4.18822000	1.85059800
H	0.33211800	-3.25315900	2.25589400

Re-TS2

C	3.77460400	0.30821000	0.19142300
C	4.30143500	0.31379800	-1.10047400
C	4.17103300	1.44560900	-1.89986100
C	3.47565900	2.54991100	-1.40942100
C	2.95891400	2.51065500	-0.11580200
C	3.11906600	1.41303600	0.71842600
C	3.87509600	-1.06960700	0.81055600
C	4.91947400	-1.77613500	-0.09850800
C	4.91437900	-1.01694100	-1.44862500

H	4.57745300	1.46698200	-2.90617700
H	3.32165200	3.42719700	-2.02811300
H	2.72720900	1.37586300	1.73353300
H	4.11626100	-1.06892300	1.87113600
H	5.89456500	-1.65976800	0.37809900
H	5.92206700	-0.93037500	-1.86140500
C	2.38399200	-2.68121700	-0.38532200
C	3.52130900	-3.54662700	-0.84164500
C	1.35403700	-1.20724500	0.89917400
H	3.61277200	-3.50234800	-1.93275600
H	4.30488500	-1.52840000	-2.20132800
N	2.57528100	-1.76541500	0.62781500
N	1.16327500	-2.70918100	-0.80304800
N	0.51861300	-1.76812400	-0.02219800
O	4.71334600	-3.17218900	-0.18515600
H	3.32196400	-4.58354200	-0.56144000
C	-0.79647700	-1.39306100	-0.37726100
C	-1.87631000	-2.20611600	-0.03517400
C	-1.04376000	-0.20042300	-1.06267400
C	-3.17709800	-1.86085600	-0.37674200
C	-2.33380400	0.16777500	-1.41815500
C	-3.38324100	-0.67369900	-1.06944700
H	-4.00952600	-2.49148100	-0.09099500
H	-2.51965600	1.10977300	-1.91899300
Br	1.86659900	3.94339100	0.48070400
Br	0.38021300	0.98267400	-1.38915100
Br	-5.14421500	-0.15911200	-1.49519000
Br	-1.55431800	-3.73907700	1.00208300
C	-1.28245100	0.40635200	1.99862400
C	0.03324100	0.64585500	1.95839100
H	-1.61898500	-0.60741000	2.21947100
H	0.41416600	1.65917600	1.81156900
C	-2.33736600	1.36747300	1.64258600
C	-3.67760000	1.02953600	1.86940100
C	-2.05134300	2.56832800	0.97401900
C	-4.70703100	1.86807300	1.45418400
H	-3.90855400	0.08834800	2.36260600
C	-3.08113700	3.40957800	0.56804500

H	-1.02371000	2.82985000	0.73554100
C	-4.41185500	3.06354200	0.80313100
H	-5.73968900	1.58303500	1.62956000
H	-2.84537500	4.33287400	0.04784100
H	-5.21231700	3.71627900	0.47005200
C	1.07656800	-0.40164600	2.04435700
O	2.18150700	-0.15690000	2.92365500
H	1.20012000	-1.06596900	3.01093400

Re-TS2^A

C	-3.85643600	-0.47823500	-0.11743600
C	-5.03707100	-0.67807800	-0.82480000
C	-5.43260600	-1.97263500	-1.15727000
C	-4.62051200	-3.04766600	-0.80168000
C	-3.43979200	-2.81114800	-0.09885000
C	-3.04593800	-1.53594400	0.27733200
C	-3.53721100	0.99400500	0.02725200
C	-4.63141300	1.71607500	-0.84430700
C	-5.70109300	0.63638400	-1.14596700
H	-6.34960900	-2.14964700	-1.71034800
H	-4.89257000	-4.06034200	-1.07685700
H	-2.13585300	-1.36192800	0.84095700
H	-3.55123300	1.35133700	1.05749800
H	-5.05064900	2.55427200	-0.28815500
H	-6.58147900	0.79230800	-0.51465300
C	-2.00476500	1.30153900	-1.88339900
C	-3.21444200	1.47896100	-2.74121500
C	-0.97984500	1.09877100	0.05872700
H	-3.65933300	0.50328500	-2.98241000
H	-6.03133400	0.71385000	-2.18624500
N	-2.19765200	1.23593300	-0.52590100
N	-0.75355300	1.24583600	-2.20056700
N	-0.11758400	1.09661800	-0.98513100
O	-4.10910700	2.30609000	-2.02493700
H	-2.94940500	1.98580000	-3.66888400
C	1.25352500	0.72369200	-1.00741400
C	2.24317800	1.69403800	-1.15614300
C	1.62835200	-0.61774700	-0.90090600

C	3.58538300	1.34690300	-1.22180100
C	2.96531800	-0.98945700	-0.95995900
C	3.92443500	0.00199800	-1.13101600
H	4.34696000	2.10855900	-1.32968100
H	3.25352500	-2.02805500	-0.85323600
Br	-2.29331000	-4.26222500	0.33029600
Br	0.31843700	-1.93224100	-0.59495100
Br	5.74149400	-0.48604000	-1.21972500
Br	1.73846000	3.50318800	-1.16682200
C	1.09036800	-0.38012800	2.36986400
C	0.70571300	0.76329200	1.79334500
H	0.32473800	-1.08920800	2.67903600
H	1.45374700	1.46349900	1.42426200
C	2.48716700	-0.83440700	2.39175500
C	2.74006100	-2.20653300	2.26262100
C	3.57356400	0.05258600	2.37892000
C	4.03913600	-2.67779300	2.08915800
H	1.90196200	-2.89894800	2.25653900
C	4.86903700	-0.41847400	2.20399700
H	3.39697100	1.11760200	2.50245600
C	5.10703700	-1.78505200	2.05053200
H	4.21590800	-3.74308100	1.97629200
H	5.69871200	0.28159400	2.17963700
H	6.11871600	-2.14887000	1.90237500
C	-0.70462500	1.10137200	1.48134600
O	-1.65582200	0.34493800	2.19309600
H	-0.95049600	2.43300400	1.81724600
C	-2.39483300	3.49087500	2.86914800
O	-1.28849000	3.54960600	2.21386400
O	-3.00742400	2.43985400	3.13000800
H	-2.18338400	0.99726000	2.71385900
C	-2.93463700	4.82361600	3.33648700
H	-3.00109600	5.50967100	2.48974000
H	-3.91110800	4.69935600	3.80178200
H	-2.23562600	5.25734000	4.05585200
Re-TS2 ^E			
C	-3.64298900	0.77730100	0.20272600

C	-4.86270700	1.04628800	-0.40802000
C	-5.50945100	0.04018600	-1.12435800
C	-4.90803400	-1.21128800	-1.24212300
C	-3.68019400	-1.44538400	-0.62330800
C	-3.03551500	-0.46947500	0.12216100
C	-3.04205500	2.01863600	0.82057300
C	-4.01913000	3.17709700	0.40527100
C	-5.27263500	2.47976700	-0.18517700
H	-6.46125600	0.22781500	-1.61100500
H	-5.38098500	-1.99833600	-1.81826100
H	-2.08450300	-0.68433600	0.60173800
H	-2.89953700	1.94672500	1.89726300
H	-4.26989200	3.77620400	1.27946300
H	-6.10447400	2.54206300	0.52283000
C	-1.60084100	2.74968500	-1.04835100
C	-2.77008400	3.50798200	-1.58993000
C	-0.56359900	1.56103800	0.47743100
H	-3.42922200	2.83017700	-2.15109700
H	-5.59230200	2.98648700	-1.10098200
N	-1.71156600	2.21871000	0.21577200
N	-0.45094200	2.48984900	-1.58266800
N	0.18967400	1.75719800	-0.61568400
O	-3.43020900	4.10346500	-0.49437400
H	-2.43241400	4.30081400	-2.25740500
C	1.43216600	1.14049300	-0.90349000
C	2.63135500	1.70417000	-0.47539200
C	1.44258500	-0.06561200	-1.60771500
C	3.84098100	1.08312200	-0.76579900
C	2.63806600	-0.69618300	-1.91660800
C	3.82398700	-0.10231400	-1.49156800
H	4.77374700	1.51474000	-0.42544200
H	2.64624000	-1.63548900	-2.45495900
Br	-2.81256600	-3.11780400	-0.83530100
Br	-0.19771400	-0.90361000	-1.99349100
Br	5.45571700	-0.95650900	-1.87856700
Br	2.59394400	3.26858200	0.54901600
C	-0.22964700	-1.53666800	2.32039400
C	0.22625100	-0.55589200	1.53141500

H	-0.87689600	-1.26718100	3.15220000
H	0.93042900	-0.79312100	0.73857500
C	0.09026500	-2.96350800	2.14231000
C	0.04863000	-3.82965800	3.24191100
C	0.41150000	-3.49420100	0.88427800
C	0.35037100	-5.18068900	3.09835800
H	-0.21578200	-3.43288800	4.21853400
C	0.71335900	-4.84368100	0.74095400
H	0.38942400	-2.84695000	0.01195700
C	0.68845900	-5.69218300	1.84755100
H	0.32032600	-5.83473100	3.96412900
H	0.95504500	-5.23882400	-0.24106400
H	0.91962400	-6.74623700	1.73221400
C	-0.15210700	0.87892000	1.71823000
O	-1.08074500	1.09513000	2.74587000
H	0.75033500	1.56474200	2.21676100
C	3.16626100	1.20314300	3.46133200
C	1.82316700	1.41499000	4.16344300
H	3.66216700	2.16514000	3.30013700
H	3.83004500	0.55300900	4.04125500
H	3.01046000	0.74304700	2.47693100
H	1.35756100	0.41764100	4.30937400
H	2.02083000	1.79758100	5.18308900
O	0.99340000	2.28141700	3.46203200
H	-0.47746900	1.66198000	3.34656500

Si-M02^A

C	3.12636200	-1.07050200	0.79969900
C	4.10841500	-1.86002800	1.38901400
C	4.47699500	-3.06073900	0.78611000
C	3.83031900	-3.46348900	-0.38009900
C	2.83708400	-2.65569200	-0.93280800
C	2.47335700	-1.43900100	-0.37119300
C	2.80159000	0.12994800	1.65794900
C	3.59180600	-0.11183100	2.99511200
C	4.59921700	-1.24416000	2.67463600
H	5.23823400	-3.69537500	1.22834000
H	4.07919200	-4.40747400	-0.85142100

H	1.68294900	-0.83441000	-0.81700000
H	3.07739500	1.07736600	1.19609100
H	4.09883600	0.80464000	3.29479900
H	5.60314700	-0.82707100	2.55091400
C	0.81111600	-0.73983600	2.81846000
C	1.73748500	-1.36513500	3.81050500
C	0.33834100	0.55844500	1.12189800
H	2.14746200	-2.30208000	3.40798800
H	4.64377400	-1.95447900	3.50552600
N	1.34689500	0.13212500	1.89941600
N	-0.47102500	-0.86136800	2.66639000
N	-0.74604100	-0.04721300	1.60664400
O	2.74547000	-0.41707000	4.09165800
H	1.20628800	-1.58301100	4.73689400
C	-2.02076500	-0.11656800	0.97649200
C	-2.99942500	0.83989900	1.22008500
C	-2.28312100	-1.18797100	0.11971900
C	-4.25354300	0.72545300	0.63416100
C	-3.52968700	-1.32354700	-0.46851400
C	-4.49667300	-0.36328700	-0.19302700
H	-5.01448700	1.47509600	0.81046100
H	-3.73807100	-2.14713700	-1.13923800
Br	1.89494300	-3.24897700	-2.46680700
Br	-0.91414900	-2.40854400	-0.28239600
Br	-6.19246100	-0.53438000	-0.99707300
Br	-2.59661400	2.30890400	2.30798500
C	2.34641500	2.19562400	-1.32109200
C	1.55496000	2.26492400	-0.24837000
H	2.06469300	1.48448600	-2.09565700
H	1.75162700	2.95259900	0.57384500
C	3.57259300	2.97383800	-1.56322200
C	4.36474600	2.64222400	-2.66949300
C	3.98703400	4.02893500	-0.73739700
C	5.54094300	3.33412100	-2.94193000
H	4.05038500	1.82980800	-3.31889000
C	5.16085300	4.72128700	-1.00887700
H	3.38260900	4.32141400	0.11607400
C	5.94365100	4.37623000	-2.11131600

H	6.14034000	3.06082500	-3.80431800
H	5.46445100	5.53866800	-0.36256500
H	6.85794900	4.92120200	-2.32237800
C	0.30742500	1.42724400	-0.12758500
O	0.08799700	0.58609100	-1.20524800
H	-0.55549800	2.10642600	0.01500200
C	-2.71773400	2.11485700	-1.73241100
O	-2.27058400	2.92724100	-0.90544100
O	-2.15832700	1.02062100	-2.08860200
H	-0.89341500	0.78619900	-1.59237600
C	-4.04858000	2.40269300	-2.41871200
H	-4.54053700	3.26429000	-1.96667300
H	-3.87088200	2.60290200	-3.47926800
H	-4.69893600	1.52653500	-2.35882600

Si-M02^E

C	3.36581000	-1.64394400	-0.31839200
C	4.45134400	-2.15242800	-1.02165300
C	5.64409700	-1.43108400	-1.05576500
C	5.71341200	-0.19538900	-0.41388000
C	4.59813600	0.28805100	0.27062200
C	3.41675200	-0.43143500	0.35420300
C	2.13273800	-2.49827600	-0.49888500
C	2.54777800	-3.54481200	-1.59447600
C	4.09296100	-3.46035700	-1.68161900
H	6.50629600	-1.80492700	-1.59905300
H	6.62019700	0.39743100	-0.45598400
H	2.57127900	-0.05122300	0.91485300
H	1.77185900	-2.93752000	0.43050100
H	2.21157800	-4.54094600	-1.30882800
H	4.54577900	-4.30304300	-1.14987500
C	1.05113800	-1.21416900	-2.31675600
C	1.92229700	-1.96423800	-3.27223500
C	0.19884800	-0.84918700	-0.33578800
H	2.93296700	-1.53327000	-3.28677600
H	4.41414500	-3.52557600	-2.72555500
N	1.05960700	-1.62428600	-1.00530100
N	0.22011900	-0.23562900	-2.50709500

N	-0.29469400	-0.01777800	-1.25552700
O	1.92247000	-3.31308200	-2.85050300
H	1.50505600	-1.92169600	-4.27818000
C	-1.16576000	1.07612300	-1.01031400
C	-2.50414400	1.00560000	-1.39295900
C	-0.67928400	2.23088000	-0.38918500
C	-3.36212600	2.07474700	-1.17657300
C	-1.52475900	3.30922200	-0.16286600
C	-2.85303100	3.21480200	-0.56469400
H	-4.40279200	2.01449100	-1.46884700
H	-1.15530600	4.20334000	0.32338800
Br	4.64847000	2.00892200	1.07025200
Br	1.10236300	2.29506700	0.20871900
Br	-4.00650300	4.66818400	-0.24523000
Br	-3.15230200	-0.57736900	-2.16900800
C	-1.70064300	-2.81980000	1.75996300
C	-1.52884500	-1.65836100	1.12913300
H	-0.84974900	-3.20073300	2.32254200
H	-2.33791000	-1.18307500	0.57402100
C	-2.94470900	-3.60794500	1.77805300
C	-3.12371000	-4.59052300	2.75968500
C	-3.96139500	-3.41870900	0.82958900
C	-4.29106200	-5.34723400	2.81047300
H	-2.33853100	-4.75436200	3.49283500
C	-5.12682900	-4.17372800	0.87992200
H	-3.82754300	-2.69070900	0.03382600
C	-5.29874500	-5.13944200	1.87208900
H	-4.41256200	-6.10119700	3.58176200
H	-5.90128800	-4.01718300	0.13559300
H	-6.20787600	-5.73103300	1.90561900
C	-0.18377600	-0.93358100	1.14963000
O	0.78532300	-1.50137500	1.88076500
H	-0.39963400	0.12659500	1.41277100
C	-0.13732700	1.44572600	3.72210200
C	1.33692700	1.14226900	3.96667200
H	-0.70107700	0.51719700	3.57999600
H	-0.57933300	1.98833200	4.56324200
H	-0.23594300	2.05349000	2.81683200

H	1.87149500	2.08031300	4.16627300
H	1.43225100	0.52782700	4.87789300
O	1.96180900	0.53388600	2.86905700
H	1.47709300	-0.31890200	2.59986400

Si-TS2

C	2.65508800	-1.19001800	1.02251600
C	3.41754500	-2.10223600	1.74741800
C	3.62158600	-3.38649000	1.24770700
C	3.03868700	-3.74266800	0.03546500
C	2.27281700	-2.80879900	-0.66146500
C	2.06722400	-1.51447700	-0.19905000
C	2.50198200	0.10965700	1.78227500
C	3.18463700	-0.14415200	3.17221100
C	3.91128200	-1.50583500	3.04112500
H	4.21066600	-4.11217800	1.79946100
H	3.16512200	-4.74089200	-0.36773900
H	1.44746600	-0.82277900	-0.77622100
H	2.96788700	0.94859000	1.26807000
H	3.88751200	0.66060800	3.38473100
H	4.99426800	-1.35356500	3.01466100
C	0.35282700	-0.29769800	2.90651000
C	1.10593300	-0.87197800	4.06488100
C	0.20200000	0.71342400	0.95470000
H	1.34436700	-1.92555100	3.85906700
H	3.69936700	-2.13543800	3.91120700
N	1.06889100	0.39805500	1.95692400
N	-0.89755700	-0.40571300	2.59614000
N	-0.98433000	0.23165700	1.38139900
O	2.26857900	-0.09660000	4.25479200
H	0.51101000	-0.82197000	4.97711500
C	-2.20700600	0.26092300	0.67177200
C	-3.07287600	1.34435500	0.79496400
C	-2.55602400	-0.80547100	-0.15902400
C	-4.28197100	1.37451700	0.11077600
C	-3.76024900	-0.80133200	-0.84656700
C	-4.60661400	0.29263200	-0.69789800
H	-4.94932700	2.22154000	0.20504000

H	-4.02768900	-1.62654400	-1.49417400
Br	1.44142400	-3.33610400	-2.28195100
Br	-1.34592200	-2.21531100	-0.38958900
Br	-6.23198500	0.31919000	-1.65271500
Br	-2.57302800	2.79792700	1.87533500
C	2.36159900	2.06918900	-1.67039100
C	1.70597900	2.06530100	-0.49663800
H	1.94714600	1.45474000	-2.46676000
H	2.06547200	2.65358800	0.34798800
C	3.59126900	2.81396700	-1.96697300
C	4.31560700	2.50641300	-3.12839300
C	4.08469000	3.83251100	-1.13525300
C	5.49676800	3.17335600	-3.43849100
H	3.94396300	1.72816900	-3.78969900
C	5.26484600	4.49779600	-1.44296300
H	3.53095700	4.11961300	-0.24626000
C	5.97994200	4.17133100	-2.59556000
H	6.04009900	2.91385100	-4.34182100
H	5.62509800	5.28276700	-0.78504700
H	6.89897100	4.69559700	-2.83632700
C	0.44654500	1.34943900	-0.30431300
O	-0.11932600	0.63856400	-1.44388400
H	-0.53722400	1.73460500	-0.83565700

Si-TS2^A

C	3.16152200	-1.13972700	0.77452200
C	4.14390600	-1.88527200	1.41893300
C	4.53286200	-3.11512100	0.89387300
C	3.91243500	-3.58894000	-0.25887300
C	2.92485600	-2.82140900	-0.87653700
C	2.53451200	-1.58081300	-0.38794800
C	2.81732300	0.10222000	1.56766800
C	3.60987700	-0.04798100	2.91350900
C	4.62529900	-1.19068800	2.66713500
H	5.29417700	-3.71356400	1.38406500
H	4.18101200	-4.55390500	-0.67344200
H	1.75795600	-1.00595900	-0.89279800
H	3.08013400	1.02319100	1.04830000

H	4.10910100	0.88873100	3.15862600
H	5.62726900	-0.77598600	2.52078600
C	0.86550500	-0.80519600	2.73821400
C	1.78957000	-1.29275000	3.80975100
C	0.38581900	0.34091200	0.92003700
H	2.24242100	-2.24728600	3.50603500
H	4.67275700	-1.84987300	3.53917600
N	1.36695800	0.09470300	1.82309400
N	-0.36099400	-1.12473100	2.48077200
N	-0.64368300	-0.41421900	1.34211700
O	2.75946900	-0.29029000	4.02368900
H	1.24764600	-1.44464800	4.74353400
C	-1.94999000	-0.41949800	0.79625600
C	-2.90740900	0.44909300	1.31847400
C	-2.28859900	-1.28143900	-0.24653500
C	-4.18588800	0.49852900	0.78438100
C	-3.55891900	-1.23690500	-0.80649100
C	-4.47908900	-0.33224600	-0.29096900
H	-4.92385900	1.18604500	1.17878700
H	-3.81816300	-1.87944400	-1.63822300
Br	2.05247100	-3.50724500	-2.41501400
Br	-1.00853800	-2.48468100	-0.91201600
Br	-6.17228900	-0.17428100	-1.10169200
Br	-2.43258600	1.58626100	2.72975800
C	2.17352300	2.39902100	-1.49010600
C	1.50487400	2.14616800	-0.35449900
H	1.93079600	1.80028600	-2.36523200
H	1.73305000	2.71014600	0.55178200
C	3.22936000	3.41085900	-1.64194800
C	4.13126400	3.31446700	-2.71138200
C	3.37620000	4.48441000	-0.74981100
C	5.15993500	4.23838400	-2.86892300
H	4.02405600	2.49779500	-3.42036500
C	4.40502600	5.40586500	-0.90450300
H	2.66334100	4.61294100	0.05915700
C	5.30485500	5.28683000	-1.96316100
H	5.84880800	4.14028900	-3.70222400
H	4.49699500	6.22981800	-0.20359600

H	6.10302600	6.01144400	-2.08676900
C	0.36784400	1.21372300	-0.24663800
O	0.09370400	0.47334000	-1.41196900
H	-0.72881100	2.07485100	-0.11902600
C	-2.53313400	2.39165700	-1.12184900
O	-1.71385100	2.81001200	-0.21899100
O	-2.30031500	1.46406100	-1.91411000
H	-0.79048800	0.77956800	-1.74402500
C	-3.85905900	3.11703200	-1.19228400
H	-4.10565500	3.56248800	-0.22796900
H	-3.78680300	3.91494700	-1.93695100
H	-4.63951700	2.42190300	-1.50852800

Si-TS2^E

C	3.76730200	1.34287800	-0.02805000
C	5.00884400	1.53453600	0.56917400
C	6.00303700	0.56899600	0.41569800
C	5.72402700	-0.58846200	-0.30916700
C	4.46728700	-0.74206200	-0.89332100
C	3.47382600	0.22023800	-0.79204900
C	2.78758200	2.42513000	0.36440800
C	3.56351700	3.28918100	1.42712400
C	5.04178800	2.83070200	1.33789700
H	6.97833900	0.69692700	0.87461100
H	6.47052300	-1.36752100	-0.41446300
H	2.52433300	0.06414700	-1.31208900
H	2.43001700	3.01847000	-0.47311800
H	3.45413000	4.34703500	1.19058300
H	5.63577500	3.58222200	0.80875600
C	1.68479000	1.32284700	2.28020400
C	2.79585400	1.83502900	3.13748400
C	0.52116500	1.20989100	0.42254400
H	3.68749700	1.20209600	3.02876600
H	5.46670000	2.73280200	2.34154800
N	1.61362900	1.77024400	0.98035000
N	0.70033300	0.53851100	2.57612300
N	-0.01420900	0.46606700	1.40714400
O	3.03835300	3.16786700	2.73969700

H	2.49015500	1.83906200	4.18353700
C	-1.01573100	-0.53422700	1.29110100
C	-2.30885300	-0.30617500	1.75962200
C	-0.68618500	-1.77930900	0.75078300
C	-3.27903500	-1.29496300	1.68575700
C	-1.64525800	-2.78139400	0.66399900
C	-2.92773300	-2.52228200	1.13321600
H	-4.28465000	-1.10771400	2.04049200
H	-1.39601000	-3.74278400	0.23236000
Br	4.03864500	-2.34100900	-1.82505900
Br	1.04397900	-2.08478200	0.08621600
Br	-4.23651200	-3.86849200	0.99084200
Br	-2.74490600	1.38691800	2.43747000
C	-1.92546400	2.40706100	-2.00983200
C	-1.42223800	1.59928800	-1.07192400
H	-1.23801900	2.86824400	-2.71514400
H	-2.09240700	1.08403900	-0.39004200
C	-3.35761100	2.70438000	-2.18349100
C	-3.80998100	3.18719500	-3.41838400
C	-4.29356600	2.52989200	-1.15268900
C	-5.15785800	3.46067200	-3.63085800
H	-3.09236800	3.33845000	-4.22032400
C	-5.64001700	2.80238400	-1.36528300
H	-3.96129300	2.20401500	-0.17046300
C	-6.07976500	3.26502100	-2.60561200
H	-5.48826000	3.82738400	-4.59764300
H	-6.35022600	2.66476100	-0.55588200
H	-7.13113200	3.47994400	-2.76708300
C	0.03549000	1.28004700	-0.96901100
O	0.84953000	2.11996300	-1.74993000
H	0.30456600	0.22684700	-1.51791900
C	-0.87510800	-1.54920400	-3.08098400
C	0.63131400	-1.37478600	-3.28772200
H	-1.40635700	-0.64407500	-3.39416400
H	-1.27387000	-2.40437800	-3.63737500
H	-1.08550300	-1.70806600	-2.01633300
H	1.13030400	-2.30132100	-2.93647400
H	0.82328700	-1.33574200	-4.37957000

O	1.13041200	-0.25999300	-2.64757700
H	1.12908000	1.49147200	-2.46064700
Re-M2			
C	-3.95903200	0.01696800	0.76400000
C	-5.26976700	0.20536700	0.33635300
C	-5.91444700	-0.79263600	-0.39132900
C	-5.22523700	-1.96198900	-0.70465000
C	-3.91462400	-2.12339000	-0.25876000
C	-3.26712300	-1.16010800	0.50312100
C	-3.40471500	1.25442600	1.43403600
C	-4.54243800	2.33132000	1.26308000
C	-5.78630200	1.55644700	0.75875500
H	-6.93536000	-0.65952900	-0.73544900
H	-5.69458200	-2.73990400	-1.29597700
H	-2.25145900	-1.31030800	0.85208700
H	-3.18393900	1.08849900	2.48663000
H	-4.73496500	2.81490700	2.22077900
H	-6.52289000	1.45631200	1.56203800
C	-2.23558800	2.38732700	-0.41100000
C	-3.55444700	2.97396100	-0.79337700
C	-0.87387800	1.21708400	0.91222900
H	-4.16115100	2.23234600	-1.33298100
H	-6.26981500	2.10796900	-0.05353200
N	-2.17437900	1.69922900	0.77929000
N	-1.10695400	2.47826400	-1.01737600
N	-0.22151400	1.77943600	-0.18950100
O	-4.18765200	3.39791300	0.39800300
H	-3.41147900	3.84439100	-1.43364700
C	0.94926300	1.26902600	-0.78842500
C	2.15264800	1.97318900	-0.69195700
C	0.96129200	0.02827100	-1.43299600
C	3.34358300	1.45348100	-1.18136000
C	2.13862700	-0.52285400	-1.92426400
C	3.31713400	0.19921700	-1.77849100
H	4.27356200	1.99542800	-1.06475500
H	2.13920600	-1.50158600	-2.38790900
Br	-2.94604200	-3.67990000	-0.74827500

Br	-0.63487100	-0.96005400	-1.55605300
Br	4.94499600	-0.58335100	-2.31587100
Br	2.18037100	3.59486900	0.25303000
C	1.49389400	-1.02609000	2.70672400
C	1.01095500	-0.02239400	1.94340500
H	0.82052900	-1.58744700	3.35078400
H	1.72045900	0.56252900	1.36846400
C	2.90431700	-1.43326500	2.70185000
C	3.45358300	-2.11250700	3.79926000
C	3.73770800	-1.19246000	1.59620100
C	4.78908500	-2.50394300	3.80573900
H	2.82299400	-2.32630100	4.65844300
C	5.07138100	-1.58107500	1.60119900
H	3.32449800	-0.72483700	0.70751600
C	5.60773700	-2.23544800	2.70997600
H	5.19247700	-3.02206000	4.67051700
H	5.68006200	-1.38887500	0.72206400
H	6.64749800	-2.54612300	2.71375100
C	-0.36559400	0.38306100	1.86815000
O	-1.27464300	-0.20874900	2.74026800
H	-1.00137300	0.00210300	3.64424100

Si-M2

C	2.85722400	-1.36727200	0.83047800
C	3.70830500	-2.40866800	1.18859700
C	4.20742800	-3.26626700	0.21106900
C	3.81565700	-3.09290100	-1.11428800
C	2.94607300	-2.05413600	-1.44197900
C	2.47224600	-1.16036900	-0.48998600
C	2.34158400	-0.62880900	2.04739800
C	2.86039600	-1.48193500	3.26857200
C	3.91688400	-2.44962400	2.67994700
H	4.86933800	-4.08478300	0.47568800
H	4.16321800	-3.76921200	-1.88670900
H	1.78074600	-0.37245300	-0.77074700
H	2.74084200	0.38331700	2.13606800
H	3.29956700	-0.81965900	4.01441000
H	4.92501400	-2.11528600	2.94428200

C	0.12953600	-1.61969000	2.44674000
C	0.84729300	-2.73835700	3.12611900
C	0.03393100	0.35574500	1.41446800
H	1.29557900	-3.41133600	2.38058900
H	3.78620300	-3.45005800	3.10333200
N	0.88913700	-0.54784900	2.04021300
N	-1.12755600	-1.47445200	2.23167900
N	-1.23053700	-0.21513100	1.61725200
O	1.82891400	-2.15898100	3.96533200
H	0.15963900	-3.30904500	3.74959100
C	-2.29838600	-0.09149200	0.69125100
C	-2.28742300	-0.77552700	-0.52611800
C	-3.41710400	0.68655300	0.99135100
C	-3.36353600	-0.72286600	-1.40333600
C	-4.50727600	0.76466600	0.13705900
C	-4.46679400	0.04304000	-1.05011500
H	-3.34052400	-1.26813300	-2.33836600
H	-5.36628400	1.37217400	0.39156100
Br	2.31466100	-1.89103300	-3.22083000
Br	-3.42000200	1.70474300	2.57541500
Br	-5.95129000	0.10628200	-2.21186100
Br	-0.76422000	-1.77280300	-1.01521700
C	1.72363300	3.32085800	-0.11411400
C	1.54485600	2.09616800	0.42393200
H	0.86052200	3.97482600	-0.20945900
H	2.41349400	1.45660700	0.54519500
C	3.00901400	3.85875100	-0.56552300
C	3.14118900	5.24164200	-0.76894300
C	4.13161500	3.04999800	-0.81385600
C	4.34831100	5.79935000	-1.17642000
H	2.28132800	5.88307500	-0.59338100
C	5.33882400	3.60756300	-1.21656400
H	4.05376900	1.97051400	-0.71422600
C	5.45715300	4.98561400	-1.39804200
H	4.42292000	6.87279200	-1.32143700
H	6.19056100	2.96093300	-1.40510000
H	6.39969600	5.41663300	-1.71959600
C	0.26601100	1.55742500	0.80434100

O	-0.85602400	2.29393300	0.43561800
H	-1.24617600	2.68312200	1.23173200
TS3RR			
C	1.10510500	1.81076300	-2.19047500
C	0.91774200	0.50164700	-1.71481000
H	0.29551500	2.21727000	-2.79460100
H	1.77713500	0.00723200	-1.27992600
C	2.45290100	2.31232500	-2.51927500
C	2.58252400	3.61119200	-3.03996500
C	3.63089000	1.59022800	-2.26936800
C	3.83118700	4.18394400	-3.25530000
H	1.68687600	4.18023500	-3.28110500
C	4.88015500	2.16282500	-2.48598700
H	3.58596700	0.55743300	-1.93853900
C	4.99040400	3.46667200	-2.96473600
H	3.89868600	5.19160600	-3.65286000
H	5.77400200	1.58157700	-2.28193200
H	5.96648400	3.91134400	-3.12685900
C	-0.26833600	-0.19906300	-1.72966400
O	-1.39902400	0.37313300	-2.29666400
H	-1.95810300	0.73661300	-1.59326300
C	3.58865800	2.49246500	1.69819200
C	2.82439300	2.92143800	0.62509800
C	1.44574700	2.64979300	0.59640700
C	0.84073200	1.95974300	1.66833900
C	1.62792500	1.55663400	2.75818700
C	2.98697100	1.81873500	2.77105300
H	0.98830800	3.88572300	-1.13479700
H	4.65445700	2.69379100	1.71725700
H	3.28241200	3.46825300	-0.19419700
C	0.62058700	3.06514800	-0.52592200
C	-0.58413800	1.75056300	1.63320300
H	1.14924900	1.04435800	3.58855400
H	3.59347400	1.49736300	3.61180200
C	-1.32243300	2.29653700	0.64454400
H	-1.07502300	1.21439700	2.43350500
H	-2.40697200	2.24757300	0.63112400

N	-0.73464000	3.03818100	-0.36749100
C	-1.58337600	3.64326600	-1.40917200
H	-0.97201400	4.39609500	-1.91451500
H	-1.84011100	2.87765100	-2.15223500
C	-2.83002800	4.27341900	-0.84001300
C	-2.72217200	5.35049800	0.04419300
C	-4.09075200	3.78442900	-1.17817600
C	-3.86503600	5.93316800	0.57891300
H	-1.73831300	5.72659700	0.31350500
C	-5.23791200	4.37125900	-0.64525200
H	-4.17691300	2.94421100	-1.86274400
C	-5.12540900	5.44445500	0.23295300
H	-3.77556300	6.76963600	1.26409700
H	-6.21601600	3.98728700	-0.91548400
H	-6.01725700	5.90063700	0.64982100
C	-3.62816300	-1.80765600	-0.85725800
C	-4.79477800	-2.56422500	-0.83813800
C	-5.66412600	-2.46178100	0.24531100
C	-5.33535700	-1.62606700	1.31086900
C	-4.14302500	-0.90537700	1.27647400
C	-3.27537200	-0.97213600	0.19493800
C	-2.79583500	-2.11484500	-2.07995100
C	-3.47987800	-3.38038700	-2.71248000
C	-4.88217500	-3.44934600	-2.05548100
H	-6.57800700	-3.04582600	0.28105900
H	-5.98637100	-1.55232200	2.17426400
H	-2.32997800	-0.43427900	0.22746200
H	-2.76873400	-1.29793700	-2.79654300
H	-3.54994700	-3.25989900	-3.79300800
H	-5.64172000	-3.08381500	-2.75329800
C	-1.13468500	-3.63086200	-1.10350800
C	-2.14879300	-4.71749800	-1.26051400
C	-0.37890600	-1.57163300	-1.37364900
H	-2.89835500	-4.65372000	-0.45908800
H	-5.13349600	-4.48635200	-1.81464300
N	-1.42236300	-2.40418300	-1.65279700
N	0.02736900	-3.65240200	-0.54367600
N	0.50405900	-2.37055300	-0.71613600

O	-2.72685200	-4.56831900	-2.54048100
H	-1.66505100	-5.69279400	-1.21481700
C	1.61945500	-1.99928200	0.07376400
C	2.90980500	-1.99933500	-0.45530000
C	1.43216300	-1.69400800	1.42241300
C	4.00529200	-1.68515300	0.33646100
C	2.51653000	-1.41672600	2.24269300
C	3.78769000	-1.39902800	1.68014800
H	5.00258600	-1.66243200	-0.08525500
H	2.37204400	-1.19711400	3.29287400
Br	-3.64178900	0.15654400	2.76184400
Br	-0.31680200	-1.60651900	2.11026900
Br	5.25280200	-0.93201000	2.76206300
Br	3.14149600	-2.34734700	-2.28178400

TS3RS

C	0.43528700	1.65721300	-1.46892800
C	0.53599300	0.31317500	-1.08895800
H	-0.45715100	1.93957600	-2.02370700
H	1.50366600	-0.00714800	-0.73522100
C	1.65324500	2.42839400	-1.78780900
C	1.59765200	3.44183700	-2.75332100
C	2.87926500	2.19836100	-1.14001600
C	2.72927500	4.18732600	-3.07505200
H	0.65606100	3.63755500	-3.25953600
C	4.01264500	2.93133900	-1.47214500
H	2.95721300	1.44247700	-0.35998000
C	3.94288000	3.93135200	-2.44219100
H	2.66149200	4.96452300	-3.82971300
H	4.95172900	2.71387400	-0.97271300
H	4.82646800	4.50582500	-2.69927300
C	-0.52294100	-0.57416500	-1.02176800
O	-1.74789400	-0.24060800	-1.54083800
H	-2.14542600	0.47523600	-1.00818400
C	-1.28423300	5.79564200	-1.21717200
C	-0.45632700	4.85316100	-0.63161000
C	-1.00546400	3.66145700	-0.13086700
C	-2.39702800	3.43688500	-0.20606600

C	-3.21870900	4.39629600	-0.81831700
C	-2.66414900	5.56040200	-1.32089400
H	0.85901500	2.83313900	0.66810200
H	-0.86434900	6.71887700	-1.60120400
H	0.61301200	5.02427900	-0.55577000
C	-0.17048000	2.60582700	0.40290900
C	-2.92353400	2.23266500	0.38763800
H	-4.28575400	4.20578200	-0.88989000
H	-3.30140000	6.30162200	-1.79151900
C	-2.11102700	1.41642600	1.10343400
H	-3.98563300	2.03506800	0.35124500
H	-2.47397100	0.54779900	1.64442500
N	-0.76020200	1.65657300	1.18905800
C	0.10977700	0.80945900	2.00841200
H	-0.50149200	-0.00542200	2.40637400
H	0.86329700	0.36159900	1.35386300
C	0.78937300	1.58522400	3.11245200
C	2.17769300	1.55961900	3.23410000
C	0.03129800	2.32552100	4.02243500
C	2.80646000	2.25772800	4.26371800
H	2.76937800	0.99425800	2.51777600
C	0.65747200	3.02585600	5.04740700
H	-1.05087000	2.35623600	3.92139200
C	2.04672500	2.98944900	5.17126700
H	3.88758500	2.23379700	4.35124600
H	0.06349000	3.60027100	5.75057000
H	2.53470300	3.53476900	5.97233600
C	-4.33836200	-2.39666700	0.99295300
C	-3.80333500	-1.86708000	-0.18801300
C	-4.37262400	-0.73864400	-0.77262600
C	-5.41302600	-0.10879800	-0.09684200
C	-5.87779300	-0.55852200	1.13656500
C	-5.34552400	-1.72615600	1.67841600
C	-3.82190700	-3.79107800	1.22123500
C	-3.46643000	-4.17184900	-0.23654600
C	-2.84718100	-2.86667600	-0.81839800
H	-4.05469400	-0.38148000	-1.74479900
H	-5.75570300	-2.13209400	2.59730000

H	-2.94280100	-3.79291800	1.87572000
H	-4.39615900	-4.33728300	-0.78555400
H	-4.56664000	-4.46186700	1.65256500
H	-2.84828200	-2.83573600	-1.90842000
N	-1.40695800	-2.84596400	-0.38224400
O	-2.70008000	-5.32825000	-0.43036600
C	-0.41477600	-1.90736000	-0.53161600
C	-0.78102500	-4.00649300	0.04740900
N	0.71809300	-2.55082700	-0.13680500
N	0.48884200	-3.85222700	0.20869200
C	-1.49224900	-5.30188000	0.28577400
H	-1.65274600	-5.44772400	1.36096400
H	-0.86494000	-6.11520000	-0.08076000
C	2.06428100	-2.11232400	-0.19644500
C	2.74610700	-1.76711000	0.97159600
C	2.70992100	-1.97530200	-1.42894700
C	4.01764600	-1.20886200	0.91485200
C	3.97002200	-1.39941600	-1.51010500
C	4.59479100	-0.99812700	-0.33344200
H	4.53502300	-0.92567300	1.82346400
H	4.44333300	-1.24694000	-2.47198700
Br	1.92389500	-2.01664800	2.63979000
Br	6.24319300	-0.10207300	-0.43938700
Br	1.80704100	-2.46422500	-2.99576000
H	-6.68252300	-0.03224800	1.63699500
Br	-6.25034900	1.39004600	-0.90276500

TS3SR

C	4.32487600	1.38805900	0.45319900
C	5.60234800	1.55968600	0.97540300
C	6.69871000	1.01896500	0.30576500
C	6.49355500	0.28466500	-0.86002700
C	5.19872500	0.12346600	-1.35231200
C	4.09769000	0.68959500	-0.72621000
C	3.26599700	1.93038200	1.38425400
C	4.06009300	2.37637400	2.66813600
C	5.55794400	2.32751100	2.27149300
H	7.70336500	1.13869400	0.69827800

H	7.32829400	-0.17376100	-1.37768300
H	3.09967700	0.55897200	-1.13145400
H	2.69994200	2.75460500	0.95991900
H	3.75487000	3.38269600	2.95304800
H	5.94530800	3.34189200	2.13807300
C	2.67484500	-0.11178600	2.63256900
C	3.80222000	0.19802900	3.56293300
C	1.29001700	0.32798300	0.97169500
H	4.75614300	-0.12068000	3.11992100
H	6.14500000	1.86299500	3.06969300
N	2.32426900	0.83672600	1.69961300
N	1.92626400	-1.16148900	2.56968100
N	1.07158600	-0.89531900	1.52724000
O	3.76861900	1.58733000	3.80841300
H	3.66241900	-0.32265800	4.51013700
C	0.22464300	-1.93267500	1.06592600
C	-0.94449300	-2.24883600	1.76094800
C	0.52088800	-2.60996400	-0.12205900
C	-1.84204800	-3.18239400	1.25744200
C	-0.37312200	-3.53210700	-0.65017200
C	-1.55310000	-3.79065000	0.04066100
H	-2.75490500	-3.41205400	1.79306000
H	-0.16366100	-4.02410100	-1.59174000
Br	4.89774800	-0.94791800	-2.88879100
Br	2.08723800	-2.19292300	-1.07539000
Br	-2.81968100	-4.95535600	-0.71656800
Br	-1.33872100	-1.36684000	3.36803700
C	-1.23481900	1.01581200	-1.75837600
C	-0.47240000	0.39603500	-0.75900600
H	-0.75241600	1.82841700	-2.29705400
H	-0.83752700	-0.54786800	-0.38381600
C	-2.22762800	0.23684100	-2.52766300
C	-2.68957500	0.73288700	-3.75442600
C	-2.76446200	-0.97778600	-2.06741900
C	-3.63458600	0.03626200	-4.50347900
H	-2.31365000	1.69086800	-4.10321600
C	-3.69346900	-1.68294600	-2.82223300
H	-2.46230000	-1.39269100	-1.10856800

C	-4.13349100	-1.18100900	-4.04689500
H	-3.97459500	0.44343800	-5.45048900
H	-4.06352700	-2.63348100	-2.45030900
H	-4.85931000	-1.73203500	-4.63536400
C	0.61761800	0.95306100	-0.12212200
O	1.19304400	2.11659200	-0.57497700
H	0.59058000	2.87211300	-0.42687400
C	-3.29363900	4.67996000	-3.44647500
C	-3.36526000	3.58278600	-2.60562700
C	-2.54244200	3.51738700	-1.46932600
C	-1.65945300	4.57963200	-1.17423500
C	-1.59574200	5.68039300	-2.04336400
C	-2.40013100	5.72501100	-3.16870000
H	-3.35162000	1.63894300	-0.68331600
H	-3.93236500	4.73197600	-4.32134200
H	-4.04828400	2.76790800	-2.81861900
C	-2.53103300	2.34805400	-0.61241100
C	-0.89352200	4.50713200	0.04882900
H	-0.91809900	6.49724400	-1.81518700
H	-2.34861600	6.58012400	-3.83422000
C	-1.13691700	3.50884800	0.93594200
H	-0.21082400	5.30542300	0.31496100
H	-0.67051000	3.45940000	1.91370700
N	-2.00854700	2.48736100	0.64370200
C	-2.26469100	1.41642200	1.60992200
H	-1.60007000	1.57495700	2.46372100
H	-1.97730300	0.46842000	1.14417500
C	-3.71339100	1.33769700	2.02887100
C	-4.37552800	2.45872100	2.53393200
C	-4.39410200	0.12561400	1.92155500
C	-5.70486400	2.36314400	2.93133700
H	-3.85018200	3.40748700	2.61110000
C	-5.72479400	0.02805400	2.32349200
H	-3.88043300	-0.74445900	1.51760800
C	-6.38023100	1.14683100	2.82869500
H	-6.21549200	3.23718400	3.32202300
H	-6.24848300	-0.91791100	2.23412600
H	-7.41755400	1.07505400	3.13869300

TS3SS

C	-2.51559700	-3.40358900	-0.11636300
C	-3.34848000	-4.43721500	0.29686400
C	-4.45711000	-4.78015100	-0.47464700
C	-4.73385500	-4.05498500	-1.63083800
C	-3.88016100	-3.02149700	-2.01625000
C	-2.74137200	-2.69878500	-1.29174000
C	-1.44512000	-3.11063200	0.90886300
C	-1.80367700	-4.04313900	2.12794600
C	-2.87736300	-5.02663500	1.60011000
H	-5.11944100	-5.58388600	-0.16959900
H	-5.61200500	-4.28001500	-2.22515900
H	-2.07318800	-1.90827600	-1.61678100
H	-0.43790400	-3.29661600	0.54167800
H	-0.90951700	-4.56874700	2.46301500
H	-2.43697000	-6.01582900	1.44323200
C	-2.47658000	-1.27204900	2.20114900
C	-3.18912100	-2.31937800	2.99158000
C	-0.95762500	-0.59009300	0.76304400
H	-4.04920600	-2.71008000	2.43090400
H	-3.67617300	-5.14381100	2.33855300
N	-1.52689800	-1.69601300	1.30077400
N	-2.53853800	0.01588200	2.27622100
N	-1.59568100	0.44639100	1.36907700
O	-2.23736600	-3.32791200	3.27248300
H	-3.53919700	-1.90512700	3.93642800
C	-1.70663200	1.77982400	0.88919600
C	-2.48192700	2.04912300	-0.24182700
C	-1.07958500	2.83679600	1.54776700
C	-2.61297800	3.34620500	-0.71860600
C	-1.19815900	4.14164100	1.09194000
C	-1.96659800	4.37579400	-0.04294400
H	-3.20897000	3.55132000	-1.59900800
H	-0.69643000	4.95262400	1.60475600
Br	-4.30481500	-1.96846900	-3.53287200
Br	-0.00192800	2.46888000	3.04144100
Br	-2.12956900	6.13313100	-0.69314600

Br	-3.34514700	0.63924800	-1.14118300
C	2.11931500	0.70590500	-0.93751000
C	0.90534900	0.60252900	-0.24259700
H	2.26829600	0.01943500	-1.77142000
H	0.66834800	1.39701600	0.45556700
C	2.78182800	2.02123900	-1.06630600
C	3.51351900	2.33065800	-2.22122900
C	2.73773200	2.97662500	-0.03682100
C	4.17127500	3.55024100	-2.35034000
H	3.55421400	1.60830000	-3.03281000
C	3.39081200	4.19736500	-0.16984200
H	2.18502400	2.77888400	0.88020400
C	4.11281700	4.49119900	-1.32518800
H	4.72613100	3.76715400	-3.25759600
H	3.33820800	4.92156700	0.63703500
H	4.62364800	5.44301400	-1.42428800
C	0.10358500	-0.51267400	-0.18309200
O	0.28331200	-1.62436000	-0.96849000
H	1.20308700	-1.94301000	-0.90483800
C	1.28018600	-0.90107700	3.39960400
C	2.12442900	-0.27071400	2.50288600
C	2.68999800	-0.98664100	1.43601900
C	2.39547000	-2.35640100	1.27563300
C	1.56715100	-2.99240400	2.21914400
C	1.00549600	-2.27188000	3.25934700
H	3.93917700	0.64182400	0.69039500
H	0.82572500	-0.33671600	4.20710900
H	2.35198600	0.78638300	2.60837100
C	3.49282200	-0.31472100	0.43432600
C	2.97069900	-3.04173400	0.14394700
H	1.38334200	-4.05895500	2.11872000
H	0.34365300	-2.76400600	3.96567900
C	3.90150200	-2.40882000	-0.61675800
H	2.74033600	-4.08330200	-0.04516600
H	4.43943000	-2.90221000	-1.41819800
N	4.24729600	-1.10150100	-0.39385100
C	5.25974400	-0.48470700	-1.26790900
H	5.41221400	0.53503300	-0.90364700

H	4.85726600	-0.41405900	-2.28442000
C	6.55414300	-1.26291000	-1.26225600
C	7.13684900	-1.66924700	-2.46105500
C	7.18488100	-1.56470300	-0.05198400
C	8.34719400	-2.36149900	-2.45489000
H	6.64460700	-1.44252000	-3.40287500
C	8.38920000	-2.25876900	-0.04517000
H	6.72666500	-1.25562400	0.88429800
C	8.97350200	-2.65657400	-1.24811500
H	8.79457300	-2.67421300	-3.39263600
H	8.87467000	-2.48869100	0.89761500
H	9.91332200	-3.19880300	-1.24151700

M3RR

C	1.05496800	2.14651300	-1.60770100
C	0.83038400	0.67722100	-1.42448900
H	0.29599300	2.51166800	-2.31043900
H	1.71304000	0.05887700	-1.34746200
C	2.41952200	2.38340700	-2.23410800
C	2.54349600	3.33375700	-3.25080900
C	3.56668300	1.70527300	-1.80752800
C	3.77981500	3.60036900	-3.83255100
H	1.65905300	3.86433300	-3.59521100
C	4.80444100	1.96997000	-2.38826700
H	3.51115300	0.97837400	-0.99999700
C	4.91448600	2.91539900	-3.40472500
H	3.85462400	4.33757000	-4.62532600
H	5.68295800	1.43218700	-2.04610400
H	5.87821400	3.11512200	-3.86133000
C	-0.35207300	0.05218500	-1.47238600
O	-1.55691600	0.67756300	-1.61344500
H	-1.71193500	1.20077100	-0.80258900
C	3.14151700	1.79056900	2.49584800
C	2.70094800	2.42711400	1.33786500
C	1.35727800	2.37880400	0.96989600
C	0.42944300	1.69427200	1.77857100
C	0.87862600	1.08258000	2.95641900
C	2.22321300	1.12623300	3.30776600

H	1.49201700	3.92919900	-0.49590000
H	4.19118100	1.81835500	2.76898800
H	3.40370400	2.97439700	0.71554300
C	0.87806400	3.04276400	-0.30195500
C	-0.98875400	1.77575700	1.44050900
H	0.15984300	0.57545200	3.59486800
H	2.56218900	0.64478500	4.22104700
C	-1.38176800	2.73865700	0.57128100
H	-1.72807300	1.22767100	2.01467900
H	-2.43078500	2.98943000	0.42711900
N	-0.49101900	3.50784400	-0.13497500
C	-1.00688300	4.46026200	-1.11400800
H	-0.14867400	5.03905400	-1.47452200
H	-1.43809200	3.94722600	-1.98704800
C	-2.03721300	5.39882400	-0.52546200
C	-1.80153500	6.02712000	0.70066800
C	-3.21782800	5.66971300	-1.21526400
C	-2.73106900	6.92078500	1.22143300
H	-0.88811200	5.80343900	1.24514700
C	-4.14884700	6.56878200	-0.69635600
H	-3.41010700	5.17634000	-2.16446200
C	-3.90642500	7.19581600	0.52202800
H	-2.54008900	7.40458900	2.17395000
H	-5.06425800	6.77329700	-1.24208300
H	-4.63100800	7.89342200	0.92924800
C	-3.68430000	-1.83309400	-1.05908200
C	-4.77713600	-2.67929800	-1.21216100
C	-5.62226200	-2.91524600	-0.12894700
C	-5.33693400	-2.33165400	1.10359500
C	-4.22431800	-1.50109400	1.22835300
C	-3.39807300	-1.21669400	0.15159000
C	-2.83137600	-1.80183600	-2.30712700
C	-3.45531800	-2.90861000	-3.23736500
C	-4.82799100	-3.24963600	-2.60606600
H	-6.47881600	-3.57432900	-0.22655100
H	-5.95994000	-2.53496200	1.96701400
H	-2.53357200	-0.57529000	0.28024700
H	-2.80461600	-0.83122000	-2.79724200

H	-3.56260900	-2.51609600	-4.24756700
H	-5.63258300	-2.78852400	-3.18652300
C	-1.11119400	-3.47436900	-1.70760400
C	-2.06020000	-4.52493000	-2.18660900
C	-0.44055400	-1.40929700	-1.44997200
H	-2.82130500	-4.72822300	-1.42098300
H	-4.99424000	-4.33072200	-2.62509100
N	-1.45002700	-2.16052500	-1.92207900
N	0.05299400	-3.58055700	-1.14740000
N	0.46455300	-2.28694200	-0.98839600
O	-2.62167000	-4.04431700	-3.38949800
H	-1.52016900	-5.44602000	-2.40375200
C	1.54276800	-2.04231400	-0.08823600
C	2.86296800	-1.98028400	-0.52880100
C	1.25693800	-1.91357200	1.27154500
C	3.89860000	-1.77165500	0.37326300
C	2.28143700	-1.75312700	2.19061000
C	3.58780800	-1.66262300	1.72472300
H	4.92137800	-1.69319600	0.02562100
H	2.06223800	-1.67108600	3.24693100
Br	-3.74699000	-0.79294100	2.92185700
Br	-0.52909000	-1.88114500	1.85693200
Br	4.95889800	-1.33686000	2.96624200
Br	3.22108100	-2.07783900	-2.36580300

M3RS

C	0.46811000	1.60081700	-1.01074300
C	0.16619200	0.28890800	-0.36243600
H	-0.02039700	1.60262100	-1.99091300
H	0.75844200	0.00577700	0.49917100
C	1.96815600	1.63657300	-1.25747300
C	2.46783900	1.36956600	-2.53341100
C	2.86658200	1.86241800	-0.20792500
C	3.84243500	1.35205900	-2.76456400
H	1.77564600	1.17074700	-3.34727400
C	4.23816100	1.85518400	-0.44054300
H	2.49679200	2.04275100	0.80034400
C	4.72982800	1.59920200	-1.72003700

H	4.21810500	1.14737300	-3.76222700
H	4.92731700	2.02326600	0.38119500
H	5.80071800	1.58200300	-1.89636800
C	-0.71583900	-0.59300100	-0.85691000
O	-1.59691800	-0.37375600	-1.86568300
H	-1.87736700	0.56319700	-1.83758600
C	0.07274100	5.69514100	-2.80228300
C	0.44282500	4.87144600	-1.73979600
C	-0.43588300	3.90026600	-1.27392400
C	-1.70747400	3.74386200	-1.85868800
C	-2.06524200	4.57385400	-2.92714100
C	-1.17880000	5.53762700	-3.39718000
H	0.77186100	3.26318200	0.38506300
H	0.76135300	6.44821500	-3.17029900
H	1.42290800	4.97275300	-1.28072300
C	-0.03815300	2.87696000	-0.23624000
C	-2.63123500	2.79119400	-1.24844500
H	-3.04845800	4.46773800	-3.37709900
H	-1.46756000	6.17373200	-4.22777900
C	-2.36552000	2.35895100	0.01445000
H	-3.62481900	2.64913100	-1.65818300
H	-3.11545100	1.85243600	0.61572300
N	-1.17187200	2.60056700	0.63320200
C	-0.93831300	2.06379100	1.97269600
H	-1.89753400	2.10393900	2.49938600
H	-0.63617700	1.00670800	1.93965500
C	0.09937800	2.85165800	2.73871300
C	1.16653400	2.19875900	3.35643900
C	-0.00216200	4.24240400	2.83743400
C	2.11816700	2.92522900	4.07263100
H	1.25493300	1.11681000	3.27888400
C	0.94834800	4.96712900	3.54758200
H	-0.82378400	4.75129200	2.33993100
C	2.01071300	4.30904000	4.16875100
H	2.94392600	2.40823200	4.55071800
H	0.86260400	6.04670900	3.61776100
H	2.75284400	4.87537800	4.72182900
C	-4.54851300	-2.69392300	0.91597700

C	-3.92406500	-1.96284900	-0.10184000
C	-4.28331400	-0.64432500	-0.35749300
C	-5.24604100	-0.06704600	0.46488300
C	-5.82987600	-0.75817300	1.52318600
C	-5.48507100	-2.08877700	1.74460700
C	-4.14653900	-4.14215000	0.86140800
C	-3.68179800	-4.25738800	-0.60631500
C	-3.04449100	-2.87621200	-0.92860500
H	-3.86738800	-0.09105900	-1.18992400
H	-5.97360300	-2.65099600	2.53351800
H	-3.33714100	-4.34836700	1.57061400
H	-4.56215300	-4.34143200	-1.24693900
H	-4.96580900	-4.82748800	1.08433700
H	-3.03043000	-2.64201400	-1.99285500
N	-1.61315700	-2.94657600	-0.48846400
O	-2.86579400	-5.35282800	-0.93430500
C	-0.66434300	-1.99101500	-0.43657000
C	-0.99704200	-4.12708500	-0.13406800
N	0.45271700	-2.61511200	-0.04163600
N	0.25501900	-3.94153600	0.15808700
C	-1.70401700	-5.44729600	-0.14806200
H	-1.91807500	-5.77013000	0.87735400
H	-1.04960100	-6.18751900	-0.61031300
C	1.78945200	-2.12416300	0.05403800
C	2.33124700	-1.82991400	1.30252700
C	2.56734400	-1.97015500	-1.09232800
C	3.65869400	-1.44840700	1.42857200
C	3.89945800	-1.59520300	-0.98931800
C	4.43037200	-1.35892100	0.27413500
H	4.07600200	-1.21830800	2.40088700
H	4.50495800	-1.47509000	-1.87890000
Br	1.19998000	-1.83897600	2.79983200
Br	6.23189700	-0.84736900	0.41629300
Br	1.78367500	-2.19389400	-2.77850900
H	-6.57524100	-0.27006900	2.14062800
Br	-5.82091600	1.70033900	0.09746400

M3SR

C	-4.41574900	1.19931400	-0.81032400
C	-5.73512000	1.19848900	-1.25023000
C	-6.75683700	0.87953700	-0.35687100
C	-6.43767500	0.53292600	0.95425900
C	-5.10381700	0.53792700	1.36151600
C	-4.07641100	0.89423000	0.50147500
C	-3.45276100	1.43889300	-1.95251600
C	-4.36266700	1.44906300	-3.23742100
C	-5.81698400	1.54430100	-2.71434700
H	-7.79299900	0.87151100	-0.67918000
H	-7.21569600	0.24926300	1.65375400
H	-3.04934300	0.91315200	0.84532200
H	-2.86611500	2.35052100	-1.85604500
H	-4.10187300	2.30119400	-3.86336300
H	-6.19872500	2.56022700	-2.85242800
C	-2.91429100	-0.90713200	-2.52704700
C	-4.13364300	-0.91403600	-3.39213600
C	-1.38840100	0.06203000	-1.30314300
H	-5.03386200	-1.07114500	-2.78230100
H	-6.46749800	0.87503800	-3.28502300
N	-2.51598100	0.29445800	-1.99515100
N	-2.09794300	-1.86507100	-2.20740300
N	-1.16648000	-1.25428500	-1.42221900
O	-4.15301800	0.32288100	-4.07255400
H	-4.06302100	-1.71094500	-4.13205300
C	-0.20217600	-2.05466800	-0.74303600
C	0.92332900	-2.50977800	-1.42627800
C	-0.36613000	-2.35963200	0.60895100
C	1.85674600	-3.31900800	-0.79697100
C	0.55675000	-3.17020500	1.25628000
C	1.64508400	-3.65311100	0.53728200
H	2.73373600	-3.66630900	-1.32880600
H	0.43829200	-3.40687600	2.30612000
Br	-4.63934800	0.00317500	3.11909400
Br	-1.78719300	-1.60156100	1.58021700
Br	2.89378400	-4.75338500	1.40733000
Br	1.22538200	-1.88404300	-3.16856900
C	1.47062600	1.44349600	0.81527500

C	0.69458700	0.71838200	-0.23324700
H	0.75895000	2.04679200	1.38859600
H	1.17847100	-0.11725300	-0.72247900
C	2.00653000	0.36237500	1.74094200
C	1.27706000	0.02291300	2.88318100
C	3.13739500	-0.39157700	1.40728900
C	1.68470900	-1.03332200	3.69516700
H	0.37609300	0.57988600	3.12703000
C	3.54805000	-1.44266300	2.22191200
H	3.69841700	-0.17094000	0.50102100
C	2.82337100	-1.76627000	3.36813300
H	1.10968400	-1.28511300	4.58070200
H	4.42027200	-2.02795800	1.94856500
H	3.13787600	-2.59663600	3.99245200
C	-0.58427700	0.99761300	-0.52475300
O	-1.28751600	2.07193500	-0.08253700
H	-0.69709900	2.85392300	-0.04452900
C	3.41180100	4.70807300	3.21418800
C	3.50590300	3.66630800	2.29227300
C	2.62886200	3.60960300	1.21509800
C	1.64836600	4.60426400	1.03701100
C	1.56142000	5.64234300	1.97115500
C	2.43379100	5.68931000	3.05366500
H	3.53969200	1.91875000	0.25400800
H	4.09126500	4.74777000	4.05886000
H	4.25187400	2.88594100	2.41866900
C	2.57508500	2.42863700	0.27362200
C	0.83052800	4.55356000	-0.17226300
H	0.81408400	6.41918100	1.83618400
H	2.35508400	6.49813700	3.77301400
C	1.25704700	3.78113800	-1.20791300
H	0.04991800	5.28745900	-0.33492600
H	0.81994900	3.86109600	-2.19985100
N	2.29498800	2.89947400	-1.07690700
C	2.70018900	2.08105500	-2.21886000
H	2.55556100	2.69413400	-3.11478500
H	2.06259800	1.19159700	-2.33409000
C	4.14480800	1.64553700	-2.12325400

C	5.14889700	2.58839200	-1.88332900
C	4.48936100	0.30158600	-2.26758400
C	6.47786800	2.19118900	-1.79120100
H	4.87727900	3.63283200	-1.75328700
C	5.82347500	-0.09683200	-2.17912200
H	3.71235800	-0.43610800	-2.45701400
C	6.81819700	0.84616400	-1.94003000
H	7.25055200	2.92975200	-1.60387600
H	6.08159100	-1.14466800	-2.29378200
H	7.85553200	0.53622200	-1.86732700

M3SS

C	-3.41524300	-2.73018700	-0.21766000
C	-4.54690900	-3.48403700	0.07204900
C	-5.59493700	-3.53113800	-0.84554300
C	-5.50839000	-2.78822100	-2.02051300
C	-4.36372500	-2.03253500	-2.27524800
C	-3.28815400	-2.01234200	-1.40032200
C	-2.46189700	-2.69620600	0.95567900
C	-3.23390500	-3.43227300	2.11305300
C	-4.43509800	-4.12997100	1.42863400
H	-6.48777700	-4.11222400	-0.63891000
H	-6.32914800	-2.77975200	-2.72863300
H	-2.39852100	-1.43452700	-1.62480100
H	-1.48894900	-3.14419400	0.75643300
H	-2.57205800	-4.14911300	2.59884000
H	-4.24180100	-5.20267700	1.33418300
C	-3.17554900	-0.57403600	2.02031800
C	-4.23858000	-1.35816100	2.72090600
C	-1.35089500	-0.39952700	0.83582300
H	-5.08758900	-1.54303400	2.04914500
H	-5.33554000	-4.01643000	2.03939900
N	-2.23860200	-1.28333700	1.31025200
N	-2.91644700	0.69891500	2.01256700
N	-1.78510700	0.79642800	1.25719100
O	-3.62746700	-2.55624800	3.15650800
H	-4.59008800	-0.81509500	3.59769500
C	-1.28626000	2.06442600	0.84464300

C	-1.52231600	2.50687700	-0.45810600
C	-0.48736400	2.81860700	1.70244700
C	-0.94354800	3.68537800	-0.91023400
C	0.08828600	4.00428400	1.27225400
C	-0.14118400	4.41398800	-0.03737200
H	-1.10487000	4.02315700	-1.92622300
H	0.72654800	4.57909300	1.93200400
Br	-4.27975600	-0.93709600	-3.81894500
Br	-0.06489600	2.12617500	3.39490600
Br	0.69936100	5.97807000	-0.65070700
Br	-2.57053100	1.46158400	-1.62348800
C	2.28999700	-0.05915200	-0.30968000
C	0.93228600	0.11560100	0.28012200
H	2.21347200	-0.65323100	-1.22833800
H	0.84237300	0.88050000	1.03887200
C	2.82895400	1.31657100	-0.65636100
C	3.13440700	1.65308200	-1.97520400
C	2.94677100	2.29834100	0.33604400
C	3.54208000	2.94528000	-2.30190000
H	3.03410800	0.90329500	-2.75585000
C	3.34472400	3.59067800	0.01037500
H	2.69895400	2.06547900	1.37186000
C	3.63889500	3.91901600	-1.31236200
H	3.77034800	3.19213100	-3.33362800
H	3.41646100	4.34635500	0.78686500
H	3.93418500	4.93138100	-1.56758800
C	-0.13523800	-0.66329600	0.06997600
O	-0.22315600	-1.74750300	-0.74155400
H	0.62964000	-2.22637400	-0.75807300
C	1.06017900	-1.40226500	3.76507700
C	2.05667100	-0.89614500	2.93191500
C	2.40259400	-1.56392300	1.76199100
C	1.79478400	-2.78914000	1.43701200
C	0.80855100	-3.30126500	2.29127600
C	0.42688100	-2.59968200	3.43289700
H	3.92744000	-0.17601500	1.15492900
H	0.77226600	-0.85992100	4.65958100
H	2.53557000	0.05078800	3.17306300

C	3.23169900	-0.88573300	0.69588800
C	2.22529100	-3.45587800	0.21246500
H	0.34709400	-4.25796100	2.05652900
H	-0.35546300	-2.99489400	4.07391800
C	3.33938300	-3.00650400	-0.42316500
H	1.77721200	-4.39683400	-0.08468300
H	3.78880300	-3.55606400	-1.24500200
N	4.00123600	-1.86837300	-0.04269600
C	5.07073100	-1.35152200	-0.89856900
H	5.51790700	-0.50572400	-0.36425000
H	4.66774400	-0.95389900	-1.84134200
C	6.12808200	-2.39107500	-1.19061900
C	6.57590700	-2.59704500	-2.49440100
C	6.68584800	-3.13887800	-0.14948900
C	7.57906700	-3.52900600	-2.75783100
H	6.13839300	-2.02526900	-3.30855200
C	7.68281600	-4.07195500	-0.41118300
H	6.32591900	-2.98734700	0.86450800
C	8.13337100	-4.26750200	-1.71703800
H	7.92135700	-3.68017700	-3.77649600
H	8.11137400	-4.64734300	0.40321400
H	8.91144300	-4.99634400	-1.91957500

TS4RR

C	2.53032300	-1.02964200	-0.06627000
C	1.34315400	-0.41361500	0.60595500
H	2.45886800	-2.11491900	0.06265900
H	1.50216900	0.51905400	1.12749100
C	3.78779800	-0.52951600	0.62096100
C	4.68413000	-1.42475300	1.20253800
C	4.05366400	0.84283200	0.70042600
C	5.83490700	-0.96246700	1.83868700
H	4.47990100	-2.49103100	1.15822800
C	5.20063200	1.30652100	1.33656400
H	3.35155300	1.55653400	0.27180700
C	6.09709000	0.40278900	1.90652900
H	6.52415200	-1.67506800	2.28152400
H	5.39245900	2.37333400	1.39275000

H	6.99146400	0.76336600	2.40423800
C	0.14543300	-1.03463700	0.70060100
O	-0.20081000	-2.16361600	0.13541200
H	-0.09691900	-1.96662500	-1.20274800
C	1.14613700	2.47987100	-2.88742000
C	2.06587000	1.56219200	-2.38570700
C	1.69268000	0.23247400	-2.20492100
C	0.39639100	-0.19123600	-2.52112800
C	-0.52163700	0.73175800	-3.02376900
C	-0.14360700	2.05837300	-3.20960400
H	3.67853900	-0.49152500	-1.85301800
H	1.42991200	3.51955500	-3.01836300
H	3.07981900	1.87438800	-2.14953700
C	2.64758100	-0.79308400	-1.65353100
C	0.09219500	-1.65339200	-2.42852000
H	-1.52185900	0.39934500	-3.28548400
H	-0.85787600	2.76563800	-3.62093300
C	1.24183000	-2.45449800	-2.70548100
H	-0.80207100	-1.97264400	-2.96412400
H	1.15604800	-3.43538200	-3.16681900
N	2.44627800	-2.06090200	-2.38644000
C	3.63307300	-2.85136300	-2.75516400
H	3.30175500	-3.59877800	-3.48023700
H	4.32260700	-2.17673400	-3.26929000
C	4.31921800	-3.51915900	-1.58563700
C	5.68218000	-3.32434600	-1.37222300
C	3.61118100	-4.39610800	-0.75803700
C	6.33861700	-4.00664500	-0.34806100
H	6.23578100	-2.64081300	-2.01016300
C	4.26260000	-5.07052700	0.26922200
H	2.54606700	-4.55175800	-0.91724800
C	5.63100000	-4.88000500	0.47191900
H	7.40023100	-3.84851800	-0.18937800
H	3.70586900	-5.74878700	0.90727500
H	6.13987300	-5.41026300	1.27009600
C	-3.37820200	-2.46119700	0.86002400
C	-4.60692000	-2.97028200	1.26554600
C	-5.67660300	-2.98470600	0.37117800

C	-5.50742900	-2.46385700	-0.91007600
C	-4.26322100	-1.95587200	-1.28182900
C	-3.17800800	-1.96253800	-0.42058000
C	-2.37796400	-2.44875400	1.99387000
C	-3.20674200	-2.90813800	3.25278700
C	-4.55655900	-3.43160600	2.69868300
H	-6.64379800	-3.37577600	0.67029200
H	-6.33486900	-2.44179200	-1.61010100
H	-2.21870500	-1.56449200	-0.72540400
H	-1.51241000	-3.08132200	1.80564600
H	-2.66095700	-3.68905800	3.78047700
H	-4.59065600	-4.52341200	2.75831600
C	-2.62069100	-0.14127600	2.86961400
C	-3.76915800	-0.63884100	3.68404600
C	-0.89270100	-0.40975300	1.55310600
H	-4.66919700	-0.72178400	3.05874200
H	-5.38482300	-3.05118900	3.30441900
N	-1.88699600	-1.06747700	2.17152800
N	-2.13298200	1.05167100	2.73633300
N	-1.05098400	0.87773500	1.91110800
O	-3.37434100	-1.88440100	4.21994800
H	-3.97165200	0.04282700	4.50947000
C	-0.60426300	2.02894500	1.19550400
C	0.45555900	2.81910000	1.63143800
C	-1.33074900	2.41125200	0.06424900
C	0.82050100	3.96174800	0.92817100
C	-1.00702600	3.56748100	-0.62599600
C	0.07937200	4.31762000	-0.19182500
H	1.66270300	4.55947200	1.25335700
H	-1.57784200	3.86705200	-1.49492900
Br	-4.02022400	-1.17725700	-2.99509700
Br	-2.73852900	1.32830500	-0.54607800
Br	0.57655100	5.83371400	-1.18740500
Br	1.42643200	2.31927200	3.15587700
TS4RS			
C	-0.91198000	1.17386000	1.55661100
C	-0.47006000	-0.07941200	0.87528700

H	-0.15856000	1.41466000	2.31329900
H	-1.25957400	-0.69225100	0.47793200
C	-2.24875200	0.94098000	2.23801500
C	-2.38886500	1.11907900	3.61354200
C	-3.36421500	0.52950400	1.49870000
C	-3.61336200	0.88119000	4.23820700
H	-1.53286100	1.44021100	4.20060400
C	-4.58304900	0.27790800	2.11771100
H	-3.28674400	0.39719000	0.42054200
C	-4.71015900	0.45469700	3.49517400
H	-3.70581000	1.02434300	5.31000900
H	-5.42254100	-0.06267200	1.51900100
H	-5.65947500	0.26242200	3.98400500
C	0.83198800	-0.47792000	0.84397900
O	1.84010700	0.21758500	1.28730300
H	1.81638000	1.34989900	0.56996500
C	0.32134900	5.42905400	2.64719800
C	-0.57528100	4.53179100	2.07264900
C	-0.10822100	3.56180600	1.19017700
C	1.24963000	3.48543900	0.86425300
C	2.14313600	4.38672300	1.44439800
C	1.67821200	5.35064200	2.33479000
H	-2.04568100	2.82623500	0.61738100
H	-0.03692600	6.18425100	3.33851200
H	-1.63351500	4.57656800	2.31535200
C	-1.00646000	2.49207600	0.63143400
C	1.66821400	2.44203900	-0.11691900
H	3.19740900	4.32782100	1.19199600
H	2.37833400	6.04846700	2.78243200
C	0.64384900	2.08934100	-1.04500500
H	2.63450100	2.60619500	-0.59196800
H	0.88310500	1.69311300	-2.02972800
N	-0.62741200	2.21306200	-0.75337600
C	-1.67667000	1.75161700	-1.66470100
H	-1.21058300	1.56389500	-2.63598300
H	-2.05026200	0.78976400	-1.28959000
C	-2.80827300	2.74487200	-1.78463900
C	-4.13127600	2.30433300	-1.77186600

C	-2.53569200	4.10762400	-1.92936600
C	-5.17448900	3.21717900	-1.91549900
H	-4.35840800	1.24679600	-1.65527000
C	-3.57800200	5.01838500	-2.06346100
H	-1.50537800	4.45413200	-1.92643400
C	-4.89961300	4.57392700	-2.05948400
H	-6.20112200	2.86623600	-1.90601700
H	-3.35961000	6.07562600	-2.17160500
H	-5.71182500	5.28557700	-2.16407100
C	5.26162100	-1.51569000	-0.83289600
C	4.41772700	-0.90246000	0.09968700
C	4.45935700	0.47784100	0.28187100
C	5.28223900	1.21678400	-0.56090900
C	6.05952300	0.62798800	-1.55466300
C	6.06487700	-0.75744700	-1.67689200
C	5.24402300	-3.00827600	-0.67538800
C	4.72454500	-3.13900900	0.77281700
C	3.72462100	-1.95722200	0.94964100
H	3.89802100	0.95894100	1.07003800
H	6.71533500	-1.23657400	-2.40129300
H	4.56972600	-3.46874300	-1.40545100
H	5.54950700	-2.94247700	1.46107800
H	6.22699100	-3.46663200	-0.79798200
H	3.57296600	-1.65890500	1.98561500
N	2.38991700	-2.44575900	0.44440200
O	4.20833000	-4.39379800	1.13617000
C	1.19042900	-1.82598500	0.32125200
C	2.18888600	-3.75947900	0.06719600
N	0.37711900	-2.75356400	-0.20752300
N	0.97786800	-3.95984600	-0.35159100
C	3.20818800	-4.84215800	0.25667400
H	3.61356000	-5.16932700	-0.70691700
H	2.71290700	-5.69350700	0.72598200
C	-0.99834600	-2.62698500	-0.53611200
C	-1.38298100	-1.97141000	-1.70292300
C	-1.96336800	-3.03655100	0.38585500
C	-2.72268700	-1.69349900	-1.94389300
C	-3.30401100	-2.74500700	0.17633800

C	-3.65700600	-2.04988900	-0.97624700
H	-3.02184000	-1.16326400	-2.84047300
H	-4.04634600	-3.00373300	0.92128900
Br	-0.07528600	-1.29647300	-2.86651600
Br	-5.42775200	-1.45204800	-1.16757200
Br	-1.41055500	-3.80334400	2.00069800
H	6.68240300	1.24425700	-2.19266700
Br	5.37783400	3.09941500	-0.33164700

TS4SR

C	4.45876700	0.93667200	0.73724000
C	5.77946200	0.83029500	1.15857000
C	6.75714200	0.41337000	0.25614900
C	6.38806100	0.07752800	-1.04452400
C	5.05373700	0.19531700	-1.43310700
C	4.07241300	0.65176300	-0.56679300
C	3.53337100	1.26055500	1.88901400
C	4.46347500	1.23957200	3.15877000
C	5.91332700	1.19404000	2.61494000
H	7.79391200	0.32137600	0.56326000
H	7.12634400	-0.28411000	-1.75099800
H	3.04316400	0.77063100	-0.88747300
H	2.99616300	2.19936300	1.76873200
H	4.28416300	2.13132100	3.75817800
H	6.38741300	2.17348400	2.72840100
C	2.84617900	-1.03016500	2.54231300
C	4.06712900	-1.09221700	3.40205500
C	1.38755400	0.01061400	1.29015200
H	4.95012900	-1.32995000	2.79347300
H	6.51016100	0.47980500	3.19019600
N	2.53058700	0.17801700	1.97284600
N	1.96356800	-1.93771300	2.25538600
N	1.07163100	-1.28357200	1.45479100
O	4.17752900	0.16360600	4.03852700
H	3.94981300	-1.85704000	4.16933700
C	0.05373500	-2.03660400	0.80011000
C	-1.10444000	-2.38955600	1.49014000
C	0.18574000	-2.37954100	-0.54597000

C	-2.10580100	-3.12657300	0.87630200
C	-0.80642500	-3.11591900	-1.18049400
C	-1.93174100	-3.49137800	-0.45501300
H	-3.00647400	-3.39022200	1.41622400
H	-0.71285600	-3.37438600	-2.22777700
Br	4.52545500	-0.33163300	-3.17549800
Br	1.65701000	-1.76224900	-1.54029900
Br	-3.27832800	-4.48381500	-1.31258900
Br	-1.36525600	-1.70105600	3.21780200
C	-1.37969100	1.50731300	-0.82940600
C	-0.63902200	0.75306400	0.21695400
H	-0.61975800	2.02564300	-1.42230300
H	-1.15872800	-0.05276500	0.71460100
C	-2.04110200	0.48008900	-1.73103500
C	-1.32960500	0.03070700	-2.84706000
C	-3.25893600	-0.12800300	-1.41393500
C	-1.83437400	-0.99131000	-3.64651400
H	-0.36355900	0.47358200	-3.07619600
C	-3.76392500	-1.15137300	-2.21274100
H	-3.81724700	0.18483900	-0.53393200
C	-3.05527100	-1.58421000	-3.33216200
H	-1.27151400	-1.32518200	-4.51285200
H	-4.70527900	-1.62428400	-1.95031100
H	-3.44793700	-2.38787800	-3.94701600
C	0.66813100	1.00781400	0.47068900
O	1.37070500	2.02181100	0.03290700
H	0.61503700	3.13621300	0.20681100
C	-2.50138400	5.39217700	-2.91584900
C	-2.87719300	4.28648000	-2.15531200
C	-2.08785800	3.89214900	-1.08137600
C	-0.92332000	4.59544100	-0.74713500
C	-0.55745600	5.70420300	-1.50916100
C	-1.34164400	6.09424500	-2.59308500
H	-3.39480000	2.31899200	-0.40716300
H	-3.10962800	5.70178800	-3.75883100
H	-3.77355400	3.72432900	-2.40208600
C	-2.35770400	2.63374700	-0.29809600
C	-0.17465000	4.15100800	0.46872500

H	0.33494500	6.26566400	-1.24859900
H	-1.04893600	6.95627300	-3.18354200
C	-1.03028300	3.55984100	1.44989400
H	0.50022300	4.89485400	0.89061400
H	-0.77797100	3.59309400	2.50775300
N	-2.11902000	2.90659100	1.13105400
C	-2.79350800	2.10817000	2.18001400
H	-2.75916500	2.70904500	3.09307900
H	-2.19470700	1.20452600	2.35139800
C	-4.21289700	1.72504800	1.85604300
C	-5.14724900	2.68245200	1.45106600
C	-4.60567100	0.39377800	1.99571600
C	-6.45592700	2.30440400	1.17037000
H	-4.84220900	3.72080100	1.34246200
C	-5.92081700	0.01797700	1.72617000
H	-3.87746600	-0.34807800	2.31700000
C	-6.84427500	0.97169000	1.30847300
H	-7.17484300	3.04927300	0.84562000
H	-6.21914500	-1.01933000	1.83637300
H	-7.86608800	0.68001900	1.08943100

TS4SS

C	-3.67580300	-2.41764300	-0.21929100
C	-4.81670700	-3.09013100	0.20306900
C	-6.02767400	-2.86927300	-0.45099700
C	-6.08065700	-1.94789800	-1.49352300
C	-4.91726500	-1.28742100	-1.88931300
C	-3.69115600	-1.52983200	-1.28831800
C	-2.50316200	-2.68814300	0.69411000
C	-3.10122300	-3.56769500	1.85527900
C	-4.51818500	-3.97958100	1.38140100
H	-6.93062800	-3.38373500	-0.13841800
H	-7.01898000	-1.73100900	-1.99097400
H	-2.78345000	-1.03658600	-1.62134400
H	-1.66467600	-3.16693400	0.19278300
H	-2.46658700	-4.43774200	2.02181100
H	-4.52482300	-5.03292800	1.08594700
C	-2.67749000	-0.77672100	2.26097800

C	-3.64431000	-1.59247600	3.05560300
C	-1.17243300	-0.50289300	0.69619100
H	-4.64040800	-1.56485400	2.59289500
H	-5.23617600	-3.87115700	2.19990100
N	-2.02720100	-1.39560100	1.22183100
N	-2.27619500	0.44693300	2.41424000
N	-1.34245200	0.60809300	1.42778200
O	-3.11602900	-2.90228700	3.10707900
H	-3.71435800	-1.20975700	4.07325600
C	-0.89978000	1.92377700	1.11638000
C	-1.54071100	2.63647200	0.10131500
C	0.14217100	2.51464000	1.82724900
C	-1.14619000	3.93176500	-0.20103900
C	0.55260200	3.80839700	1.53899700
C	-0.10753100	4.50065100	0.52853100
H	-1.63873100	4.48603000	-0.98981400
H	1.36970600	4.26326700	2.08480300
Br	-5.01035700	0.03715700	-3.24356400
Br	1.04480300	1.50228000	3.12676000
Br	0.42500900	6.25990200	0.12437400
Br	-2.92173800	1.81887600	-0.88369800
C	2.16387800	-0.42357300	-1.11187800
C	0.97170700	-0.08279000	-0.29552400
H	1.82563200	-0.79725400	-2.08531400
H	1.12569600	0.59056000	0.53572300
C	3.08303900	0.76413100	-1.31022000
C	3.46408200	1.16944700	-2.59010900
C	3.59445900	1.45165900	-0.20330500
C	4.35840000	2.22526700	-2.76466500
H	3.05422900	0.65922000	-3.45848800
C	4.48685100	2.50463800	-0.37533500
H	3.28356800	1.17501100	0.80356000
C	4.87841700	2.88927200	-1.65744200
H	4.64633800	2.52662400	-3.76657500
H	4.87782800	3.02613700	0.49245800
H	5.57858200	3.70715900	-1.79063300
C	-0.20277600	-0.75356300	-0.39592900
O	-0.53341500	-1.68501600	-1.25273500

H	0.31057700	-2.75867100	-1.16247800
C	1.83230800	-2.08650400	3.15225200
C	2.58851200	-1.66936900	2.05849300
C	2.34725300	-2.20974000	0.79928600
C	1.37271700	-3.19716300	0.63053900
C	0.64441000	-3.63985100	1.73487300
C	0.85949000	-3.07140000	2.98885900
H	3.99131300	-1.25597800	-0.17855700
H	2.00327500	-1.64531800	4.12873700
H	3.35073100	-0.90382500	2.18245100
C	2.99978900	-1.63843300	-0.42928900
C	1.11520700	-3.67575100	-0.75834100
H	-0.08761700	-4.43362700	1.61091700
H	0.27107200	-3.40343100	3.83810200
C	2.25013400	-3.57930200	-1.62190300
H	0.58416800	-4.62236300	-0.84552100
H	2.36085500	-4.22844400	-2.48677500
N	3.17689700	-2.67491700	-1.44637300
C	4.28025600	-2.47438000	-2.40758400
H	4.09312700	-1.53112900	-2.93151500
H	4.22792800	-3.28883200	-3.13312900
C	5.61893900	-2.43437200	-1.71332700
C	6.16992100	-3.60927400	-1.19660100
C	6.29882500	-1.22510700	-1.55792700
C	7.39198600	-3.57636900	-0.53420800
H	5.64077900	-4.55133200	-1.31687900
C	7.52356600	-1.19295600	-0.89331800
H	5.86697500	-0.30760900	-1.95418700
C	8.06984000	-2.36681200	-0.38181400
H	7.81721300	-4.49278600	-0.13859800
H	8.04729100	-0.25009900	-0.77543000
H	9.02341000	-2.34143700	0.13541300

M4RR

C	2.07851100	-0.88798400	1.54739000
C	0.81913600	-0.07357100	1.42118800
H	1.91264000	-1.64958700	2.32127600
H	0.92627700	0.99066800	1.54734100

C	3.26060200	-0.04632100	2.00329400
C	4.22977600	-0.61709400	2.83236100
C	3.43039000	1.27898900	1.59130800
C	5.33657900	0.11721000	3.24968200
H	4.11146300	-1.64773100	3.16041500
C	4.53540300	2.01704800	2.00702300
H	2.71216300	1.73363600	0.91466900
C	5.49033600	1.43984200	2.84024400
H	6.07437000	-0.34146100	3.90003600
H	4.64801700	3.04499500	1.67668200
H	6.34946200	2.01638000	3.16717700
C	-0.44311200	-0.59205000	1.41296000
O	-0.84824500	-1.80471100	1.38409900
H	-0.58748400	-1.19385400	-1.06559100
C	3.54311900	0.76843300	-2.44761500
C	3.57429400	-0.04174600	-1.31692300
C	2.48414500	-0.85850200	-1.00629200
C	1.37949600	-0.88538400	-1.85764200
C	1.36751000	-0.10256900	-3.01149800
C	2.44048200	0.73354200	-3.29989400
H	3.49302700	-2.09265100	0.42418100
H	4.38335800	1.41693500	-2.67224200
H	4.44417000	-0.03722400	-0.66743900
C	2.49217500	-1.68080500	0.25777600
C	0.21247600	-1.77476500	-1.53741400
H	0.50245900	-0.14049400	-3.66930100
H	2.42035700	1.35972800	-4.18653300
C	0.54869000	-2.86490500	-0.59795500
H	-0.23297800	-2.21517000	-2.43550400
H	-0.09863500	-3.73571700	-0.54157600
N	1.59936800	-2.86521800	0.13496000
C	1.90956500	-4.01641000	1.00946100
H	1.94259000	-3.65885500	2.04031700
H	1.07627400	-4.71647700	0.92337500
C	3.22017900	-4.65347400	0.61516600
C	4.27159800	-4.72165500	1.52816100
C	3.38258200	-5.18309000	-0.66761800
C	5.47651600	-5.32118600	1.16599800

H	4.14437200	-4.31335100	2.52730600
C	4.58609300	-5.77668900	-1.03047600
H	2.56507200	-5.13197200	-1.38288600
C	5.63433000	-5.84679200	-0.11299500
H	6.28951300	-5.37445200	1.88224200
H	4.70679800	-6.18832600	-2.02689500
H	6.57243500	-6.31199800	-0.39728800
C	-4.11159800	-1.50454800	1.02114800
C	-5.49036700	-1.62388700	1.14481100
C	-6.25186100	-1.97183800	0.02883900
C	-5.62199100	-2.16124500	-1.20014900
C	-4.23560100	-2.03426800	-1.28590500
C	-3.45732300	-1.73396400	-0.18084900
C	-3.47452500	-0.98001800	2.28740500
C	-4.69494000	-0.67657900	3.23670600
C	-5.93102000	-1.31664600	2.55267700
H	-7.33032500	-2.06950100	0.10089300
H	-6.20125200	-2.39822800	-2.08527700
H	-2.37668700	-1.68091600	-0.22820200
H	-2.74437600	-1.66165700	2.71951500
H	-4.50987600	-1.10953500	4.21887800
H	-6.21838300	-2.23229300	3.07799900
C	-3.45043700	1.44853700	1.79993900
C	-4.84514900	1.51326500	2.33108500
C	-1.52718500	0.45501200	1.45025400
H	-5.56012000	1.17076200	1.57049100
H	-6.78605800	-0.63584500	2.60323200
N	-2.76415100	0.26930300	1.94299800
N	-2.71458000	2.36476400	1.25234200
N	-1.52003100	1.73442600	1.03277800
O	-4.87372100	0.70739000	3.49053700
H	-5.09263300	2.53533000	2.61640600
C	-0.59114900	2.37040700	0.16012600
C	0.37385500	3.25451300	0.63934800
C	-0.68629200	2.13809400	-1.21178500
C	1.28233200	3.85086300	-0.22603900
C	0.19175300	2.74617400	-2.09611100
C	1.18620300	3.57100100	-1.58465400

H	2.05227600	4.51001500	0.15593300
H	0.11729500	2.56159500	-3.16000200
Br	-3.35794100	-2.21153100	-2.96042500
Br	-1.98141600	0.94235500	-1.87285100
Br	2.45161800	4.29518500	-2.77227200
Br	0.49666700	3.57179900	2.48145000

M4RS

C	0.43316300	1.51928700	-1.01759300
C	0.12796300	0.21528600	-0.35930100
H	-0.12337000	1.52636300	-1.96135700
H	0.73132300	-0.07816900	0.48855300
C	1.91667800	1.57381400	-1.34688500
C	2.34326700	1.21436300	-2.62758900
C	2.87918700	1.86807900	-0.37477100
C	3.70069000	1.16500500	-2.93733700
H	1.60337600	0.95656100	-3.38092300
C	4.23555200	1.83292600	-0.68654600
H	2.58040600	2.11502100	0.64240700
C	4.65160400	1.48017100	-1.96897900
H	4.01375900	0.88161400	-3.93753500
H	4.97146500	2.05340700	0.08040100
H	5.71031600	1.44001000	-2.20543100
C	-0.76180800	-0.65877300	-0.92156200
O	-1.58600000	-0.50769400	-1.87789600
H	-2.38070200	1.93720400	-1.95544800
C	0.35727700	5.88083900	-2.39685800
C	0.65435500	4.89157400	-1.46285100
C	-0.30088300	3.92637900	-1.15977600
C	-1.54944900	3.94249300	-1.78270300
C	-1.84923800	4.94255100	-2.70316100
C	-0.89176000	5.90567600	-3.01397300
H	0.76574000	3.07754600	0.49602200
H	1.09827200	6.63558000	-2.63753700
H	1.62409600	4.86262200	-0.97372300
C	-0.00307500	2.78919900	-0.21950200
C	-2.54412400	2.87413700	-1.38871900
H	-2.82704500	4.96854100	-3.17485100

H	-1.12440900	6.68189400	-3.73523800
C	-2.36938800	2.49850000	0.03868200
H	-3.57866400	3.17460600	-1.56125100
H	-3.22452400	2.22113800	0.65111400
N	-1.21189000	2.48049400	0.58696700
C	-1.03245900	2.01718400	1.98899000
H	-2.02039600	2.04738800	2.45458900
H	-0.70410700	0.97552400	1.92835500
C	-0.03202500	2.85675900	2.73874200
C	1.12105900	2.26722600	3.25886500
C	-0.24465900	4.22845400	2.89956400
C	2.05691700	3.04701700	3.93673400
H	1.28223700	1.19727900	3.14414000
C	0.69370200	5.00522500	3.56979900
H	-1.14254300	4.68695900	2.49249100
C	1.84584600	4.41441700	4.08864000
H	2.95066300	2.58528800	4.34285100
H	0.52662000	6.07034400	3.69009200
H	2.57720600	5.02114900	4.61211600
C	-4.64823000	-2.69355000	0.83422800
C	-3.91586900	-1.99822800	-0.13311000
C	-4.19234700	-0.66619000	-0.43025400
C	-5.21421000	-0.05656100	0.28999300
C	-5.92038500	-0.71289900	1.29529100
C	-5.63584300	-2.04766300	1.56882300
C	-4.27205200	-4.14959100	0.85113200
C	-3.67044300	-4.31450300	-0.56083600
C	-3.00004800	-2.94744300	-0.87705300
H	-3.63655800	-0.15677600	-1.21096800
H	-6.20710600	-2.58060400	2.32191900
H	-3.53736500	-4.34856000	1.63966500
H	-4.48731100	-4.42724100	-1.27686000
H	-5.12067000	-4.81628200	1.01361000
H	-2.92313600	-2.72641600	-1.94082400
N	-1.60089900	-3.01120000	-0.36795400
O	-2.83522600	-5.42867700	-0.76501600
C	-0.65629300	-2.05314900	-0.36783100
C	-0.99782100	-4.17410700	0.05471100

N	0.45448800	-2.66204800	0.06737500
N	0.25510100	-3.98263200	0.33676500
C	-1.72907300	-5.47908600	0.10476500
H	-2.02161000	-5.71319700	1.13495900
H	-1.06505400	-6.26815200	-0.25018500
C	1.79173200	-2.17162800	0.12719800
C	2.35304000	-1.82534400	1.35281100
C	2.55492200	-2.05525700	-1.03368900
C	3.67599400	-1.41811400	1.44492000
C	3.88236100	-1.65721500	-0.96719200
C	4.42741000	-1.35813700	0.27620600
H	4.10406500	-1.14474800	2.40112400
H	4.47153200	-1.56372100	-1.87072000
Br	1.24853700	-1.79223600	2.87163700
Br	6.22278900	-0.80417600	0.36801300
Br	1.75145000	-2.34956400	-2.69922700
H	-6.70692100	-0.19413000	1.83123800
Br	-5.72891400	1.72043000	-0.15195700

M4SR

C	-4.17442600	1.80323400	-0.38050100
C	-5.47977300	2.09588000	-0.75907500
C	-6.53288000	1.75758800	0.08972600
C	-6.26130500	1.09531200	1.28481300
C	-4.94018300	0.80771000	1.62847300
C	-3.87325100	1.17880300	0.82340900
C	-3.19223500	2.11291500	-1.48649100
C	-4.09179800	2.53873000	-2.70355700
C	-5.51352900	2.74226800	-2.12071500
H	-7.56023400	1.97604800	-0.18362800
H	-7.06833800	0.79038100	1.94110200
H	-2.84656200	0.97462500	1.10955100
H	-2.45031600	2.85916300	-1.21353200
H	-3.70321800	3.45712500	-3.14222300
H	-5.73637000	3.81044400	-2.03966400
C	-3.05523100	-0.11193800	-2.55388300
C	-4.24970600	0.26362600	-3.36945400
C	-1.41292800	0.30294400	-1.16080200

H	-5.16915500	0.12733200	-2.78301300
H	-6.26174300	2.30752600	-2.79033400
N	-2.46564000	0.86114200	-1.78791600
N	-2.42580600	-1.24262300	-2.45752100
N	-1.41850800	-0.97367800	-1.57645100
O	-4.06712100	1.60438400	-3.77139900
H	-4.30566400	-0.35793500	-4.26288100
C	-0.59382900	-2.03564400	-1.12238800
C	0.52604700	-2.40997400	-1.86046000
C	-0.85091100	-2.63687800	0.10967500
C	1.38981600	-3.38972900	-1.39259400
C	0.00734200	-3.61122000	0.60167300
C	1.11451400	-3.97335400	-0.15981000
H	2.26785700	-3.67021400	-1.96061000
H	-0.17003000	-4.06449900	1.56882000
Br	-4.56844200	-0.17421300	3.20689300
Br	-2.29476800	-2.03688300	1.15422200
Br	2.31118500	-5.25163800	0.52619900
Br	0.93445600	-1.45845600	-3.42508700
C	1.55149500	0.93914600	1.20025300
C	0.63469700	0.35034000	0.17231700
H	0.94925600	1.59427900	1.84107400
H	0.91575400	-0.59188400	-0.26524200
C	2.20747600	-0.11912900	2.06560900
C	2.19284300	-0.00678500	3.45617400
C	2.84932100	-1.21894800	1.48487800
C	2.78940000	-0.98121700	4.25395600
H	1.70873700	0.85057400	3.91630200
C	3.44358600	-2.19612200	2.27811900
H	2.89015100	-1.31682900	0.40068400
C	3.41007700	-2.08061000	3.66717500
H	2.76480600	-0.88146000	5.33433800
H	3.92007800	-3.05187400	1.81146800
H	3.86951800	-2.84293000	4.28798200
C	-0.50575800	1.01027400	-0.19088500
O	-0.90653300	2.16363700	0.19005900
H	0.37628100	3.74400400	1.48901000
C	4.86879200	3.37189000	3.23632500

C	4.41795000	2.49526800	2.25350700
C	3.24536700	2.78309100	1.56009700
C	2.52100500	3.94344800	1.84066300
C	2.98367500	4.82439200	2.81495100
C	4.15165700	4.53374400	3.51603500
H	3.43371500	1.18884800	0.11901300
H	5.78091800	3.15088500	3.78000300
H	4.96761300	1.58574100	2.02771300
C	2.66211800	1.82612300	0.55722500
C	1.26545700	4.21391200	1.04243600
H	2.43224000	5.73634000	3.02415300
H	4.50713400	5.22075500	4.27661800
C	1.36425300	3.64219500	-0.32795500
H	1.05754100	5.28310500	0.96430600
H	0.88130800	4.13275800	-1.16849600
N	2.06637600	2.59714700	-0.57312300
C	2.28299900	2.09405900	-1.95051600
H	1.83703900	2.82591600	-2.62842200
H	1.74420000	1.14960700	-2.04977800
C	3.75532500	1.90007900	-2.22234700
C	4.65672100	2.95064500	-2.03403600
C	4.22028200	0.65636400	-2.65003500
C	6.01228200	2.75757500	-2.27759600
H	4.29838300	3.91721500	-1.68840700
C	5.57774200	0.46710600	-2.90211900
H	3.51559600	-0.15927000	-2.79302800
C	6.47344400	1.51576400	-2.71445400
H	6.71016700	3.57451000	-2.12793900
H	5.93384500	-0.50062300	-3.23908900
H	7.53110200	1.36668200	-2.90491500

M4SS

C	-4.34211400	-1.55114600	-0.00904300
C	-5.65818800	-1.84966200	0.32602900
C	-6.69152500	-1.43404500	-0.51216100
C	-6.38856700	-0.69598000	-1.65464400
C	-5.05611600	-0.41627500	-1.95810000
C	-4.00775500	-0.86219500	-1.16798300

C	-3.38264300	-1.96221100	1.08575600
C	-4.31776500	-2.45052000	2.25647700
C	-5.72522800	-2.60305400	1.62924100
H	-7.72650300	-1.65428200	-0.27083400
H	-7.17852700	-0.33064700	-2.30083300
H	-2.96580200	-0.68051100	-1.41687700
H	-2.65530900	-2.71241100	0.77159700
H	-3.94726500	-3.39247700	2.65905100
H	-5.94640100	-3.66052500	1.45478900
C	-3.18866900	0.17882300	2.32896000
C	-4.44576800	-0.19873700	3.04340200
C	-1.47680600	-0.28081100	1.04933800
H	-5.32352500	-0.00255100	2.41309600
H	-6.48650000	-2.22272300	2.31659300
N	-2.63157400	-0.77157400	1.51097200
N	-2.44306100	1.24002100	2.40175500
N	-1.38157800	0.94345100	1.59021500
O	-4.31617300	-1.56948800	3.37002500
H	-4.53994400	0.36464800	3.97124300
C	-0.50224900	1.98067800	1.15879400
C	-0.74165400	2.60868300	-0.06580100
C	0.59679600	2.36654300	1.92159500
C	0.11701100	3.59289400	-0.53386800
C	1.46848600	3.34922300	1.47184500
C	1.21276300	3.94993600	0.24539000
H	-0.06307200	4.07215500	-1.48783000
H	2.33230100	3.62882300	2.06151300
Br	-4.63383700	0.65804100	-3.46431600
Br	0.94515700	1.49025800	3.54135900
Br	2.37789800	5.28622500	-0.38255300
Br	-2.21880500	2.09001900	-1.11370300
C	1.86235300	-0.88633000	-0.61363400
C	0.77799300	-0.64446800	0.38060300
H	1.37432600	-0.91624700	-1.59708200
H	1.03681900	-0.17495100	1.32017800
C	2.82538100	0.28579600	-0.56489600
C	2.90645100	1.19240000	-1.62392900
C	3.59634200	0.51470500	0.57999300

C	3.75459700	2.29595700	-1.55107000
H	2.29478200	1.03552900	-2.50923600
C	4.44419800	1.61635300	0.65610100
H	3.53021600	-0.16985900	1.42424300
C	4.52842300	2.50842100	-0.41206900
H	3.79966500	2.99864900	-2.37721000
H	5.03721100	1.77985600	1.55061700
H	5.18015800	3.37383400	-0.35196000
C	-0.52478700	-0.90388400	0.07405400
O	-1.04273500	-1.53031200	-0.91024000
H	0.03735900	-3.09488500	-1.93327600
C	1.32238500	-4.35400400	2.43816000
C	2.06586600	-3.42978400	1.71127700
C	1.86473800	-3.30336800	0.33815300
C	0.93546100	-4.11109500	-0.30904700
C	0.19844900	-5.04480800	0.41578300
C	0.38685800	-5.15947500	1.78993100
H	3.59210200	-2.09398400	0.00710200
H	1.47690900	-4.45101700	3.50742700
H	2.79941000	-2.80137600	2.20962700
C	2.61760600	-2.26691600	-0.45451600
C	0.76182900	-3.92331100	-1.79268200
H	-0.51828700	-5.68016500	-0.09629100
H	-0.18790300	-5.88631100	2.35427400
C	2.02644200	-3.49745700	-2.43585300
H	0.37040100	-4.80923500	-2.29479300
H	2.24268900	-3.76337300	-3.46771400
N	2.89076700	-2.76859500	-1.82414200
C	4.07242400	-2.21018300	-2.53311800
H	3.83872000	-1.16266600	-2.74665400
H	4.15597900	-2.74843900	-3.47958600
C	5.33254100	-2.30922900	-1.71475500
C	5.86285500	-3.55866700	-1.38371600
C	5.96855700	-1.14621400	-1.27937900
C	7.02438200	-3.64187100	-0.62363400
H	5.36623700	-4.46464600	-1.72249100
C	7.13441600	-1.23183300	-0.52111200
H	5.54872900	-0.17387400	-1.52912600

C	7.66110000	-2.47769000	-0.19279900
H	7.43553400	-4.61316000	-0.36947800
H	7.62495300	-0.32420600	-0.18489200
H	8.56826600	-2.54382300	0.39890100

TS5RR

C	-1.81970000	2.02004400	0.60749900
C	-1.01526600	0.75848600	0.72134100
H	-1.11414000	2.85489100	0.68138500
H	-1.45547500	-0.11962300	1.17900800
C	-2.89714100	2.21724600	1.65237400
C	-3.25224500	3.52573000	1.99223000
C	-3.60514600	1.15805900	2.22696900
C	-4.29156600	3.77551800	2.88477500
H	-2.70760300	4.35566300	1.54587500
C	-4.64059200	1.40571100	3.12403400
H	-3.35776700	0.12829200	1.98237800
C	-4.98952200	2.71355700	3.45408700
H	-4.55184500	4.79855600	3.13719000
H	-5.17837700	0.57243300	3.56520600
H	-5.79752300	2.90274600	4.15324800
C	0.37826600	0.88796600	0.75995600
O	1.06511500	1.86921500	0.40446400
H	-1.90347700	-1.35481400	-0.81623300
C	-6.06674600	0.97768300	-0.90367500
C	-4.95755100	1.81151700	-0.81655500
C	-3.67758500	1.29701900	-1.02497500
C	-3.51553500	-0.05249700	-1.32893400
C	-4.62869300	-0.88893700	-1.41939600
C	-5.90248600	-0.37559000	-1.20225600
H	-2.69625500	3.20662100	-1.04713500
H	-7.05969600	1.38163000	-0.73694000
H	-5.07957800	2.86229400	-0.56751400
C	-2.45342500	2.16089500	-0.85531400
C	-2.13413700	-0.59581100	-1.55975100
H	-4.48516900	-1.94175000	-1.65607400
H	-6.76763000	-1.02710600	-1.26676200
C	-1.06268100	0.45848200	-1.56924600

H	-2.07962400	-1.09797800	-2.53821200
H	-0.07325200	0.15330000	-1.91142700
N	-1.37620700	1.73072100	-1.73413300
C	-0.36549800	2.67708000	-2.29635900
H	0.61529900	2.36912300	-1.93045000
H	-0.39956200	2.54476100	-3.38134500
C	-0.62888300	4.12020600	-1.95455000
C	-0.02801700	4.70766000	-0.83829400
C	-1.48788100	4.88040200	-2.75295200
C	-0.29513100	6.03742300	-0.51912700
H	0.64134100	4.10997700	-0.22572600
C	-1.75678900	6.20784700	-2.43192500
H	-1.94920900	4.42668300	-3.62655700
C	-1.16188700	6.78651800	-1.31215000
H	0.17688700	6.48988800	0.34695600
H	-2.42490400	6.79145900	-3.05658500
H	-1.36892900	7.82226000	-1.06305700
C	4.19240500	0.96717900	0.92193600
C	5.51708900	0.94843400	1.34363900
C	6.53303100	0.74074200	0.41156800
C	6.20139100	0.51825000	-0.92283300
C	4.86159500	0.53477800	-1.30992400
C	3.83836700	0.78618000	-0.40901600
C	3.24068100	1.07499200	2.09200900
C	4.16620600	0.97754100	3.36160900
C	5.61267300	1.14738600	2.83387200
H	7.57358000	0.72195700	0.71902300
H	6.97339800	0.32019500	-1.65747300
H	2.80061100	0.81629300	-0.72179600
H	2.63404800	1.97794000	2.08029600
H	3.89918700	1.76089200	4.06979700
H	5.98263000	2.14986100	3.06885000
C	2.73464200	-1.31987200	2.45760200
C	3.97285000	-1.39237900	3.29208300
C	1.17636500	-0.25346800	1.35566400
H	4.86149000	-1.47270600	2.65119800
H	6.28062000	0.43389500	3.32545700
N	2.32387900	-0.08376300	2.02939300

N	1.90449000	-2.24832100	2.09026500
N	0.93907800	-1.56911800	1.40382200
O	3.98860500	-0.22731200	4.08894400
H	3.93161000	-2.25913000	3.95102100
C	0.02907200	-2.33172600	0.62002400
C	-1.14428000	-2.83767500	1.17534600
C	0.36571300	-2.63894200	-0.70090100
C	-1.99613800	-3.63166000	0.41791800
C	-0.46596300	-3.44177300	-1.46928600
C	-1.64411100	-3.91636700	-0.89811400
H	-2.92317000	-4.00029700	0.83925600
H	-0.22002200	-3.66390000	-2.50045900
Br	4.39351400	0.13809600	-3.10483800
Br	1.90430200	-1.87270100	-1.46947400
Br	-2.84871800	-4.88391900	-1.96506300
Br	-1.60225200	-2.36945200	2.92991500

TS5RS

C	-0.55948000	1.38539000	1.32312000
C	-0.05472600	0.26284600	0.46567800
H	0.08052900	1.43448300	2.21040200
H	-0.69670300	-0.03586300	-0.34943500
C	-1.97689800	1.07122900	1.78299300
C	-2.14854300	0.31815900	2.94847800
C	-3.11304400	1.45270900	1.06259300
C	-3.42042700	-0.03176600	3.39222400
H	-1.27178600	-0.00123900	3.50630400
C	-4.38838700	1.11104000	1.50836000
H	-3.02431700	2.04337900	0.15409700
C	-4.54745600	0.36706800	2.67403900
H	-3.52996000	-0.61516700	4.30147700
H	-5.25714300	1.41429800	0.93274300
H	-5.54119600	0.09644400	3.01707000
C	0.93060000	-0.62826000	0.86779100
O	1.80618500	-0.50634100	1.75549400
H	2.39916600	1.31413000	0.77476400
C	1.19859700	5.52395800	2.68235800
C	0.20497900	4.75825100	2.07706000

C	0.56403000	3.69060800	1.26047100
C	1.90570600	3.38751500	1.03115100
C	2.89578800	4.16129700	1.63075300
C	2.54084100	5.22386400	2.45926900
H	-1.41894900	3.30641200	0.55184000
H	0.92536900	6.35610400	3.32229700
H	-0.84465900	4.98697700	2.23831400
C	-0.45302900	2.80332500	0.59292300
C	2.22615400	2.20470100	0.14847900
H	3.94037100	3.92487400	1.45527100
H	3.31577100	5.82053900	2.92895100
C	1.14128700	1.91346300	-0.84184600
H	3.15260600	2.36682100	-0.41276600
H	1.39303300	1.42258300	-1.77940900
N	-0.01169900	2.53656300	-0.77835400
C	-1.03323600	2.34176000	-1.81086800
H	-0.51363800	2.08851100	-2.73963200
H	-1.65687500	1.47783400	-1.54008500
C	-1.89683100	3.56843800	-1.98178700
C	-3.25930200	3.42015400	-2.24316000
C	-1.34494400	4.84931000	-1.90420300
C	-4.06279700	4.54099800	-2.43900700
H	-3.69304700	2.42351200	-2.29289200
C	-2.15009600	5.96825500	-2.09142500
H	-0.28636500	4.96809500	-1.68780300
C	-3.50896500	5.81608500	-2.36286100
H	-5.12118500	4.41659500	-2.64226200
H	-1.71620100	6.96042200	-2.02420300
H	-4.13499800	6.69026800	-2.50822700
C	4.83136800	-2.16969700	-1.27039700
C	4.17656200	-1.65754400	-0.14474900
C	4.46163800	-0.38402500	0.33579100
C	5.36822600	0.38275500	-0.39012100
C	5.97123500	-0.08030600	-1.55714400
C	5.71160700	-1.37595800	-1.99478800
C	4.52927400	-3.63234900	-1.44698900
C	4.08670200	-4.00887700	-0.01550300
C	3.35470600	-2.74416300	0.51335900

H	4.01786600	-0.02466200	1.25614700
H	6.22154300	-1.76629500	-2.86942800
H	3.72922300	-3.77928100	-2.18115200
H	4.97656900	-4.12940600	0.60633000
H	5.39144800	-4.21552900	-1.77487200
H	3.30951400	-2.67314400	1.59923200
N	1.93764600	-2.83849200	0.03767800
O	3.35389900	-5.19928300	0.13061900
C	0.92733100	-1.95154500	0.13017500
C	1.40768300	-3.99247900	-0.49530800
N	-0.13947100	-2.58340500	-0.37483700
N	0.14467500	-3.85409900	-0.76284200
C	2.20180200	-5.24950200	-0.67399200
H	2.44077400	-5.39900200	-1.73340400
H	1.59788000	-6.09323100	-0.33725300
C	-1.51975600	-2.22406900	-0.33958300
C	-2.14855500	-1.70155200	-1.46603700
C	-2.25539200	-2.45525300	0.82059300
C	-3.50984400	-1.43260800	-1.45538300
C	-3.62157700	-2.21613800	0.84709200
C	-4.22892500	-1.71092500	-0.29679500
H	-3.99590400	-1.01468800	-2.32820400
H	-4.19375800	-2.40241400	1.74684400
Br	-1.10639900	-1.25761800	-2.96397500
Br	-6.07407700	-1.35760600	-0.26143900
Br	-1.36640400	-3.03573800	2.36281500
H	6.66890100	0.55358700	-2.09249300
Br	5.85927900	2.09805100	0.25557600

TS5SR

C	4.52908100	0.53090600	0.72186000
C	5.82171300	0.31173900	1.18512800
C	6.78904000	-0.18841400	0.31431000
C	6.43641900	-0.49085800	-0.99929700
C	5.12995300	-0.26141900	-1.42955700
C	4.16383900	0.27642900	-0.59426000
C	3.60318400	0.95458000	1.84184800
C	4.48231100	0.82070400	3.14334300

C	5.93955800	0.66322900	2.64554200
H	7.80331300	-0.36833600	0.65567900
H	7.16529500	-0.91067100	-1.68300200
H	3.15873200	0.48116800	-0.94235800
H	3.18541100	1.95246700	1.71208000
H	4.35832300	1.70556700	3.76644100
H	6.48434000	1.60309500	2.77617400
C	2.64737400	-1.25128400	2.43248500
C	3.84925900	-1.47161200	3.29307000
C	1.30871500	-0.00518400	1.24209100
H	4.71053800	-1.77415300	2.68286700
H	6.45950800	-0.09653700	3.23656400
N	2.47897100	-0.00159500	1.89310200
N	1.65242600	-2.03303400	2.13820800
N	0.83157900	-1.24468400	1.38403400
O	4.07347400	-0.25399300	3.97487600
H	3.64806600	-2.24591100	4.03273600
C	-0.25165300	-1.85500200	0.68588600
C	-0.15080700	-2.10633000	-0.68551300
C	-1.37709600	-2.28261200	1.38670100
C	-1.16207200	-2.78732700	-1.34702700
C	-2.39780200	-2.96513900	0.73934900
C	-2.27260200	-3.20487500	-0.62338200
H	-1.08999200	-2.97926400	-2.40973300
H	-3.26764700	-3.30883800	1.28439800
Br	4.61302300	-0.73477700	-3.19155200
Br	-1.50596500	-1.91215400	3.22076500
Br	-3.65786800	-4.10267300	-1.52232400
Br	1.36155100	-1.55079400	-1.65661800
C	-1.31498200	1.92287900	-0.75434100
C	-0.65346500	1.27803200	0.43550800
H	-0.50862400	2.39077500	-1.32744900
H	-1.24305100	0.58203500	1.03054500
C	-1.95123000	0.88578200	-1.66038600
C	-1.29269900	0.51886100	-2.83715500
C	-3.15470500	0.25150100	-1.33852900
C	-1.84019700	-0.43752700	-3.69061200
H	-0.34034600	0.98257900	-3.08158400

C	-3.71205700	-0.69096900	-2.19699000
H	-3.66464600	0.49627800	-0.41333000
C	-3.05779700	-1.03805900	-3.37873600
H	-1.31485700	-0.70816900	-4.60142700
H	-4.64796300	-1.17213000	-1.92791600
H	-3.48769000	-1.78229000	-4.04219100
C	0.73394200	1.10868200	0.40592100
O	1.58194100	1.79587000	-0.20570700
H	0.85709000	3.52196300	0.54018300
C	-1.77895700	6.32027900	-2.31966900
C	-2.34468600	5.11980500	-1.89436000
C	-1.75918300	4.41764800	-0.84771700
C	-0.61231200	4.90296200	-0.21132200
C	-0.06161000	6.11054800	-0.63202700
C	-0.64027900	6.81390900	-1.68807000
H	-3.32265000	2.92847300	-0.65056100
H	-2.23039200	6.87042800	-3.13856000
H	-3.23753100	4.72899500	-2.37376100
C	-2.29638100	3.10708900	-0.32234900
C	-0.00424100	4.09309200	0.91526900
H	0.82264100	6.50152800	-0.13622400
H	-0.20197100	7.75128500	-2.01453200
C	-1.01876200	3.20021500	1.59417300
H	0.38766700	4.75860600	1.69342600
H	-0.89154000	3.00437900	2.65676900
N	-2.26021700	3.18180300	1.13259800
C	-3.45304700	3.02639700	1.97272600
H	-4.06983700	3.91679200	1.81004500
H	-3.10986200	3.04946600	3.00998600
C	-4.26082400	1.78290600	1.70474200
C	-5.40579700	1.83477900	0.90751100
C	-3.86518800	0.56401200	2.25885500
C	-6.13044600	0.67408300	0.64073100
H	-5.72909500	2.78507300	0.49003900
C	-4.59576700	-0.59234000	2.00595600
H	-2.98969800	0.52375100	2.90186800
C	-5.72339500	-0.54141900	1.18635900
H	-7.01336600	0.72019000	0.01206400

H	-4.29489800	-1.52632900	2.46882500
H	-6.28996600	-1.44488500	0.98510100
TS5SS			
C	4.17975400	1.56449800	0.62529500
C	5.51090500	1.69453700	1.00496400
C	6.51775100	1.49882500	0.06017400
C	6.17408900	1.14646000	-1.24308300
C	4.82841300	1.02602400	-1.58951800
C	3.80984200	1.25830100	-0.67861600
C	3.24821700	1.68754100	1.81109200
C	4.20995100	1.81492600	3.05286300
C	5.62709100	2.03606300	2.46760500
H	7.56332000	1.59434000	0.33478400
H	6.94289700	0.96048300	-1.98434200
H	2.76447600	1.19966400	-0.95943900
H	2.53921300	2.50966500	1.72447300
H	3.89596800	2.65204300	3.67508700
H	5.92977800	3.07900000	2.60015200
C	3.01195700	-0.70178900	2.43773600
C	4.25076900	-0.55350300	3.25960300
C	1.34141900	0.07802700	1.26895600
H	5.14270600	-0.61416500	2.62148000
H	6.35706400	1.42057000	3.00221500
N	2.46600900	0.43629000	1.90321600
N	2.29189400	-1.74809500	2.16466800
N	1.26330800	-1.24921700	1.41770100
O	4.14722200	0.69203900	3.91805100
H	4.30132600	-1.33798100	4.01431800
C	0.40260900	-2.17325300	0.75338100
C	0.54833000	-2.42013000	-0.61404100
C	-0.56492200	-2.86444400	1.47841100
C	-0.21205300	-3.40254700	-1.23128800
C	-1.33263100	-3.85333300	0.87987100
C	-1.12296800	-4.12374400	-0.46717200
H	-0.10660500	-3.59223400	-2.29224600
H	-2.08331600	-4.38876500	1.44727700
Br	4.34150700	0.49042200	-3.34246000

Br	-0.89892800	-2.35336900	3.25453800
Br	-2.13898800	-5.46771000	-1.30072700
Br	1.72926200	-1.38688600	-1.65100800
C	-1.72428200	0.99041600	-0.76554800
C	-0.88615600	0.51867500	0.37723600
H	-1.06182400	1.55869200	-1.42917400
H	-1.19978500	-0.36648200	0.91557500
C	-2.24589400	-0.20004100	-1.54893600
C	-1.79391000	-0.39659300	-2.85625900
C	-3.07057500	-1.17621000	-0.97229900
C	-2.17725600	-1.52082900	-3.58617300
H	-1.12286000	0.33252700	-3.30238600
C	-3.46858500	-2.28859300	-1.70602200
H	-3.39965100	-1.07630600	0.05874000
C	-3.02312900	-2.46717400	-3.01517400
H	-1.81030300	-1.65510800	-4.59879500
H	-4.10152600	-3.03980400	-1.24278600
H	-3.31836700	-3.34933700	-3.57457800
C	0.41949800	0.97142000	0.48528700
O	0.93770600	2.00357700	-0.01248700
H	-1.99022200	0.68439400	2.93312100
C	-6.17086200	0.44522200	0.48964700
C	-5.15047800	1.10099500	-0.18968700
C	-3.96426800	1.42316400	0.46899800
C	-3.80740100	1.11520000	1.82126900
C	-4.83536200	0.45836200	2.49919300
C	-6.00821300	0.11452600	1.83454700
H	-3.18582400	2.61732000	-1.13747500
H	-7.08914400	0.19027500	-0.02824200
H	-5.26172000	1.34771900	-1.24181500
C	-2.81923400	2.04106900	-0.28466900
C	-2.55635800	1.53846700	2.54832000
H	-4.71441500	0.22145900	3.55286900
H	-6.80012200	-0.40067400	2.36781300
C	-1.66413600	2.41330100	1.72127500
H	-2.82586200	2.13958700	3.42941100
H	-0.83195500	2.90574500	2.22001900
N	-2.04529200	2.92858200	0.58110400

C	-1.33815000	4.04747300	-0.06009800
H	-0.71694400	3.65390500	-0.86972300
H	-0.66215000	4.47146200	0.68689200
C	-2.31784200	5.08006700	-0.56892200
C	-3.43983400	5.43914400	0.18232200
C	-2.08634600	5.70251600	-1.79551000
C	-4.31396700	6.41457300	-0.28708900
H	-3.63289500	4.94936500	1.13333500
C	-2.95622600	6.68610500	-2.26076700
H	-1.22149000	5.41737800	-2.38824600
C	-4.07185200	7.04259900	-1.50777000
H	-5.18505100	6.68533600	0.30044400
H	-2.76714700	7.16542600	-3.21566800
H	-4.75449100	7.80280800	-1.87290100

M5RR

C	-1.91335300	1.11348800	1.53656200
C	-0.67899100	0.58058700	0.75848600
H	-1.53407700	1.67751100	2.39293200
H	-0.93323900	-0.34032000	0.23315400
C	-2.84738500	0.04175400	2.04659100
C	-3.06000200	-0.05869400	3.42480300
C	-3.48673900	-0.87899500	1.20643800
C	-3.88622000	-1.04558200	3.95654900
H	-2.56336900	0.64326200	4.08970700
C	-4.32978700	-1.85330300	1.73514100
H	-3.32902800	-0.85125700	0.13127500
C	-4.52925800	-1.94476900	3.11032300
H	-4.02994900	-1.10753500	5.03044700
H	-4.83283500	-2.54288600	1.06232800
H	-5.18229700	-2.70943700	3.51813700
C	0.51335100	0.37571700	1.64709500
O	0.78551400	1.07077900	2.59572300
H	-0.31045100	0.31821600	-1.97119200
C	-5.13229300	0.65907100	-1.68814400
C	-4.52319800	1.41272400	-0.68794600
C	-3.13715900	1.55579600	-0.65023300
C	-2.35130800	0.98798600	-1.66813800

C	-2.96751400	0.21686400	-2.65436300
C	-4.34982800	0.03993700	-2.66042900
H	-3.10851800	2.89797700	1.05298900
H	-6.21078700	0.54072100	-1.69849200
H	-5.12389100	1.86321000	0.09843800
C	-2.44859300	2.18651100	0.54799700
C	-0.85409900	1.22222000	-1.68209200
H	-2.35744700	-0.24489500	-3.42815700
H	-4.81113600	-0.57636000	-3.42538300
C	-0.37930600	1.70076200	-0.30713600
H	-0.60141100	1.97708400	-2.43743900
H	0.67748700	1.99234600	-0.34743400
N	-1.17631200	2.82055400	0.19544500
C	-1.27418800	3.96712400	-0.70260700
H	-0.25067000	4.24510300	-0.98374300
H	-1.81730200	3.73212000	-1.63207100
C	-1.95608900	5.12730800	-0.01538900
C	-1.42926400	5.65123200	1.16888600
C	-3.11958100	5.68300000	-0.54512500
C	-2.04767900	6.72445100	1.80102800
H	-0.53236300	5.20578800	1.59047300
C	-3.74203300	6.75969300	0.08623900
H	-3.54159800	5.26867000	-1.45722000
C	-3.20544900	7.28353600	1.25836500
H	-1.62830500	7.12778000	2.71739500
H	-4.64681000	7.18455400	-0.33653300
H	-3.68762100	8.12139700	1.75154600
C	4.31966700	0.88484700	0.79466700
C	5.70197800	0.97468500	0.91322600
C	6.46564800	1.29152000	-0.20867000
C	5.83493400	1.47604800	-1.43778300
C	4.44929000	1.34780200	-1.53024100
C	3.66999300	1.06504000	-0.41783100
C	3.68902200	0.43796400	2.09588200
C	4.90657700	-0.03213400	2.96775100
C	6.13968200	0.63795000	2.31629000
H	7.54611500	1.36475300	-0.14164100
H	6.41551700	1.69710000	-2.32603600

H	2.59719800	0.94272800	-0.52729000
H	3.09602900	1.20121500	2.59726800
H	4.77141400	0.27476100	4.00390400
H	6.40880200	1.54239900	2.87057400
C	3.37011000	-1.90027300	1.43578700
C	4.79992800	-2.12847100	1.81310100
C	1.53445900	-0.72368500	1.34986100
H	5.46262000	-1.78099000	1.00896800
H	6.99850000	-0.03770400	2.35315100
N	2.80659000	-0.70180800	1.77628600
N	2.50914200	-2.67006700	0.83183200
N	1.38185200	-1.91979600	0.77518300
O	5.01396200	-1.44581100	3.02971100
H	4.97542900	-3.19048000	1.98322600
C	0.26852100	-2.39996900	0.02771400
C	-0.85162700	-2.91827300	0.66966500
C	0.30202900	-2.28189400	-1.36328600
C	-1.94732600	-3.32814500	-0.07761900
C	-0.79806100	-2.65918400	-2.11927500
C	-1.91653000	-3.16114800	-1.45753500
H	-2.82766600	-3.71685100	0.41769900
H	-0.79568600	-2.53816100	-3.19554300
Br	3.58711100	1.50656900	-3.20712500
Br	1.78612600	-1.47879500	-2.19477100
Br	-3.46526700	-3.54494000	-2.44475400
Br	-0.94086600	-2.89512900	2.53757100

M5RS

C	-0.76981900	1.28661800	1.51246800
C	0.02337400	0.55852400	0.39025400
H	-0.10417300	1.40972400	2.37226200
H	-0.67731400	-0.02922800	-0.19307500
C	-1.99426900	0.52937000	1.99149300
C	-1.83422800	-0.44642700	2.98134700
C	-3.28501700	0.77973900	1.51214000
C	-2.92787300	-1.14721200	3.48285800
H	-0.83935300	-0.65283500	3.37128800
C	-4.38325500	0.08598000	2.01583200

H	-3.45756100	1.54402800	0.76163300
C	-4.20881400	-0.88000300	3.00393500
H	-2.77779200	-1.90036600	4.24985300
H	-5.37431600	0.30270500	1.63059100
H	-5.06443200	-1.41582400	3.40281400
C	1.12392000	-0.33505400	0.86380100
O	1.92454900	-0.05878400	1.72759500
H	2.47695100	1.92224500	0.24536400
C	0.60574000	5.40326800	3.01875800
C	-0.36605500	4.58433600	2.44924000
C	-0.01576200	3.66617000	1.46346500
C	1.31059400	3.55450900	1.03403400
C	2.27779700	4.37596100	1.61284000
C	1.92990500	5.29339100	2.60153800
H	-2.03243200	3.06906000	1.02287700
H	0.33087200	6.12176500	3.78418600
H	-1.40191600	4.65571200	2.77039200
C	-1.01512100	2.70401900	0.86905100
C	1.66140900	2.57605500	-0.07053000
H	3.31123200	4.29137900	1.29149000
H	2.69432500	5.92428800	3.04369800
C	0.47084700	1.74360200	-0.56256100
H	2.04529600	3.13713900	-0.93037900
H	0.67866100	1.35339900	-1.56145300
N	-0.72193800	2.57872500	-0.56858700
C	-1.81879400	2.03990700	-1.37033000
H	-1.41688200	1.84491500	-2.37261000
H	-2.19931800	1.07473300	-0.99401400
C	-2.98854900	2.99392100	-1.46795400
C	-4.29069000	2.49264000	-1.54896200
C	-2.78849900	4.37589000	-1.50766300
C	-5.37462000	3.35683300	-1.68560000
H	-4.46731800	1.41949500	-1.48475100
C	-3.87230200	5.23972300	-1.63854000
H	-1.77782300	4.76348600	-1.42399100
C	-5.16743000	4.73306000	-1.73258700
H	-6.38067800	2.95403000	-1.74591000
H	-3.70557800	6.31189800	-1.66590500

H	-6.01088800	5.40845900	-1.83269600
C	5.16806800	-1.54973000	-1.09104900
C	4.44986500	-1.00592100	-0.02030200
C	4.49100200	0.35763800	0.25211800
C	5.19174500	1.16841200	-0.63672900
C	5.85695300	0.65121400	-1.74567500
C	5.86331700	-0.72315000	-1.96404100
C	5.12317200	-3.05202000	-1.06699000
C	4.71787800	-3.31706900	0.39887600
C	3.81050700	-2.11616800	0.78505400
H	4.02277900	0.77487200	1.13563500
H	6.42253700	-1.13938100	-2.79551700
H	4.38014900	-3.42826300	-1.77895200
H	5.60435000	-3.24429100	1.03174600
H	6.07937300	-3.51629400	-1.31427600
H	3.74367700	-1.93624200	1.85712500
N	2.42070800	-2.46540700	0.31553400
O	4.14615000	-4.56999200	0.68041200
C	1.29943100	-1.72033700	0.23969300
C	2.09502800	-3.71240500	-0.15433000
N	0.37726100	-2.52037800	-0.30814000
N	0.85479400	-3.75827400	-0.55071300
C	3.04030400	-4.87480100	-0.13017700
H	3.32837800	-5.14731700	-1.15172100
H	2.52439800	-5.72494200	0.31949600
C	-1.02307000	-2.31448800	-0.50619300
C	-1.49378600	-1.68150700	-1.65406500
C	-1.91665300	-2.78758500	0.45518100
C	-2.85137100	-1.44690100	-1.81464300
C	-3.27859300	-2.56773600	0.30666100
C	-3.71899300	-1.86511800	-0.81031900
H	-3.21768600	-0.92430900	-2.69029000
H	-3.97526100	-2.90919000	1.06151300
Br	-0.27338300	-1.02968700	-2.91975000
Br	-5.53601500	-1.42357200	-0.95489800
Br	-1.26071000	-3.70888900	1.94684300
H	6.39245800	1.31778200	-2.41194700
Br	5.27011300	3.03391900	-0.32515300

M5SR

C	-4.35841700	-1.64250800	0.24760400
C	-5.69068500	-1.84627900	0.58985100
C	-6.69510800	-1.43399200	-0.28429700
C	-6.34905000	-0.78868200	-1.46904100
C	-5.00344400	-0.59098200	-1.77811800
C	-3.98783500	-1.03759400	-0.94656700
C	-3.43422900	-2.03872000	1.37754100
C	-4.39880600	-2.39311400	2.57103000
C	-5.80983100	-2.49882800	1.94237200
H	-7.74117800	-1.58312200	-0.03751800
H	-7.11594100	-0.42626000	-2.14383700
H	-2.94897800	-0.88771600	-1.21413200
H	-2.76078600	-2.85913000	1.13326300
H	-4.08583500	-3.33150100	3.02648200
H	-6.09658400	-3.54988000	1.84242400
C	-3.13463600	0.16626000	2.46685100
C	-4.39556100	-0.10182800	3.22385900
C	-1.47096400	-0.40019000	1.18501500
H	-5.26903500	0.11298000	2.59372300
H	-6.54969500	-2.02282900	2.59252200
N	-2.61355600	-0.85310100	1.71648300
N	-2.37511200	1.22430000	2.41768300
N	-1.34678700	0.85678100	1.61352600
O	-4.33714300	-1.45197600	3.62977900
H	-4.43767400	0.52347800	4.11511800
C	-0.43783600	1.86137200	1.16281000
C	-0.62657900	2.44887600	-0.08924000
C	0.60600300	2.27881700	1.98570300
C	0.19274100	3.49159200	-0.49625300
C	1.44913200	3.30311600	1.58178000
C	1.21549700	3.90701800	0.34980100
H	0.04850100	3.95904600	-1.46162900
H	2.27100200	3.61942300	2.21154800
Br	-4.51808700	0.37263900	-3.33470900
Br	0.91381800	1.36986000	3.59447000
Br	2.33377400	5.30616100	-0.20745700

Br	-1.96476000	1.80877000	-1.24632400
C	1.59143200	-1.03147600	-1.07937500
C	0.91984100	-0.89799700	0.32242900
H	0.91762200	-1.56303600	-1.75608400
H	1.09946200	0.10638100	0.70373200
C	1.90781200	0.32303100	-1.67048400
C	1.10407500	0.83970700	-2.68813800
C	2.98903500	1.08173900	-1.20508300
C	1.38113300	2.08675100	-3.24686400
H	0.25337200	0.26308500	-3.04317600
C	3.27242200	2.32112300	-1.77008900
H	3.60932300	0.68186200	-0.40559700
C	2.46975600	2.82696600	-2.79354800
H	0.74771000	2.47492300	-4.03875500
H	4.11288400	2.90304700	-1.40413800
H	2.68754400	3.79910000	-3.22518600
C	-0.54485900	-1.19529400	0.28896100
O	-1.05575500	-2.07783700	-0.36205900
H	0.23532700	-3.42345800	1.44399000
C	2.47627100	-5.38261800	-2.36168100
C	2.86261200	-4.06199400	-2.15277500
C	2.46349100	-3.38240200	-1.00228100
C	1.67701800	-4.03301300	-0.04243500
C	1.29794300	-5.35849200	-0.25743700
C	1.68816300	-6.03054200	-1.41193300
H	3.69234700	-1.63905900	-1.36522700
H	2.79040900	-5.90615400	-3.25884100
H	3.48054300	-3.54946400	-2.88614000
C	2.82114400	-1.92630900	-0.76939700
C	1.30743200	-3.32200000	1.24450400
H	0.69377900	-5.86699700	0.49000200
H	1.38330100	-7.06031700	-1.56816700
C	1.73901700	-1.84756400	1.25461700
H	1.80837400	-3.82403700	2.08158700
H	1.72856400	-1.45952400	2.27874200
N	3.06106600	-1.64514300	0.65368600
C	4.14745700	-2.40562900	1.27136500
H	3.98685100	-3.49346500	1.21567500

H	4.17210800	-2.12806100	2.33170400
C	5.46080500	-2.06574500	0.60849400
C	6.12218400	-3.00657700	-0.18023400
C	6.00530800	-0.78516400	0.74129600
C	7.31658100	-2.67958700	-0.82107500
H	5.69367700	-3.99899000	-0.29789500
C	7.19582600	-0.45506300	0.10211300
H	5.48756800	-0.04973600	1.35237200
C	7.85477000	-1.40359500	-0.68052300
H	7.82288800	-3.42081900	-1.43112700
H	7.61399200	0.54012500	0.21587900
H	8.78404800	-1.14685300	-1.17880000

M5SS

C	4.23145700	1.56671400	0.66275800
C	5.56134400	1.64246300	1.06150500
C	6.57208700	1.42821800	0.12507000
C	6.23362900	1.10894600	-1.18775900
C	4.88967500	1.03847500	-1.55438200
C	3.87027500	1.29295100	-0.65035300
C	3.29193300	1.70078200	1.83965500
C	4.24137200	1.78385900	3.09666000
C	5.67310000	1.95169000	2.53110600
H	7.61644600	1.48246900	0.41454200
H	7.00542300	0.90795300	-1.92185600
H	2.83287100	1.26123900	-0.95863300
H	2.61129700	2.54940800	1.77427200
H	3.94928500	2.63244600	3.71326200
H	6.01926100	2.97746900	2.68690500
C	2.96168700	-0.68482000	2.45693400
C	4.18810400	-0.58388500	3.30478700
C	1.34709900	0.13770500	1.25716700
H	5.08948700	-0.68416500	2.68514900
H	6.36899200	1.29501300	3.06183600
N	2.47270400	0.46739900	1.90159200
N	2.20157900	-1.70430100	2.17700600
N	1.20045600	-1.17549200	1.42494900
O	4.11676800	0.66516600	3.95783700

H	4.18732600	-1.36876800	4.06084300
C	0.33380800	-2.07459700	0.73231800
C	0.53826600	-2.33167100	-0.62669600
C	-0.63059900	-2.78956300	1.44004600
C	-0.14862500	-3.36259000	-1.24828400
C	-1.33610900	-3.81530700	0.82832800
C	-1.05761000	-4.10558200	-0.50270700
H	0.01018600	-3.57334000	-2.29839600
H	-2.08852900	-4.36942500	1.37542600
Br	4.40482800	0.53628300	-3.31501900
Br	-1.01445400	-2.29599600	3.20856500
Br	-1.98516300	-5.49966300	-1.35036000
Br	1.73245500	-1.28598000	-1.63710600
C	-1.75501500	1.06624900	-0.71888700
C	-1.04858700	0.86937200	0.64660300
H	-1.08507500	1.66019500	-1.34975200
H	-1.27026900	-0.10650800	1.08539900
C	-2.08425700	-0.20169100	-1.47112100
C	-1.59666800	-0.36512300	-2.77148600
C	-2.89216200	-1.21295500	-0.93081000
C	-1.93927400	-1.48133600	-3.53316800
H	-0.94380100	0.39482800	-3.19314800
C	-3.26238900	-2.30956400	-1.70179900
H	-3.25521100	-1.14070300	0.09125800
C	-2.79047200	-2.44861700	-3.00612500
H	-1.54764500	-1.58669600	-4.53986300
H	-3.90030500	-3.07641100	-1.27183100
H	-3.06827500	-3.31717700	-3.59503000
C	0.42190800	1.09778700	0.54953700
O	0.93406400	2.07056900	0.03841500
H	-2.28171800	0.58147900	3.06313800
C	-6.17403800	0.09401100	0.25961000
C	-5.19618200	0.87030800	-0.35532600
C	-4.06829700	1.27802600	0.35351600
C	-3.92183400	0.92626800	1.70307700
C	-4.90146500	0.13854900	2.30851600
C	-6.01986500	-0.28171500	1.59241900
H	-3.30911400	2.57632600	-1.19555700

H	-7.04806900	-0.22213500	-0.30024200
H	-5.29507100	1.14697300	-1.40173000
C	-2.94322200	2.02431100	-0.32533400
C	-2.71830800	1.40769800	2.48992400
H	-4.78432200	-0.14670400	3.35114500
H	-6.77250500	-0.89586000	2.07625100
C	-1.66771200	2.02103700	1.56159400
H	-3.03434100	2.17206200	3.20834600
H	-0.90287300	2.54737800	2.13894700
N	-2.33810100	2.92740000	0.64975900
C	-1.56669500	4.02714400	0.08160200
H	-0.85444600	3.70960000	-0.69526600
H	-0.96323000	4.45086700	0.89382400
C	-2.47376800	5.10318200	-0.48320700
C	-3.76697400	5.29337500	0.00858000
C	-2.00335700	5.94640200	-1.49235800
C	-4.56976900	6.31491100	-0.49279400
H	-4.13855400	4.62593900	0.77978900
C	-2.80200900	6.97294700	-1.98947400
H	-1.00317600	5.79742900	-1.89215600
C	-4.08940200	7.16033200	-1.49033400
H	-5.57392000	6.44983300	-0.10292700
H	-2.42207200	7.62157200	-2.77253700
H	-4.71599800	7.95578200	-1.88079300

M06RR

C	1.98836700	0.51463600	2.24112500
C	1.11220400	0.13970200	1.01285700
H	1.39960300	1.18258500	2.87709500
H	1.62383000	0.29126100	0.06263400
C	3.33174400	1.15292000	1.97798000
C	3.93471700	1.85378300	3.02816400
C	4.04583100	0.99015200	0.79021100
C	5.22094400	2.37046100	2.90281100
H	3.38372600	1.99499400	3.95576100
C	5.33518600	1.50098500	0.66394200
H	3.60907800	0.47799400	-0.06178900
C	5.92901700	2.18939200	1.71696200

H	5.66751300	2.91584500	3.72846100
H	5.87109600	1.36892300	-0.27129400
H	6.93101600	2.59323400	1.61036300
C	-0.17038500	0.92309700	0.99377600
O	-0.79761500	1.26841800	1.96886200
H	1.84164400	-2.04854100	-0.46618000
C	5.51493400	-2.48007600	2.56458800
C	4.46705200	-1.75218500	3.11897100
C	3.22824900	-1.69493100	2.48074300
C	3.03537000	-2.38138700	1.27655300
C	4.08826100	-3.11564100	0.72796900
C	5.32445200	-3.16327300	1.36333300
H	2.20438900	-0.67853300	4.08865400
H	6.47748300	-2.51472700	3.06484800
H	4.61114200	-1.20776700	4.04918200
C	2.09128800	-0.84279700	3.01146200
C	1.69363300	-2.32715100	0.58030000
H	3.93119900	-3.64562600	-0.20951200
H	6.13881100	-3.73032700	0.92360400
C	0.72197500	-1.34760600	1.25378300
H	1.24078000	-3.32881200	0.56818600
H	-0.29873000	-1.56913900	0.92675200
N	0.78016300	-1.41210000	2.71101700
C	0.45451600	-2.71443800	3.27987000
H	1.15142600	-3.51137900	2.97224600
H	0.52880400	-2.62248900	4.36984800
C	-0.95592700	-3.07247400	2.86891600
C	-1.99503600	-2.18219300	3.16006300
C	-1.23176000	-4.21843500	2.12530500
C	-3.28665700	-2.43811000	2.71895900
H	-1.76922700	-1.27396200	3.71188500
C	-2.52926400	-4.47893600	1.68113300
H	-0.42584400	-4.90892400	1.88728400
C	-3.55611100	-3.58881100	1.97540700
H	-4.08424400	-1.73431400	2.93460400
H	-2.73275400	-5.37239800	1.09898200
H	-4.56317900	-3.78045700	1.61610600
C	-3.77181600	2.49513500	0.53353100

C	-4.77903700	3.41704200	0.26724900
C	-6.10503200	2.99535000	0.21039800
C	-6.39604700	1.64272500	0.36512300
C	-5.36184100	0.73847200	0.60508200
C	-4.04086400	1.14656800	0.73350000
C	-2.40229900	3.12999100	0.40277100
C	-2.69562400	4.54669300	-0.21560700
C	-4.20435900	4.78651600	0.01855300
H	-6.90391700	3.70037200	0.00465400
H	-7.41471600	1.28338300	0.27481100
H	-3.24916600	0.43003700	0.92793600
H	-1.85224600	3.19686200	1.34035400
H	-2.08370900	5.30276200	0.27637900
H	-4.34924900	5.43570100	0.88774100
C	-1.88309100	2.36603100	-1.87969900
C	-2.69686600	3.51978100	-2.37257900
C	-0.79453900	1.26953500	-0.34645400
H	-3.76950500	3.29290900	-2.30722100
H	-4.64445900	5.29294200	-0.84494600
N	-1.61663100	2.30920600	-0.53841600
N	-1.30522000	1.39405100	-2.51971800
N	-0.64400400	0.70504000	-1.54528400
O	-2.33161300	4.63408300	-1.58298500
H	-2.44185600	3.74037100	-3.40860000
C	-0.10149500	-0.56991900	-1.89596700
C	1.13448600	-0.64551700	-2.54042900
C	-0.85354300	-1.72759800	-1.67973800
C	1.60890700	-1.86844500	-2.99958900
C	-0.37683500	-2.95943200	-2.10828600
C	0.84306400	-3.00692400	-2.77640700
H	2.57329500	-1.93292000	-3.48850600
H	-0.94141400	-3.86337200	-1.91595700
Br	-5.75252300	-1.11671000	0.65600900
Br	-2.48568900	-1.65577500	-0.73964000
Br	1.50966200	-4.67690400	-3.32758400
Br	2.19600200	0.89339600	-2.60142400
C	4.20160700	3.93743300	-1.04110900
O	4.05260500	4.68535000	-0.06366700

O	3.30283300	3.19453900	-1.56462500
C	5.56369300	3.92035400	-1.73998100
H	5.64649300	4.80300000	-2.38240900
H	6.36234500	3.97409300	-0.99677300
H	5.68363000	3.02942600	-2.35867100
C	1.24066400	4.26624200	1.82314500
C	0.96510000	4.11871000	0.33557900
H	0.95213600	5.25862900	2.18545700
H	0.68801900	3.51286500	2.39627900
H	2.31062400	4.12228600	1.99405300
H	-0.08863800	4.34594700	0.11152500
H	1.57836300	4.84122700	-0.21551700
O	1.26174900	2.81501000	-0.11356700
H	2.12072000	2.91066400	-0.66689300

M06RS

C	1.08178200	-1.52331000	2.00311000
C	0.46369700	-0.63584500	0.88046300
H	1.10703800	-0.98327800	2.95395100
H	1.02797200	-0.86541300	-0.01316700
C	2.48133000	-1.95471300	1.60522400
C	3.60828500	-1.32831800	2.13498900
C	2.65751500	-2.96181700	0.64530800
C	4.88679900	-1.72477700	1.74364200
H	3.50086000	-0.50617300	2.83631600
C	3.93292700	-3.34944300	0.24740700
H	1.78339500	-3.43111700	0.19782100
C	5.05445300	-2.73480500	0.80204800
H	5.74218100	-1.22474700	2.18457800
H	4.05053300	-4.13350400	-0.49566400
H	6.05151400	-3.03906800	0.49794200
C	0.40818200	0.84320800	1.06333800
O	0.02727900	1.40651700	2.06405600
H	-1.90744200	0.24199400	1.95569200
C	-1.90164400	-3.16943600	5.31193200
C	-0.91851300	-3.32807200	4.33891300
C	-0.94254800	-2.55340100	3.17903200
C	-1.95986200	-1.61469600	2.98475500

C	-2.94473200	-1.46421300	3.96145100
C	-2.91701400	-2.23240800	5.12132800
H	0.60566000	-3.67103200	2.18331500
H	-1.88125100	-3.77738200	6.21069900
H	-0.12920800	-4.06357200	4.47362000
C	0.07397500	-2.72121800	2.07076200
C	-2.01889700	-0.81596800	1.70322700
H	-3.74682900	-0.74757300	3.80019800
H	-3.68928100	-2.10626000	5.87352000
C	-0.95653500	-1.24889200	0.65909500
H	-3.01661600	-0.91717000	1.26240900
H	-1.33615700	-1.02437300	-0.33924700
N	-0.55924300	-2.64661900	0.74979100
C	-1.46228600	-3.70328500	0.27897200
H	-1.18810400	-3.93074000	-0.76163000
H	-1.25207600	-4.60095900	0.86963200
C	-2.94223500	-3.38047600	0.32339600
C	-3.52967700	-2.69658000	-0.74497700
C	-3.72150100	-3.67234100	1.44502800
C	-4.85922700	-2.28634900	-0.68786500
H	-2.93429700	-2.46683600	-1.62652700
C	-5.04921100	-3.25756000	1.51137100
H	-3.27233700	-4.19524400	2.28625700
C	-5.61838400	-2.55450100	0.45034500
H	-5.29704900	-1.74803200	-1.52393800
H	-5.63746200	-3.47677600	2.39696100
H	-6.65183100	-2.22698500	0.50512600
C	-1.74755100	3.81658800	0.45246900
C	-2.31486600	5.05576700	0.18060800
C	-3.65654900	5.12773100	-0.19416000
C	-4.40083200	3.95587400	-0.32550300
C	-3.79538600	2.72622500	-0.06858700
C	-2.47229200	2.64000500	0.33477700
C	-0.26762700	3.93003200	0.74081300
C	0.07211300	5.44014700	0.46442600
C	-1.29587600	6.15815000	0.31869700
H	-4.11976400	6.08500200	-0.41086100
H	-5.43703600	3.99468800	-0.64144800

H	-2.02605400	1.66965100	0.50865400
H	0.01170700	3.62725900	1.74726900
H	0.64578400	5.83707600	1.30153500
H	-1.49472100	6.76784700	1.20483100
C	0.66444200	3.45343500	-1.49501200
C	0.52631500	4.90845600	-1.80643900
C	0.60923200	1.70992500	-0.18356900
H	-0.51051100	5.12960000	-2.09692200
H	-1.27723200	6.83641600	-0.54002100
N	0.43073200	3.04004500	-0.21274300
N	0.97771500	2.45419400	-2.26528900
N	0.92666000	1.37226500	-1.44159300
O	0.92014800	5.62293900	-0.65579000
H	1.18982800	5.18343000	-2.62583200
C	0.93184000	0.07688900	-2.05192000
C	-0.26911100	-0.41707500	-2.56367200
C	2.08536700	-0.70908300	-2.07506400
C	-0.34260100	-1.71023400	-3.06100300
C	2.02033800	-2.01193400	-2.55633700
C	0.80291200	-2.49915300	-3.01574800
H	-1.27544700	-2.10646700	-3.44299500
H	2.89683400	-2.64695400	-2.51950300
Br	-4.72582700	1.09175300	-0.31805500
Br	3.62407500	-0.07155900	-1.23429500
Br	0.67191400	-4.30772100	-3.51529900
Br	-1.84445700	0.60685900	-2.42960400
C	6.00342300	1.19038900	1.44139900
O	5.75856300	1.20239200	2.65895800
O	5.18171600	1.46500700	0.50340700
C	7.39855400	0.77856400	0.96743500
H	7.77500600	1.48774000	0.22654400
H	8.09542900	0.70299900	1.80285400
H	7.32173200	-0.19634300	0.47336200
C	3.24518000	3.96580900	1.72438500
C	2.82094300	2.61927600	2.30107000
H	2.57293000	4.28328100	0.91918500
H	3.25869900	4.74451800	2.49376300
H	4.24816300	3.87523100	1.29821100

H	3.53634100	2.31366600	3.07513200
H	1.83030300	2.69099500	2.77021700
O	2.75397900	1.62591300	1.30018100
H	3.71672300	1.49722300	0.98622100

M06SR

C	4.42301400	-1.40843200	0.43069200
C	5.76018800	-1.71147700	0.19921500
C	6.75255600	-1.02303900	0.89535600
C	6.39095100	-0.01019100	1.78018200
C	5.04174200	0.28608400	1.97226800
C	4.03716600	-0.41936900	1.32693000
C	3.51501600	-2.17232700	-0.50817200
C	4.49679200	-2.88926400	-1.50720700
C	5.89982900	-2.77262900	-0.86163000
H	7.80175900	-1.24469600	0.72931300
H	7.14932000	0.56077600	2.30334500
H	2.99620700	-0.16922700	1.49615300
H	2.85397400	-2.87867200	-0.00838700
H	4.19371600	-3.92914400	-1.63285100
H	6.19079700	-3.73111300	-0.42144500
C	3.17530700	-0.47267500	-2.26799400
C	4.45453300	-0.94030300	-2.88309400
C	1.51604700	-0.61590600	-0.86697700
H	5.31232300	-0.50294100	-2.35382900
H	6.64533100	-2.52674000	-1.62364000
N	2.67784500	-1.18392900	-1.21295200
N	2.39014900	0.51543900	-2.58286800
N	1.36405400	0.42175200	-1.69165100
O	4.44789400	-2.35115000	-2.81880800
H	4.49686300	-0.64728200	-3.93164600
C	0.49031800	1.55013900	-1.59187200
C	0.89510800	2.63614300	-0.81516200
C	-0.70192000	1.60008900	-2.31206900
C	0.13781400	3.79729600	-0.79174200
C	-1.48401000	2.74733200	-2.27508200
C	-1.04064900	3.83258900	-1.52851500
H	0.44430700	4.64483200	-0.19304200

H	-2.42485700	2.78686600	-2.80967500
Br	4.53965400	1.73850500	3.08084600
Br	-1.29587500	0.03414700	-3.15629500
Br	-2.09485100	5.38828800	-1.46085900
Br	2.44367200	2.51084600	0.24791000
C	-1.17648800	-0.18597100	1.78452000
C	-0.78876200	-0.68723300	0.35339100
H	-0.42253100	-0.51784400	2.50306300
H	-1.00544700	0.10379100	-0.36029400
C	-1.27729300	1.32080600	1.84348800
C	-0.24852100	2.07406200	2.41268000
C	-2.39714400	1.98486200	1.32635200
C	-0.34280800	3.46399200	2.48508100
H	0.63371500	1.57310100	2.80717300
C	-2.49975100	3.36929800	1.41382700
H	-3.19186600	1.39966600	0.86760700
C	-1.47206700	4.11407600	1.99385400
H	0.46830000	4.03433800	2.92846700
H	-3.37446000	3.87236500	1.01267900
H	-1.55005900	5.19576600	2.05086700
C	0.64566900	-1.09466000	0.27732100
O	1.19497500	-1.78325000	1.10914800
H	-0.45487000	-3.49026200	0.32353300
C	-2.14522600	-3.51052400	4.86104100
C	-2.45982700	-2.33656400	4.18159700
C	-2.21910600	-2.22484000	2.81314700
C	-1.66735500	-3.30126100	2.10415400
C	-1.36096300	-4.47556900	2.79384400
C	-1.59077500	-4.58181500	4.16306600
H	-3.22882000	-0.32524200	2.59394300
H	-2.33588400	-3.59171100	5.92646600
H	-2.89864200	-1.49607000	4.71458000
C	-2.50754800	-0.94516100	2.05064200
C	-1.47158700	-3.20426700	0.60660400
H	-0.93946300	-5.31586700	2.24679600
H	-1.34395600	-5.50165300	4.68398400
C	-1.81035800	-1.81847600	0.04591000
H	-2.13292600	-3.91492200	0.09507900

H	-1.97165400	-1.88969300	-1.02925800
N	-2.98492900	-1.22018400	0.69015200
C	-4.21448200	-2.00177300	0.59373100
H	-4.18203900	-2.92011400	1.20176500
H	-4.31170700	-2.32034600	-0.45119700
C	-5.39224300	-1.15799400	1.02073700
C	-6.14594500	-1.48627100	2.14676700
C	-5.71977800	-0.00495200	0.29972000
C	-7.21748800	-0.68520600	2.54306800
H	-5.88782500	-2.37391000	2.71925800
C	-6.78613700	0.79698900	0.69126200
H	-5.12443800	0.25651800	-0.57208000
C	-7.53985200	0.45653100	1.81586700
H	-7.79629700	-0.95278400	3.42153700
H	-7.03466200	1.68623600	0.12021800
H	-8.37348600	1.08059700	2.12180200
C	-3.00005200	-3.02629900	-2.95786100
O	-3.19695800	-3.87291800	-2.07142400
O	-1.86205800	-2.68428000	-3.43157100
C	-4.18641100	-2.23951700	-3.51273900
H	-5.13365900	-2.72223600	-3.27047700
H	-4.16744800	-1.24221300	-3.05636700
H	-4.09199600	-2.10325500	-4.59228800
C	0.96604700	-4.90393400	-1.75655400
C	1.03683200	-3.62587900	-2.57933400
H	-0.07542000	-5.23091100	-1.67910000
H	1.55399900	-5.70600600	-2.21323600
H	1.34226100	-4.73415500	-0.74131300
H	2.07677700	-3.28032100	-2.66923300
H	0.68689600	-3.82415900	-3.60156300
O	0.26010300	-2.59347100	-2.00822300
H	-0.63691200	-2.65392000	-2.47637700
M06SS			
C	-3.83970900	-2.08250700	0.19589500
C	-5.16618200	-2.43315400	0.42162900
C	-6.11575000	-2.21634200	-0.57568400
C	-5.72897500	-1.61440500	-1.77058300

C	-4.39393500	-1.25849400	-1.96080400
C	-3.42556100	-1.50651800	-0.99892300
C	-2.99497700	-2.29507300	1.43232600
C	-4.02403100	-2.70120900	2.55110300
C	-5.35256100	-2.99278700	1.80811900
H	-7.15601100	-2.48210500	-0.41781100
H	-6.45902900	-1.40657600	-2.54434700
H	-2.39595900	-1.21358800	-1.17131700
H	-2.22423300	-3.04909400	1.30410800
H	-3.65369500	-3.58179600	3.07585000
H	-5.53519300	-4.07082000	1.77427600
C	-3.03058400	-0.03463700	2.41660900
C	-4.30944800	-0.40413100	3.09365000
C	-1.22908200	-0.43040800	1.25536600
H	-5.14870800	-0.30435400	2.39069800
H	-6.19182000	-2.54055700	2.34507600
N	-2.33715700	-1.00801800	1.75210700
N	-2.42500500	1.11131900	2.34803400
N	-1.30979700	0.85624700	1.60354700
O	-4.16441200	-1.72453400	3.56843500
H	-4.48402100	0.25004000	3.94747000
C	-0.67231000	2.00918000	1.04493600
C	-1.30441700	2.64084100	-0.03006100
C	0.44999000	2.58092300	1.63623200
C	-0.84332400	3.86267000	-0.49099700
C	0.94983100	3.78663500	1.15542300
C	0.28167700	4.41514000	0.11257800
H	-1.33133900	4.35791800	-1.32041500
H	1.83761100	4.22504400	1.59384100
Br	-3.87848500	-0.33257200	-3.53437800
Br	1.30803900	1.64849500	3.01484000
Br	0.94825100	6.04321000	-0.55600800
Br	-2.77278000	1.81899300	-0.86724200
C	1.26820500	-0.59978000	-1.44943200
C	1.15505200	-0.61134100	0.10623800
H	0.58317100	-1.36602500	-1.82708000
H	1.28801300	0.38643500	0.52494700
C	0.89188900	0.69518100	-2.12973600

C	-0.21569100	0.70451900	-2.98291600
C	1.59307400	1.89626400	-1.94187000
C	-0.60091900	1.86012900	-3.65876700
H	-0.80000400	-0.20430000	-3.11335700
C	1.23993500	3.03867000	-2.65278200
H	2.42470700	1.94264200	-1.24495100
C	0.14299400	3.02687000	-3.51492200
H	-1.48321000	1.84010300	-4.29201700
H	1.79917700	3.95714100	-2.49974100
H	-0.13793700	3.92746100	-4.05257300
C	-0.16709400	-1.20100100	0.49190000
O	-0.50007400	-2.31810700	0.14933100
H	3.17730500	-0.03993800	1.85748700
C	5.33062500	1.52234200	-2.18617800
C	4.40629200	0.51640000	-2.45459600
C	3.79300300	-0.17714700	-1.41322200
C	4.12665500	0.11172000	-0.08130500
C	5.04472100	1.13074800	0.17725500
C	5.64007100	1.83866900	-0.86473600
H	2.80336700	-1.61421200	-2.67980300
H	5.80123400	2.06112300	-3.00224900
H	4.13869400	0.27980100	-3.48144900
C	2.70625900	-1.19389700	-1.67419000
C	3.51379400	-0.69225900	1.04504200
H	5.29543800	1.36762600	1.20893300
H	6.35039900	2.62982100	-0.64592300
C	2.34808500	-1.55035900	0.55101400
H	4.26250900	-1.36694100	1.47395700
H	2.05270200	-2.24852800	1.33661200
N	2.79908700	-2.23781700	-0.65607200
C	2.14434900	-3.49313100	-0.99485300
H	1.10820900	-3.37330100	-1.34618600
H	2.08128300	-4.07830200	-0.06891300
C	2.92627500	-4.27537100	-2.03152700
C	4.31000200	-4.13751700	-2.16218200
C	2.25785200	-5.17975600	-2.85965200
C	5.00990500	-4.89634300	-3.09757600
H	4.82550100	-3.42247900	-1.52837600

C	2.95612200	-5.94485700	-3.79004300
H	1.17878400	-5.28441100	-2.77362800
C	4.33687700	-5.80437900	-3.91210500
H	6.08510900	-4.77702400	-3.19102400
H	2.42082600	-6.64398800	-4.42515400
H	4.88359200	-6.39385000	-4.64130900
C	3.32060500	-1.43704400	4.13546300
O	3.30908500	-2.53775300	3.56077700
O	2.30427700	-0.68524900	4.33327700
C	4.65241700	-0.86758500	4.61832000
H	4.52923000	-0.34176600	5.56692800
H	5.40227300	-1.65342100	4.71242000
H	5.00301500	-0.13848400	3.87870400
C	-0.87105000	-2.85493600	4.46581400
C	0.08328100	-2.76797100	3.28156700
H	-1.80461100	-2.32115200	4.25725300
H	-1.11063300	-3.89517100	4.70882600
H	-0.41265000	-2.39319000	5.34527100
H	1.03070800	-3.27263500	3.50868200
H	-0.34713100	-3.27715700	2.40464100
O	0.34218400	-1.42605500	2.92900900
H	1.15365200	-1.11831700	3.48827900

TS6RR

C	2.10617300	0.61605500	2.10214300
C	1.12450100	0.21555400	0.96917300
H	1.63095200	1.40909000	2.68723700
H	1.62189400	0.23964400	0.00217900
C	3.46057300	1.09901000	1.63618600
C	4.11034000	2.11058100	2.34515200
C	4.12184500	0.52704700	0.54263400
C	5.37924800	2.54906400	1.97261500
H	3.60608400	2.57358500	3.18982300
C	5.38785300	0.95894400	0.16730200
H	3.65120200	-0.27001700	-0.02770300
C	6.02298800	1.97312300	0.88184400
H	5.85653600	3.35171700	2.52625700
H	5.87830200	0.50429800	-0.68840000

H	7.00923300	2.31648100	0.58445800
C	-0.08951300	1.11106600	0.91453500
O	-0.74873900	1.44691900	1.88201400
H	1.67745700	-2.08649600	-0.32231900
C	5.34150100	-2.72103500	2.64491800
C	4.40517200	-1.82055500	3.14444200
C	3.15969500	-1.68143500	2.53282600
C	2.84839300	-2.46126800	1.41363100
C	3.79153400	-3.36013700	0.91195300
C	5.03512500	-3.48991000	1.52174300
H	2.30865100	-0.40788400	4.05165800
H	6.30977200	-2.82124200	3.12498600
H	4.64461900	-1.20746300	4.01010600
C	2.13476000	-0.66691300	3.00155700
C	1.50734000	-2.30874000	0.73292000
H	3.54703300	-3.93873500	0.02213100
H	5.76534300	-4.18679000	1.12276100
C	0.63934700	-1.20221000	1.35600200
H	0.97254000	-3.26824900	0.75778300
H	-0.40930300	-1.37015200	1.07986900
N	0.76626400	-1.14508100	2.81022400
C	0.34131600	-2.34509400	3.52049300
H	0.81426400	-3.26754600	3.14425900
H	0.63857900	-2.23052100	4.56858300
C	-1.16319000	-2.43344900	3.40753600
C	-1.95644800	-1.58019400	4.17801500
C	-1.77376800	-3.24634300	2.45256800
C	-3.33543600	-1.54496200	4.00467600
H	-1.47967800	-0.92865100	4.90543600
C	-3.15310600	-3.19597300	2.25678400
H	-1.16187000	-3.90599500	1.84034000
C	-3.93655200	-2.34958900	3.03806900
H	-3.94241400	-0.88299200	4.61435700
H	-3.61363600	-3.81130000	1.48923600
H	-5.00850500	-2.30205700	2.87937200
C	-4.01786000	2.02580600	0.29866600
C	-5.11992800	2.83548000	0.03867100
C	-6.38098900	2.26314900	-0.10432200

C	-6.50853400	0.87730000	-0.04882100
C	-5.38319000	0.09063200	0.19183200
C	-4.13026500	0.64712800	0.42057300
C	-2.73250200	2.82921100	0.25336700
C	-3.17699000	4.19684600	-0.37536300
C	-4.69693100	4.27323600	-0.11622400
H	-7.25089400	2.87830500	-0.31038900
H	-7.46926500	0.40486400	-0.21846600
H	-3.26825200	0.02341500	0.63256800
H	-2.25243400	2.94901200	1.22279200
H	-2.63728400	5.02447300	0.08542500
H	-4.89163200	4.83782000	0.80152300
C	-2.08243500	2.10319900	-1.99114300
C	-3.06545600	3.10630700	-2.50801200
C	-0.78097400	1.27904600	-0.43827600
H	-4.09268300	2.72917800	-2.42723700
H	-5.19688900	4.79233100	-0.93795300
N	-1.78755900	2.14294300	-0.65190300
N	-1.35675400	1.22695900	-2.61198500
N	-0.56382900	0.69860500	-1.62788500
O	-2.86006600	4.28806700	-1.75668600
H	-2.84885900	3.33108200	-3.55205600
C	0.13430900	-0.50371100	-1.96065000
C	1.43155900	-0.45604000	-2.47320700
C	-0.52723300	-1.73059000	-1.85973700
C	2.07609600	-1.62458100	-2.86281200
C	0.09997200	-2.90577400	-2.25314500
C	1.40047100	-2.83354400	-2.74052800
H	3.09576100	-1.59063400	-3.22586400
H	-0.40207000	-3.85956500	-2.14867300
Br	-5.54579000	-1.79628100	0.07990200
Br	-2.25379000	-1.82203700	-1.11258700
Br	2.31490500	-4.42696700	-3.13900000
Br	2.33888900	1.17389500	-2.46867000
C	3.84714500	4.33278500	-0.30979500
O	3.52046500	5.00718000	0.66194500
O	3.14689200	3.37211100	-0.83483700
C	5.13385000	4.62123800	-1.06546900

H	4.90148800	5.25600600	-1.92654600
H	5.83701800	5.15031300	-0.42176300
H	5.57749600	3.69566600	-1.43438700
C	0.69328000	4.28520200	2.08601100
C	0.51970800	4.00439800	0.59785200
H	0.26932000	5.26021500	2.35192600
H	0.20545700	3.51442000	2.68800000
H	1.76258700	4.29985500	2.30956900
H	-0.54737900	4.05860900	0.32325400
H	1.01157400	4.80957800	0.03065900
O	1.05907600	2.77243600	0.20705000
H	2.17776100	3.05113000	-0.27250300

TS6RS

C	-0.55437100	1.53669400	1.36493100
C	0.12233900	0.79272500	0.18785400
H	0.13959400	1.51394400	2.21060000
H	-0.65455400	0.35183100	-0.43503700
C	-1.90205900	1.07090800	1.86200700
C	-2.11566800	0.98370800	3.23993000
C	-2.99277300	0.86914300	1.01249700
C	-3.37854900	0.70679600	3.75536000
H	-1.27847900	1.13965400	3.91611000
C	-4.25675300	0.59033200	1.52071800
H	-2.86253600	0.92541700	-0.06505500
C	-4.45692100	0.51594400	2.89638400
H	-3.51924200	0.64277900	4.83022500
H	-5.07917700	0.41660700	0.83306300
H	-5.44468100	0.30523500	3.29545000
C	1.10148700	-0.28476600	0.58984500
O	2.02458600	-0.07890900	1.36019200
H	2.74930200	1.87839900	0.28646600
C	1.16614900	5.39020400	3.20044700
C	0.13310700	4.72597100	2.54092500
C	0.42101000	3.83362200	1.51329200
C	1.74487100	3.58763700	1.13011100
C	2.77103600	4.25339500	1.79906400
C	2.48590600	5.14814200	2.82982900

H	-1.63161700	3.44785100	0.96512200
H	0.94150300	6.08934200	3.99972100
H	-0.90217100	4.89838600	2.82431800
C	-0.63842900	3.01978200	0.81678900
C	2.02900000	2.63599300	-0.01885800
H	3.80242100	4.06361100	1.51806100
H	3.29748500	5.65496400	3.34246800
C	0.77245400	1.98042600	-0.62461300
H	2.50933100	3.20558500	-0.82360200
H	1.00021100	1.67089700	-1.64541500
N	-0.28856500	2.98503600	-0.61389800
C	-1.36549200	2.71780200	-1.56340300
H	-0.91460500	2.76754300	-2.56359900
H	-1.79372400	1.70713800	-1.48102200
C	-2.49080600	3.72082100	-1.46643500
C	-3.81845800	3.30947500	-1.59677600
C	-2.21668500	5.07738700	-1.26839900
C	-4.85540200	4.23964300	-1.54735300
H	-4.05473900	2.25555300	-1.73585800
C	-3.25143600	6.00548300	-1.21195600
H	-1.18390500	5.39090500	-1.14530200
C	-4.57475200	5.58940600	-1.35506500
H	-5.88321900	3.90560300	-1.64954800
H	-3.02630300	7.05571300	-1.05454700
H	-5.38208100	6.31334000	-1.30905800
C	5.43504200	-1.74751100	-1.00018400
C	4.55761700	-1.16865400	-0.07681100
C	4.67295700	0.17747400	0.25648300
C	5.60711400	0.93817400	-0.43888900
C	6.44276500	0.38997300	-1.40819900
C	6.37170900	-0.97336100	-1.67390600
C	5.24951000	-3.23484900	-1.07280300
C	4.48267200	-3.51637500	0.23638900
C	3.65302100	-2.22962900	0.52598700
H	4.07232700	0.61287100	1.04249000
H	7.05162200	-1.42401000	-2.38951400
H	4.67334400	-3.50538500	-1.96347300
H	5.20031200	-3.60252400	1.05486200

H	6.19182700	-3.78448300	-1.11424600
H	3.43041100	-2.08632400	1.58233700
N	2.33179600	-2.38434100	-0.17499700
O	3.72454800	-4.70101300	0.26250500
C	1.25337600	-1.57063700	-0.24987400
C	2.01234800	-3.52765400	-0.87580300
N	0.39603000	-2.20745100	-1.06129700
N	0.85506500	-3.42427800	-1.44745500
C	2.81965700	-4.78890900	-0.81047500
H	3.31507800	-4.99661700	-1.76466300
H	2.13300900	-5.60911300	-0.59357900
C	-0.96593700	-1.90894800	-1.35606100
C	-1.29363100	-0.97303200	-2.33681000
C	-1.98335700	-2.59456400	-0.68745000
C	-2.61041300	-0.59643000	-2.54395800
C	-3.30751900	-2.19759300	-0.84943600
C	-3.59098600	-1.17435200	-1.74265300
H	-2.85999000	0.14901000	-3.28964500
H	-4.08835500	-2.66345500	-0.26161400
Br	0.06127900	-0.18534100	-3.36777100
Br	-5.34422400	-0.50592800	-1.87833300
Br	-1.58513600	-4.08930800	0.36263800
H	7.15829200	1.01915300	-1.92498500
Br	5.76320100	2.78743400	-0.05432300
C	-2.97305100	-2.66504400	3.01365600
O	-2.29134300	-3.05221800	3.96611400
O	-2.59206000	-1.87254800	2.07488700
C	-4.39617000	-3.17200400	2.82573200
H	-4.36799700	-3.94850900	2.05213000
H	-4.78837200	-3.60451200	3.74641000
H	-5.04289700	-2.36555700	2.47257500
C	0.79214300	-3.40012600	2.88440600
C	0.43847100	-1.91624200	2.89003900
H	1.35321100	-3.67254500	1.98111900
H	1.40479700	-3.65681600	3.75500400
H	-0.12345400	-3.99443600	2.91618200
H	-0.19056600	-1.70863300	3.76584400
H	1.35286100	-1.31015000	2.99281100

O	-0.23929800	-1.52268500	1.72373900
H	-1.38207500	-1.65034000	1.93402900
TS6SR			
C	-4.20916400	1.29836400	0.85941000
C	-5.58791900	1.47910900	0.86715500
C	-6.38049200	0.68612500	1.69574800
C	-5.78123400	-0.30318900	2.47227900
C	-4.39685800	-0.46817300	2.43029100
C	-3.58457700	0.34128400	1.64851600
C	-3.54394900	2.16221600	-0.18602700
C	-4.73493900	2.82393600	-0.96973900
C	-5.99681100	2.55092400	-0.11170200
H	-7.45849700	0.80936300	1.71799500
H	-6.38403600	-0.95449900	3.09473800
H	-2.50823200	0.20188300	1.62442500
H	-2.86762300	2.90255500	0.23251600
H	-4.54700700	3.89190600	-1.08219400
H	-6.29791900	3.46316400	0.41210900
C	-3.39109900	0.55296600	-2.04970600
C	-4.78277000	0.94500400	-2.42350700
C	-1.51122500	0.79408700	-0.95152400
H	-5.50978100	0.43232800	-1.77844300
H	-6.83368500	2.25596800	-0.75201900
N	-2.76065900	1.27631400	-1.07008300
N	-2.61580100	-0.36115500	-2.53685600
N	-1.44777300	-0.22244300	-1.82842800
O	-4.85968300	2.35026300	-2.30086700
H	-4.98251900	0.68057700	-3.46160500
C	-0.60100600	-1.37368800	-1.83643500
C	-1.02505200	-2.50228400	-1.12834400
C	0.55552700	-1.43688400	-2.60845000
C	-0.31808600	-3.69122400	-1.20709800
C	1.29930600	-2.60955400	-2.66750600
C	0.84219400	-3.72067900	-1.97194400
H	-0.64426300	-4.56399400	-0.65685900
H	2.21559600	-2.64810800	-3.24287500
Br	-3.58735900	-1.88726700	3.39548400

Br	1.14891800	0.11416300	-3.46844600
Br	1.85380000	-5.30690700	-2.00325400
Br	-2.55752100	-2.41263300	-0.04306700
C	1.14533500	0.17218000	1.48457000
C	0.90901800	0.82641400	0.07974300
H	0.40304900	0.56167900	2.18560100
H	1.05064100	0.06514200	-0.68551400
C	1.07244400	-1.33659300	1.49369000
C	0.00333400	-1.98408100	2.11161500
C	2.10421700	-2.11216200	0.94583600
C	-0.03921500	-3.37569600	2.19622000
H	-0.80001200	-1.39927200	2.55410700
C	2.08075900	-3.49793000	1.05597000
H	2.93839900	-1.60819500	0.46183900
C	1.00434300	-4.13613400	1.67714100
H	-0.88988200	-3.85458500	2.67386000
H	2.89194200	-4.08663100	0.63791800
H	0.98331600	-5.21946100	1.75113500
C	-0.48434300	1.42470300	-0.00761200
O	-0.95785300	2.07474000	0.92053200
H	0.95660000	3.59347400	0.27631800
C	2.43746500	3.10581600	4.85598100
C	2.60837800	1.94527500	4.10583600
C	2.41565000	1.96100200	2.72517900
C	2.06379200	3.15162700	2.07623700
C	1.89940400	4.31082500	2.83608200
C	2.07772000	4.29141500	4.21697700
H	3.13801300	-0.04702000	2.40904300
H	2.58758300	3.08746400	5.93084800
H	2.89390100	1.01515700	4.59246000
C	2.55033400	0.71048300	1.88014200
C	1.92217000	3.18140500	0.57023800
H	1.62982700	5.23760200	2.33453500
H	1.94184100	5.20156400	4.79309100
C	2.09881400	1.80246200	-0.08347700
H	2.67319900	3.86278900	0.15149700
H	2.33716200	1.92343600	-1.14364900
N	3.14441400	1.00021500	0.56960600

C	4.47274800	1.60133800	0.60149800
H	4.50774600	2.53743500	1.18135200
H	4.73941000	1.84719800	-0.43373400
C	5.46766300	0.62055300	1.17700800
C	6.06733500	0.84723200	2.41528800
C	5.76073400	-0.55996200	0.48767100
C	6.95538400	-0.08402000	2.95450700
H	5.82884600	1.75581600	2.96308000
C	6.64462800	-1.49150500	1.02187000
H	5.28654700	-0.74025200	-0.47410200
C	7.24606500	-1.25362200	2.25841800
H	7.41598600	0.10348700	3.91944300
H	6.86860600	-2.40230300	0.47524000
H	7.93706200	-1.97903400	2.67597300
C	2.30720500	4.10121700	-3.05701000
O	2.06513300	4.92093300	-2.18568200
O	1.64475400	2.97912400	-3.22999600
C	3.42931400	4.27674400	-4.05609500
H	3.89058300	5.25545800	-3.93571400
H	4.17650900	3.49439200	-3.89892500
H	3.04333600	4.16212500	-5.07115100
C	-0.99840900	4.79118600	-0.89060700
C	-1.04053400	3.65269300	-1.90706400
H	-0.00092100	5.23680000	-0.89684300
H	-1.73185400	5.56129900	-1.15333100
H	-1.21378200	4.43379200	0.12031600
H	-2.07737000	3.29117900	-2.02509400
H	-0.77455600	4.06098000	-2.89643700
O	-0.16344600	2.59151200	-1.62922500
H	0.88784000	2.80955900	-2.46746100

TS6SS

C	-3.80707100	-2.08748700	0.23559200
C	-5.13630200	-2.45070300	0.42086600
C	-6.04284100	-2.30426000	-0.62736300
C	-5.60994300	-1.75955800	-1.83406000
C	-4.27305900	-1.39127400	-1.98364000
C	-3.34430000	-1.56942600	-0.96787900

C	-3.01485300	-2.22082400	1.51616000
C	-4.08951200	-2.56590600	2.61153200
C	-5.37213000	-2.94123600	1.82627800
H	-7.08499000	-2.58057800	-0.50341200
H	-6.30686600	-1.60530500	-2.64970900
H	-2.30872900	-1.27225400	-1.10187500
H	-2.23794800	-2.97641000	1.45745800
H	-3.73226700	-3.39493500	3.22259100
H	-5.51888500	-4.02533800	1.84274400
C	-3.11672200	0.09676600	2.33496600
C	-4.43501500	-0.24005400	2.95000300
C	-1.22522700	-0.37359600	1.34161500
H	-5.22631400	-0.21554400	2.18755100
H	-6.24916600	-2.48946600	2.29954100
N	-2.37436200	-0.91624300	1.78851000
N	-2.50817600	1.23552200	2.24505200
N	-1.33531900	0.93649600	1.59797000
O	-4.30410600	-1.51552000	3.53982200
H	-4.67629300	0.47758100	3.73372800
C	-0.69012500	2.06424100	1.00124200
C	-1.30588000	2.64930400	-0.11024400
C	0.41356000	2.67760200	1.58607000
C	-0.85579300	3.86212500	-0.60588800
C	0.90750900	3.87106800	1.07123100
C	0.24989500	4.45307400	-0.00381100
H	-1.33284300	4.31762800	-1.46418600
H	1.78043900	4.33690900	1.51089200
Br	-3.70570400	-0.55020400	-3.58716400
Br	1.26299700	1.83203100	3.02220400
Br	0.90927400	6.06627000	-0.71544200
Br	-2.73902200	1.77273600	-0.95550900
C	1.23870100	-0.66282800	-1.29695800
C	1.19724900	-0.62190100	0.25955000
H	0.54310500	-1.44691100	-1.61464800
H	1.32276400	0.39344900	0.63973400
C	0.85662800	0.59507800	-2.03853500
C	-0.19031900	0.53848900	-2.96250200
C	1.53144100	1.81504500	-1.87799400

C	-0.54581700	1.64851200	-3.72574000
H	-0.75213300	-0.38599200	-3.07729200
C	1.21160300	2.91036100	-2.67321000
H	2.32189500	1.91135500	-1.13854800
C	0.17147500	2.83384400	-3.60004100
H	-1.38356600	1.57923400	-4.41389700
H	1.74837400	3.84524200	-2.53779900
H	-0.08623000	3.69878300	-4.20371100
C	-0.10086600	-1.22348300	0.75230800
O	-0.45582300	-2.34026400	0.38922800
H	3.28048000	0.10521800	1.85462900
C	5.23311400	1.47471000	-2.34299100
C	4.30144700	0.45474700	-2.51604500
C	3.75406100	-0.20008800	-1.41483200
C	4.15839400	0.14756700	-0.11710100
C	5.08608600	1.17781400	0.04626900
C	5.61847300	1.84355200	-1.05575600
H	2.72649900	-1.70442500	-2.56562000
H	5.65160400	1.98217500	-3.20626600
H	3.97659100	0.17506200	-3.51520300
C	2.67320800	-1.24450000	-1.57391800
C	3.60045900	-0.59875100	1.07787900
H	5.39462200	1.45797400	1.05098900
H	6.33835100	2.64277800	-0.90986400
C	2.43097300	-1.50344300	0.67614400
H	4.38382200	-1.22856700	1.51552700
H	2.19037800	-2.18156000	1.49520100
N	2.85124400	-2.23706200	-0.51771000
C	2.20699300	-3.51969400	-0.76275100
H	1.14648800	-3.43753300	-1.04444700
H	2.22236900	-4.06856700	0.18745500
C	2.94359800	-4.32357200	-1.81646500
C	4.30679000	-4.13521700	-2.05680600
C	2.25924800	-5.29457400	-2.55174900
C	4.97149300	-4.90728200	-3.00652600
H	4.83267000	-3.36759900	-1.49770500
C	2.92284800	-6.07289800	-3.49648400
H	1.19512200	-5.44058600	-2.38138800

C	4.28342100	-5.88060800	-3.72783100
H	6.03036400	-4.74646100	-3.18528100
H	2.37588500	-6.82423600	-4.05780100
H	4.80171900	-6.48042500	-4.46928100
C	3.27815700	-1.48892400	4.14402500
O	3.30252800	-2.58794300	3.59782200
O	2.26667000	-0.66794100	4.12634800
C	4.48281200	-0.94554300	4.88594300
H	4.17954200	-0.51809200	5.84348800
H	5.22468000	-1.72861400	5.03566500
H	4.92354100	-0.14007600	4.28983200
C	-0.92383400	-2.47506100	4.47244900
C	0.03078200	-2.59025800	3.28790700
H	-1.83575600	-1.93186600	4.20313800
H	-1.20919900	-3.46320600	4.84790100
H	-0.43920200	-1.92643300	5.28557300
H	0.94091000	-3.12782500	3.59214000
H	-0.41858200	-3.19277800	2.48120000
O	0.38236800	-1.32813200	2.78274800
H	1.39100700	-0.98923000	3.42788700

M6RR

C	-1.53308900	1.29503400	1.96414900
C	-0.85310600	0.22836900	1.06662200
H	-0.77631200	1.62091900	2.68361700
H	-1.51550800	-0.62372700	0.89794000
C	-2.76876000	0.87023200	2.72074900
C	-3.02177600	1.44703300	3.96874300
C	-3.70355200	-0.04073800	2.21455800
C	-4.16886000	1.13098000	4.69334000
H	-2.30360700	2.15467200	4.37614700
C	-4.84959800	-0.36341900	2.93592600
H	-3.54697900	-0.49638400	1.23980000
C	-5.08824400	0.22088700	4.17844100
H	-4.33998900	1.59167300	5.66154000
H	-5.56047100	-1.07373400	2.52456100
H	-5.98146800	-0.03334000	4.74024200
C	0.40712600	-0.27382600	1.81495600

O	1.25289100	0.61072000	2.20273200
H	-1.88934900	-0.34585400	-1.35286800
C	-5.36238300	2.69983300	-0.21183200
C	-4.19436600	2.96130300	0.49926300
C	-3.00218300	2.31822100	0.16807200
C	-2.97782900	1.41363900	-0.90032900
C	-4.15446400	1.14297300	-1.60147900
C	-5.34392400	1.78006300	-1.25994100
H	-1.75704600	3.44563500	1.52529700
H	-6.28644200	3.20218300	0.05647900
H	-4.20693300	3.65687900	1.33578900
C	-1.73785500	2.49120000	0.98749200
C	-1.68585900	0.72189400	-1.27769200
H	-4.13261800	0.40466000	-2.40263300
H	-6.25474500	1.55873700	-1.80742500
C	-0.56676700	0.96761800	-0.24969100
H	-1.36430600	1.04872900	-2.27705000
H	0.40082700	0.68996400	-0.68730100
N	-0.52807200	2.37463100	0.16691700
C	-0.39233800	3.33124800	-0.92746000
H	0.42256900	2.96401000	-1.56194000
H	-1.29962300	3.39843000	-1.55129500
C	-0.03900600	4.70167700	-0.40162900
C	1.29354500	5.03137600	-0.14100100
C	-1.03535700	5.64144200	-0.13192700
C	1.62340300	6.27864900	0.38055900
H	2.07118700	4.30832500	-0.37753000
C	-0.70940600	6.88939000	0.39619700
H	-2.07364400	5.38804700	-0.33866800
C	0.62132300	7.20908200	0.65438500
H	2.66262300	6.52724800	0.57250300
H	-1.49285400	7.61222800	0.60175800
H	0.87831900	8.18172400	1.06219800
C	4.13557600	-0.02754200	0.80606600
C	5.50006600	-0.24759300	0.66234900
C	6.18716300	0.36247800	-0.38672200
C	5.48388200	1.15025900	-1.29543100
C	4.11325600	1.34556200	-1.12027000

C	3.41859100	0.79239300	-0.05619000
C	3.54154100	-0.88474800	1.89647800
C	4.73586900	-1.77731700	2.39141100
C	6.00822300	-1.18283400	1.73043000
H	7.25300700	0.20661400	-0.52053500
H	5.99001600	1.60391900	-2.13993200
H	2.36260700	0.98302900	0.11645600
H	3.06686800	-0.30021400	2.68117700
H	4.79339100	-1.73787500	3.47884100
H	6.59791800	-0.63923800	2.47468800
C	2.82649300	-2.84458600	0.57537000
C	4.19409800	-3.41301100	0.76397700
C	1.20410400	-1.41184100	0.97997300
H	4.89629600	-2.96534800	0.04700000
H	6.64357400	-1.98468500	1.34152000
N	2.48677900	-1.71088800	1.26782900
N	1.83549200	-3.28436300	-0.13200600
N	0.83420900	-2.38089600	0.12548100
O	4.56636200	-3.15729800	2.10156800
H	4.17634900	-4.49219700	0.61308700
C	-0.25630000	-2.39904100	-0.78916600
C	-1.50172800	-2.92303600	-0.45053900
C	-0.03377600	-1.92954400	-2.08794900
C	-2.52733200	-2.96190600	-1.38906900
C	-1.03109200	-1.99875400	-3.05046200
C	-2.27273900	-2.50171800	-2.67650400
H	-3.50646500	-3.33388100	-1.11454700
H	-0.86390600	-1.61170600	-4.04779600
Br	3.13462800	2.32794700	-2.41485000
Br	1.57766800	-1.04261300	-2.48735300
Br	-3.68709800	-2.44652100	-3.91700600
Br	-1.81333700	-3.50855000	1.29965100
C	1.03369200	-2.82077700	4.07567300
C	0.55608000	-1.37280200	4.02093900
H	1.40096600	-3.06683100	5.07618400
H	0.20160400	-3.48852900	3.83493700
H	1.84327600	-3.02137900	3.36732600
H	-0.10686900	-1.17692700	4.87257300

H	1.38577000	-0.66032900	4.08669800
O	-0.19876300	-1.11977700	2.85233900
M6RS			
C	-1.42818700	0.57662800	2.05850000
C	-0.22285600	0.35912400	1.08480000
H	-1.05366700	0.53266700	3.08682600
H	-0.62598500	-0.22357700	0.25589700
C	-2.54476800	-0.45588000	1.92792700
C	-2.48347200	-1.66207200	2.64051000
C	-3.67221800	-0.24830600	1.12344300
C	-3.46959200	-2.63554500	2.50883900
H	-1.64253400	-1.84022700	3.29818900
C	-4.67145100	-1.21269500	0.99675100
H	-3.80958700	0.68993200	0.60021200
C	-4.56736200	-2.42170100	1.67660000
H	-3.37875400	-3.56520400	3.06327600
H	-5.52667000	-1.01149200	0.35895200
H	-5.33863000	-3.17941000	1.57552000
C	0.97418300	-0.43157400	1.69229600
O	1.82154800	0.18595800	2.42314100
H	1.83157800	2.23939600	1.67606900
C	-1.22610300	4.29781900	4.75029500
C	-1.87386800	3.48788300	3.82057200
C	-1.18280300	2.97950600	2.72265400
C	0.17546200	3.27470200	2.54755000
C	0.81474800	4.08762300	3.48398100
C	0.12397800	4.59718000	4.58064000
H	-2.92393900	2.21101300	1.73085500
H	-1.77208900	4.69453300	5.60055000
H	-2.92715500	3.24796500	3.94505300
C	-1.84205800	2.05420300	1.72220000
C	0.91901400	2.73647800	1.34518900
H	1.86869500	4.32027200	3.35029500
H	0.63808000	5.22601500	5.30096700
C	0.06149300	1.77808800	0.50769000
H	1.19520300	3.57329600	0.68854200
H	0.48817100	1.70757500	-0.49592700

N	-1.27526600	2.38032200	0.39831500
C	-2.01499000	1.90150600	-0.76423400
H	-1.37242800	2.08599000	-1.63703100
H	-2.20780100	0.81553300	-0.75597200
C	-3.33118200	2.62069500	-0.96225600
C	-4.39814100	1.96345100	-1.58256300
C	-3.49623500	3.94716700	-0.55816800
C	-5.60140400	2.62583200	-1.81280900
H	-4.29533400	0.91664100	-1.86653400
C	-4.70128800	4.60836900	-0.78255700
H	-2.67194700	4.44501800	-0.05681100
C	-5.75564300	3.95194700	-1.41476900
H	-6.42176200	2.10275700	-2.29447100
H	-4.81837100	5.63855700	-0.46051500
H	-6.69507900	4.46719600	-1.58772400
C	5.71779800	0.64962100	-0.50839900
C	4.39607900	0.58128200	-0.08977500
C	3.40524500	1.38280000	-0.62797700
C	3.76577600	2.26875400	-1.62848800
C	5.08665500	2.38279300	-2.06179400
C	6.07066700	1.57303600	-1.49251800
C	6.54958700	-0.38748900	0.20572300
C	5.52578400	-1.31437100	0.91913900
C	4.15976000	-0.53963000	0.88637300
H	2.37859000	1.28726400	-0.30153100
H	7.09477800	1.64862700	-1.84389400
H	7.18229100	-0.97384600	-0.46753900
H	5.81618900	-1.50739400	1.95172200
H	7.20999600	0.07881500	0.94307400
H	3.81503600	-0.19740900	1.86395800
N	3.08241200	-1.37703500	0.33878400
O	5.45148100	-2.60541700	0.33294700
C	1.75212600	-1.23588100	0.45226200
C	3.33985900	-2.31528400	-0.62748200
N	1.26637200	-2.12178700	-0.43254000
N	2.24088700	-2.79620100	-1.12189600
C	4.76930400	-2.64931800	-0.90476900
H	5.19087300	-1.94145300	-1.63197900

H	4.85470700	-3.65916000	-1.30522600
C	-0.07288500	-2.19102000	-0.90523900
C	-0.45191600	-1.32028600	-1.93193600
C	-1.01705800	-3.05804300	-0.35890400
C	-1.75648800	-1.28716400	-2.39755800
C	-2.33486800	-3.03162400	-0.80470100
C	-2.68591700	-2.13443100	-1.80346500
H	-2.04863100	-0.59629500	-3.17905700
H	-3.07448600	-3.68447600	-0.35923000
Br	0.79269600	-0.07130700	-2.59777000
Br	-4.47710000	-2.03570300	-2.36914300
Br	-0.53858600	-4.27474900	0.97862300
H	5.33810000	3.08265200	-2.85057200
Br	2.37779500	3.26672700	-2.44818800
C	2.28818300	-2.97506200	2.99143800
C	1.02649000	-2.20446400	3.36577600
H	3.11118800	-2.29638100	2.75541700
H	2.60210400	-3.60153800	3.83121600
H	2.10039200	-3.62453700	2.12980800
H	0.28918900	-2.89865700	3.78568900
H	1.26059400	-1.44429800	4.11740900
O	0.35240500	-1.60369300	2.27364600

M6SR

C	-4.06122200	-1.37161800	-0.55037700
C	-5.43329100	-1.47852000	-0.74952800
C	-5.97595200	-1.15601000	-1.99147500
C	-5.13591200	-0.69458100	-3.00262100
C	-3.76509700	-0.58985300	-2.76709200
C	-3.19695300	-0.95005500	-1.55252000
C	-3.68614100	-1.63924500	0.88753100
C	-5.06082800	-1.76845700	1.63305500
C	-6.12423200	-1.92242800	0.51524200
H	-7.04426300	-1.22836500	-2.16902600
H	-5.54041700	-0.40035000	-3.96435900
H	-2.12784900	-0.86808800	-1.37359100
H	-3.03696500	-2.50689700	1.00191800
H	-5.04379300	-2.63542900	2.29330300

H	-6.44042600	-2.96749400	0.44006200
C	-3.59605400	0.67789000	1.72127600
C	-5.07221600	0.59177000	1.93253400
C	-1.61636100	-0.18665400	1.27966600
H	-5.60303200	0.73592300	0.98086700
H	-7.01354800	-1.33220200	0.75610600
N	-2.93047100	-0.47005300	1.37335100
N	-2.78119900	1.67350900	1.85881500
N	-1.55183200	1.12356100	1.57374300
O	-5.33374000	-0.67639800	2.49934400
H	-5.39974200	1.35497200	2.63825500
C	-0.52720500	2.05201400	1.23323400
C	-0.63249000	2.71588200	0.00630700
C	0.50797000	2.37753400	2.10384700
C	0.26463800	3.71185300	-0.33965500
C	1.44355800	3.34649300	1.75792300
C	1.29784300	4.00316900	0.54326200
H	0.18203300	4.22272800	-1.29005600
H	2.26349600	3.58080600	2.42510900
Br	-2.64701300	0.14600700	-4.11291100
Br	0.66959400	1.45567800	3.72895200
Br	2.57133200	5.29291200	0.03154600
Br	-2.00123800	2.24920800	-1.19568100
C	1.20711800	-1.07359300	-0.60912300
C	0.90010300	-0.98297200	0.91145100
H	0.38649000	-1.60385700	-1.10176800
H	1.09476400	0.03392300	1.26059000
C	1.44799700	0.24563100	-1.30667000
C	0.65709300	0.62658200	-2.38944000
C	2.53323000	1.06172200	-0.95170500
C	0.93360500	1.78951600	-3.10910200
H	-0.18018900	0.00106000	-2.68716300
C	2.83432400	2.20161200	-1.68787700
H	3.15912900	0.76211400	-0.11491900
C	2.02919900	2.57674300	-2.76610000
H	0.28945600	2.06914900	-3.93869300
H	3.68484500	2.81589200	-1.40723700
H	2.25768400	3.47657500	-3.32993400

C	-0.53136400	-1.42301300	1.28931800
O	-1.01153700	-2.43363800	0.67033200
H	0.67725900	-3.50902200	2.15638900
C	1.92465400	-5.44699100	-2.07309900
C	2.26349200	-4.09954600	-1.98233000
C	2.15416000	-3.42056700	-0.76953400
C	1.71424500	-4.09492100	0.37604000
C	1.38347000	-5.44733200	0.27777000
C	1.48030000	-6.12114300	-0.93695200
H	3.16260400	-1.64853100	-1.46177200
H	2.01146900	-5.96877400	-3.02107300
H	2.61942400	-3.56387000	-2.85984300
C	2.49539800	-1.95003000	-0.64762400
C	1.65923600	-3.36988300	1.70323600
H	1.04597700	-5.97648300	1.16622500
H	1.21459600	-7.17221900	-0.99591800
C	1.98426900	-1.86806400	1.58041400
H	2.39350600	-3.82650300	2.38171700
H	2.23068300	-1.47063800	2.57059600
N	3.10300600	-1.64007700	0.65272900
C	4.34191100	-2.34953700	0.94752500
H	4.23690100	-3.44514700	0.89054100
H	4.61910500	-2.10092000	1.97947500
C	5.43105700	-1.90701200	-0.00202700
C	5.93619300	-2.77409500	-0.97047400
C	5.91228600	-0.59575100	0.04995700
C	6.91622400	-2.34504300	-1.86571000
H	5.55048200	-3.78927100	-1.02829000
C	6.88987100	-0.16361300	-0.83971900
H	5.50970900	0.08402000	0.79676200
C	7.39587400	-1.04020200	-1.80051200
H	7.30114000	-3.03007700	-2.61466800
H	7.25993900	0.85561400	-0.78568500
H	8.15852700	-0.70368500	-2.49569800
C	-0.90848400	-2.60076200	4.80072200
C	-1.41284100	-2.33100800	3.39478000
H	-0.75609700	-1.65814300	5.33342800
H	-1.62517300	-3.20754100	5.35986400

H	0.04680300	-3.13174200	4.76430000
H	-1.53446400	-3.26055600	2.82604700
H	-2.39786400	-1.83482600	3.44042200
O	-0.46076900	-1.50113100	2.76126900

M6SS

C	-4.09969200	0.99743300	-0.07346900
C	-5.48912400	1.06233400	-0.06333700
C	-6.17133200	0.99465700	1.14881000
C	-5.44845600	0.81854900	2.32735900
C	-4.05712000	0.73923500	2.27874500
C	-3.35303300	0.85715100	1.08774900
C	-3.56003500	0.97669800	-1.48213500
C	-4.82993000	0.77037000	-2.37781800
C	-6.02428300	1.15883800	-1.47079400
H	-7.25520300	1.04047300	1.18259800
H	-5.95945100	0.72040500	3.27826900
H	-2.26779600	0.78966300	1.06471700
H	-2.98664200	1.86873900	-1.73197900
H	-4.77433600	1.39786900	-3.26774000
H	-6.34640800	2.18090800	-1.69487200
C	-3.16890200	-1.43473000	-1.65779600
C	-4.62555600	-1.57115700	-1.96133100
C	-1.31271100	-0.26811800	-1.40027400
H	-5.22146500	-1.49759600	-1.04154200
H	-6.87471000	0.49810100	-1.66189500
N	-2.64273000	-0.16934100	-1.59831300
N	-2.25069900	-2.33388600	-1.50897400
N	-1.10059900	-1.59759400	-1.34167000
O	-4.94400700	-0.55149900	-2.88814100
H	-4.82103600	-2.53321100	-2.43463100
C	-0.00611800	-2.32384600	-0.78591100
C	-0.10645400	-2.72137400	0.54924300
C	1.09075200	-2.73618700	-1.54163300
C	0.84297000	-3.55954600	1.11347800
C	2.09075200	-3.51517400	-0.97108900
C	1.94305900	-3.92346400	0.34935900
H	0.75915100	-3.86104700	2.14976100

H	2.96054300	-3.79839600	-1.54993400
Br	-3.08551300	0.36417300	3.86162800
Br	1.25001400	-2.19533000	-3.32558600
Br	3.31220700	-4.92131900	1.17316100
Br	-1.45064500	-2.00329400	1.64689300
C	1.10241600	1.50152400	0.35741200
C	1.04775900	0.91141200	-1.06864700
H	0.25936400	2.19675500	0.43840100
H	1.37521900	-0.13332800	-1.09192600
C	1.06860900	0.58062200	1.55273400
C	0.32822700	0.94867000	2.68270900
C	1.86656200	-0.56621600	1.63768800
C	0.39729100	0.21153700	3.86209200
H	-0.30653300	1.83162500	2.63883500
C	1.94778800	-1.29873500	2.81794300
H	2.45537100	-0.88033300	0.77754000
C	1.21153700	-0.91509500	3.93614400
H	-0.19114400	0.51631100	4.72213500
H	2.58824800	-2.17711000	2.85355900
H	1.27361700	-1.48742600	4.85641000
C	-0.35227300	1.02686400	-1.72288300
O	-1.00550500	2.10956500	-1.52100900
H	3.16956300	0.02698300	-2.51750800
C	5.42544500	0.52019600	1.72233100
C	4.33195900	1.37523400	1.61541700
C	3.65626000	1.52204700	0.40536700
C	4.09147600	0.81323000	-0.72577800
C	5.18181500	-0.04966800	-0.60682100
C	5.84643000	-0.20202000	0.60791600
H	2.41091300	3.15283800	1.06751300
H	5.93970300	0.41134200	2.67198400
H	3.97967400	1.92101600	2.48779800
C	2.41073600	2.37655400	0.29557100
C	3.38497800	0.99856000	-2.05472700
H	5.51212600	-0.60773600	-1.48014400
H	6.69110200	-0.87984800	0.68266000
C	2.08213100	1.77875700	-1.86803100
H	4.04449400	1.54687500	-2.73817800

H	1.68090000	2.08890200	-2.83317200
N	2.39415100	2.95589800	-1.04678900
C	1.46163000	4.06876200	-1.21250900
H	0.42615400	3.80916500	-0.95154300
H	1.44908800	4.30372200	-2.28530800
C	1.90428900	5.29945800	-0.45125900
C	3.25812200	5.58667200	-0.25448300
C	0.95032300	6.19461300	0.03746700
C	3.64684500	6.74889100	0.40650400
H	3.99757900	4.87976400	-0.61851200
C	1.33592800	7.36202700	0.69278400
H	-0.10534100	5.97315700	-0.09932100
C	2.68728300	7.64295300	0.87931800
H	4.70216800	6.95770600	0.55439800
H	0.58104500	8.04772500	1.06532700
H	2.99083800	8.54832100	1.39551800
C	-1.55694100	-0.30316500	-4.77104000
C	-1.09185900	0.96644700	-4.07213000
H	-1.97581200	-1.02307500	-4.05975900
H	-2.32524900	-0.07312800	-5.51475700
H	-0.71863500	-0.78940000	-5.27632900
H	-0.67079100	1.66372800	-4.80714600
H	-1.92292000	1.49181100	-3.58940200
O	-0.08470600	0.66859900	-3.12290600

TS7RR

C	-1.60672700	1.51702800	1.82417100
C	-0.86931500	0.35651400	1.09531200
H	-0.89333700	1.94873600	2.53296400
H	-1.50522300	-0.52762800	1.00834900
C	-2.86347500	1.15022700	2.57581800
C	-3.15393700	1.81001000	3.77355900
C	-3.77409700	0.19371600	2.11142200
C	-4.31424400	1.52707500	4.49131400
H	-2.45257800	2.55108900	4.15016800
C	-4.93417500	-0.09330400	2.82476300
H	-3.58584500	-0.32751300	1.17575700
C	-5.20921100	0.57110000	4.01853900

H	-4.51496600	2.04981400	5.42144900
H	-5.62655200	-0.83895600	2.44598500
H	-6.11229000	0.34302700	4.57572600
C	0.34452800	-0.02008600	1.95886700
O	1.23120900	0.82963400	2.21773500
H	-1.78756300	-0.52723600	-1.27285100
C	-5.32912900	2.60865400	-0.71296400
C	-4.20291900	2.96302500	0.02505500
C	-2.99464100	2.29175000	-0.15792900
C	-2.90846300	1.26410700	-1.10538000
C	-4.04376500	0.90349900	-1.83406100
C	-5.25063000	1.56922600	-1.63933700
H	-1.82896000	3.59206600	1.11237200
H	-6.26723600	3.13295600	-0.56067100
H	-4.26219500	3.75668800	0.76680500
C	-1.77534200	2.57951000	0.69759400
C	-1.59588300	0.54449700	-1.32523800
H	-3.97877400	0.07592000	-2.53963600
H	-6.12861100	1.27841200	-2.20755600
C	-0.53052700	0.93124800	-0.28471100
H	-1.22481900	0.74565800	-2.34048100
H	0.45604600	0.60744100	-0.63980500
N	-0.52404700	2.37877200	-0.04081900
C	-0.33556800	3.19198700	-1.23945800
H	0.49254300	2.73745600	-1.79492300
H	-1.22025200	3.19254600	-1.89829000
C	0.02397600	4.61337300	-0.87847900
C	1.35761100	4.96735400	-0.65901100
C	-0.96918100	5.58264600	-0.72319200
C	1.69179900	6.26580700	-0.28580800
H	2.13271000	4.21914100	-0.80918700
C	-0.63887700	6.88233500	-0.34360500
H	-2.00814400	5.31196900	-0.90311500
C	0.69286300	7.22525600	-0.12294100
H	2.73193900	6.53140900	-0.12406800
H	-1.41937200	7.62724600	-0.22377000
H	0.95321500	8.23799900	0.16830300
C	4.13921600	-0.07055100	0.82400400

C	5.50523400	-0.30329000	0.71774300
C	6.20606500	0.20531700	-0.37484100
C	5.51666900	0.91199800	-1.35800300
C	4.14611900	1.13052600	-1.21489300
C	3.43711600	0.67371400	-0.11494400
C	3.52932600	-0.81314100	1.98698200
C	4.72139100	-1.63817600	2.59442000
C	6.00077000	-1.12758200	1.87876400
H	7.27275900	0.03532300	-0.48163500
H	6.03446000	1.28636200	-2.23384100
H	2.37995100	0.88254100	0.02212400
H	3.05314800	-0.14233200	2.69978900
H	4.77157200	-1.46810300	3.66972000
H	6.59572200	-0.51499000	2.56277900
C	2.83388900	-2.91320300	0.89160200
C	4.19636200	-3.45835300	1.17063700
C	1.21649800	-1.40750900	1.08186100
H	4.90962000	-3.10162200	0.41405800
H	6.62902900	-1.97150400	1.57687000
N	2.48351600	-1.70790200	1.45136500
N	1.86096500	-3.41641100	0.20239700
N	0.86768600	-2.47008900	0.33875000
O	4.55521500	-3.04186600	2.47129300
H	4.18145900	-4.54807600	1.15251900
C	-0.21702500	-2.55686400	-0.57373200
C	-1.48043100	-3.00063500	-0.18861300
C	0.00670400	-2.20659300	-1.90912100
C	-2.50536400	-3.11710100	-1.12181900
C	-0.98867900	-2.35365100	-2.86527700
C	-2.23665200	-2.80573400	-2.45022100
H	-3.49285400	-3.43715300	-0.81398700
H	-0.81226400	-2.06897300	-3.89500800
Br	3.19112000	2.01520700	-2.59491600
Br	1.61556900	-1.34702200	-2.37370200
Br	-3.63528200	-2.90336300	-3.70673500
Br	-1.82346500	-3.35284900	1.61888600
C	0.23487500	0.35050900	5.10498300
C	0.52790100	-0.85168300	4.22280600

H	-0.84367500	0.43829700	5.26504800
H	0.72533000	0.24546200	6.07732900
H	0.59209500	1.25988600	4.61864400
H	1.60275300	-0.93550500	4.02320700
H	0.20930400	-1.77826700	4.71019500
O	-0.20603400	-0.79733400	3.00888200

TS7RS

C	-1.47950800	0.57215000	2.09372400
C	-0.25880400	0.34755900	1.13949100
H	-1.12470300	0.54235100	3.12970200
H	-0.63719400	-0.26944200	0.32329200
C	-2.58241800	-0.47329200	1.95086200
C	-2.49023800	-1.69478700	2.63370200
C	-3.71654300	-0.27098600	1.15517100
C	-3.45239900	-2.68853900	2.47819600
H	-1.64323900	-1.87036400	3.28455300
C	-4.69062900	-1.25737900	1.00328100
H	-3.87535000	0.67564900	0.65282500
C	-4.55583100	-2.48043800	1.65190600
H	-3.33645600	-3.63033000	3.00687700
H	-5.55052200	-1.06187300	0.36998000
H	-5.30786900	-3.25427800	1.53044100
C	0.93064200	-0.40741200	1.78074000
O	1.77318200	0.19723700	2.50016500
H	1.79151900	2.25123300	1.68461300
C	-1.28001800	4.32390200	4.73529300
C	-1.92481900	3.50159500	3.81460900
C	-1.23200500	2.98333700	2.72228600
C	0.12529700	3.28142700	2.54423600
C	0.76180600	4.10656400	3.47191000
C	0.06914200	4.62591800	4.56264300
H	-2.97158100	2.20372300	1.73677000
H	-1.82749400	4.72824900	5.58096200
H	-2.97726200	3.25942500	3.94182800
C	-1.89011300	2.04398200	1.73355600
C	0.87164400	2.73142700	1.34842600
H	1.81507000	4.34085200	3.33599000

H	0.58089600	5.26440700	5.27608600
C	0.01950000	1.75243100	0.53029600
H	1.13861500	3.55942400	0.67705200
H	0.44828000	1.65638700	-0.47037100
N	-1.31867700	2.34801100	0.40665700
C	-2.05544200	1.84597700	-0.74778000
H	-1.40903000	2.00778500	-1.62245400
H	-2.25202300	0.76120200	-0.71454200
C	-3.36774200	2.56680900	-0.96512400
C	-4.42979300	1.90621600	-1.59017700
C	-3.53439000	3.89677700	-0.57354200
C	-5.62977600	2.56840900	-1.83701000
H	-4.32459300	0.85765900	-1.86589700
C	-4.73642400	4.55788600	-0.81446200
H	-2.71409300	4.39768100	-0.06872200
C	-5.78585700	3.89793500	-1.45096600
H	-6.44633900	2.04276900	-2.32232700
H	-4.85484500	5.59084400	-0.50190500
H	-6.72290500	4.41314500	-1.63656100
C	5.70401800	0.71105200	-0.51547400
C	4.38416100	0.62898800	-0.09391700
C	3.38415500	1.42038100	-0.63066400
C	3.73378700	2.31215000	-1.62965600
C	5.05267400	2.44042400	-2.06525300
C	6.04543300	1.63910600	-1.49956300
C	6.54989800	-0.31708800	0.19458600
C	5.54183800	-1.23908200	0.93733200
C	4.15959800	-0.49363000	0.88324100
H	2.35843900	1.31120500	-0.30532200
H	7.06813100	1.72564900	-1.85264600
H	7.16993500	-0.90872100	-0.48607800
H	5.83652000	-1.39230100	1.97542500
H	7.22528000	0.15655900	0.91328200
H	3.80250800	-0.15304900	1.85775900
N	3.10828500	-1.35604800	0.33146300
O	5.49047000	-2.54998900	0.39519900
C	1.77540300	-1.20653400	0.41889200
C	3.38875500	-2.31684000	-0.60651100

N	1.31385800	-2.11883000	-0.45156100
N	2.30047100	-2.81349100	-1.10935400
C	4.82606800	-2.64390600	-0.85005500
H	5.25059200	-1.95373500	-1.59281800
H	4.93228000	-3.66475900	-1.21617300
C	-0.02225300	-2.19572400	-0.92807100
C	-0.41397500	-1.31878700	-1.94454200
C	-0.96144300	-3.06854300	-0.38112100
C	-1.72171000	-1.29032600	-2.40342200
C	-2.28194300	-3.04723400	-0.81826500
C	-2.64304700	-2.14767200	-1.81139200
H	-2.02228500	-0.59567100	-3.17841300
H	-3.01599600	-3.70486200	-0.37061800
Br	0.82024000	-0.06093000	-2.61408600
Br	-4.43840500	-2.06188300	-2.36815800
Br	-0.47182700	-4.28325300	0.95553000
H	5.29589800	3.14497600	-2.85246900
Br	2.33377100	3.29847300	-2.44315500
C	2.33145900	-2.95234400	2.98119700
C	1.04504000	-2.23509200	3.37228000
H	3.13223100	-2.24049400	2.76820600
H	2.66065300	-3.59156200	3.80528200
H	2.16812200	-3.58330100	2.10107500
H	0.32199200	-2.96424100	3.75441600
H	1.24731800	-1.49714400	4.15419500
O	0.36515900	-1.61067000	2.29418100

TS7SR

C	-4.01953300	-1.40541700	-0.60473900
C	-5.38526300	-1.56334200	-0.81274000
C	-5.93250300	-1.25054400	-2.05523400
C	-5.10530200	-0.74854700	-3.05796600
C	-3.74158700	-0.58918000	-2.81214700
C	-3.16876500	-0.93524600	-1.59609000
C	-3.63859500	-1.67814700	0.83038600
C	-5.01039100	-1.86302900	1.56896100
C	-6.06497800	-2.04131900	0.44593100
H	-6.99621900	-1.36251200	-2.23993600

H	-5.51548400	-0.46410600	-4.02026000
H	-2.10757300	-0.79709500	-1.40673500
H	-2.96418800	-2.52858800	0.93934400
H	-4.96753900	-2.73631400	2.21985200
H	-6.34759200	-3.09523100	0.36087100
C	-3.62104800	0.62783600	1.69672900
C	-5.09461400	0.49411700	1.90089300
C	-1.61233000	-0.18240800	1.23761900
H	-5.62650800	0.63677200	0.94952700
H	-6.97332300	-1.48156200	0.68863300
N	-2.92142100	-0.49607300	1.33392300
N	-2.83356600	1.64324500	1.84963700
N	-1.59059600	1.12394900	1.55791900
O	-5.32152300	-0.79054800	2.44687800
H	-5.44937400	1.23503000	2.61706200
C	-0.57633000	2.06918000	1.23916200
C	-0.66631200	2.73905500	0.01412500
C	0.44969700	2.39260000	2.12161600
C	0.23611900	3.73463100	-0.31952800
C	1.39051200	3.36167700	1.78959700
C	1.26072600	4.02087500	0.57485500
H	0.16465900	4.24821300	-1.26940500
H	2.20272300	3.59335600	2.46707500
Br	-2.64248300	0.19914400	-4.14370700
Br	0.59335700	1.47011400	3.74892500
Br	2.54589300	5.30637200	0.07989600
Br	-2.02050600	2.27738300	-1.20644800
C	1.21703200	-1.10131500	-0.58580100
C	0.94345600	-1.01228300	0.94010600
H	0.38918200	-1.63179400	-1.06641800
H	1.09307300	0.01508200	1.28179600
C	1.43972900	0.22232000	-1.28237700
C	0.64170000	0.59698100	-2.36242200
C	2.51334500	1.05322000	-0.92617700
C	0.90147300	1.76581200	-3.07894800
H	-0.18865900	-0.03656500	-2.66299200
C	2.79697900	2.20004100	-1.65830400
H	3.14391600	0.76021500	-0.09125100

C	1.98633000	2.56695700	-2.73514300
H	0.25063400	2.03966300	-3.90528800
H	3.63839800	2.82584900	-1.37546800
H	2.20108300	3.47214000	-3.29586200
C	-0.45374200	-1.50450000	1.34865500
O	-0.93121800	-2.52406900	0.77476200
H	0.82886500	-3.50022100	2.28512700
C	1.88287100	-5.50221500	-1.97327500
C	2.21779400	-4.15181200	-1.92354100
C	2.16241100	-3.44989500	-0.72010800
C	1.77908300	-4.10483400	0.45749700
C	1.45301000	-5.46078300	0.40005600
C	1.49725900	-6.15710500	-0.80481600
H	3.14339600	-1.69252800	-1.49013400
H	1.92779200	-6.04176900	-2.91413800
H	2.52892300	-3.63113700	-2.82670200
C	2.50478700	-1.97503500	-0.64671300
C	1.78130000	-3.35460000	1.77232100
H	1.16019000	-5.97455100	1.31297600
H	1.23598000	-7.21060200	-0.83124600
C	2.07224700	-1.85239400	1.59597900
H	2.55964200	-3.78279700	2.41912600
H	2.34376200	-1.42126700	2.56563200
N	3.15377900	-1.63164400	0.62457200
C	4.41188600	-2.31855600	0.89016700
H	4.32272200	-3.41614500	0.84531400
H	4.71318100	-2.05667100	1.91206500
C	5.46800300	-1.86619700	-0.09145700
C	5.97011300	-2.73540500	-1.05952800
C	5.92312500	-0.54470300	-0.06671100
C	6.92069800	-2.29786200	-1.98212100
H	5.60637600	-3.75970000	-1.09466400
C	6.87070900	-0.10399200	-0.98399700
H	5.52446400	0.13625700	0.68107600
C	7.37356400	-0.98246100	-1.94482300
H	7.30356300	-2.98477500	-2.73039500
H	7.21984600	0.92350400	-0.95167200
H	8.11288900	-0.63907300	-2.66150600

C	-0.94987400	-2.36479600	4.91256600
C	-1.37559600	-2.29307300	3.45853300
H	-0.87682000	-1.35703400	5.33051700
H	-1.67099100	-2.93825300	5.49997600
H	0.03014600	-2.84227100	4.99715300
H	-1.41749300	-3.28538200	2.99546700
H	-2.38019700	-1.84580900	3.38098600
O	-0.42039900	-1.48912800	2.79117500

TS7SS

C	-4.00696400	-1.49375400	0.09987300
C	-5.34563200	-1.83164900	0.27384900
C	-6.25039000	-1.62322500	-0.76321700
C	-5.80765600	-1.02228100	-1.94007300
C	-4.46528900	-0.66994300	-2.07256900
C	-3.53061100	-0.93411500	-1.07855500
C	-3.23034000	-1.67416500	1.38597900
C	-4.34539700	-1.85841900	2.46874100
C	-5.58439300	-2.33399900	1.67603300
H	-7.29914900	-1.87797400	-0.64808600
H	-6.50312400	-0.80082000	-2.74148700
H	-2.48603600	-0.66043000	-1.20267400
H	-2.51122100	-2.49534700	1.35673300
H	-4.03721600	-2.58144600	3.22518400
H	-5.64273900	-3.42746100	1.69503700
C	-3.14521900	0.69636800	1.98891300
C	-4.55629300	0.53729500	2.45720700
C	-1.18697200	-0.12896000	1.37401100
H	-5.25346400	0.52809900	1.60939800
H	-6.49949800	-1.94541800	2.13064900
N	-2.46709100	-0.44708400	1.64419800
N	-2.37105400	1.73402500	1.94160800
N	-1.16226600	1.20709700	1.55150300
O	-4.60064300	-0.66646400	3.20355300
H	-4.82277200	1.35475500	3.12704100
C	-0.17939700	2.11403900	1.06584700
C	-0.30458500	2.59409000	-0.24053900
C	0.89351300	2.53345000	1.85009500

C	0.65744300	3.43713900	-0.78203000
C	1.87080400	3.36852300	1.32334200
C	1.74813100	3.78961600	0.00441300
H	0.56853500	3.79182300	-1.80132200
H	2.71343800	3.67591300	1.93037900
Br	-3.91754000	0.30335400	-3.60633900
Br	1.04718300	1.93768500	3.61612400
Br	3.09974200	4.87051700	-0.73421100
Br	-1.76841600	2.06256100	-1.29257400
C	1.43289600	-1.56254400	-0.61615900
C	1.30215800	-0.86980700	0.75690900
H	0.92636000	-2.52670200	-0.51674800
H	1.26981300	0.21561700	0.62645100
C	0.80903700	-0.86637000	-1.80092000
C	-0.15900200	-1.55023300	-2.54677400
C	1.17008200	0.42169800	-2.21848400
C	-0.73541400	-0.98479500	-3.68073800
H	-0.46243600	-2.54386300	-2.22539900
C	0.61057400	0.98125200	-3.36433900
H	1.89944600	0.99411700	-1.65116400
C	-0.34508400	0.28478600	-4.09844400
H	-1.50095600	-1.52687900	-4.22708500
H	0.91495200	1.97662500	-3.67712800
H	-0.79314600	0.73204800	-4.98073300
C	0.01868700	-1.33724900	1.50470900
O	-0.48042000	-2.46887900	1.21013500
H	3.13264400	0.83156300	1.94972900
C	4.74771600	0.87590600	-2.61192900
C	4.17862900	-0.35498000	-2.29271200
C	3.76522000	-0.63275100	-0.99195700
C	3.97280500	0.31653200	0.02319100
C	4.52074800	1.55515500	-0.30967200
C	4.89723400	1.84315900	-1.62120500
H	3.18955700	-2.66961100	-1.39529600
H	5.05231000	1.08594500	-3.63236500
H	4.01498100	-1.09744400	-3.06993000
C	2.96509000	-1.87686100	-0.67565700
C	3.59500700	-0.02629300	1.44956300

H	4.65173100	2.30793100	0.46562600
H	5.30258500	2.82098400	-1.86245600
C	2.64586700	-1.22516800	1.48073500
H	4.50239800	-0.27475800	2.01288900
H	2.47914600	-1.55236200	2.50741400
N	3.28127800	-2.29772900	0.69632600
C	2.74729200	-3.61562500	1.06380200
H	1.64687600	-3.64867600	1.06057300
H	3.06100800	-3.79077300	2.10125700
C	3.29966800	-4.71336000	0.18703000
C	4.67569300	-4.80747600	-0.04640200
C	2.45109000	-5.65322600	-0.39781200
C	5.19079900	-5.82778900	-0.83839200
H	5.33324000	-4.06206500	0.39183300
C	2.96460100	-6.68090100	-1.18883800
H	1.37933700	-5.57733100	-0.23113900
C	4.33547200	-6.77075700	-1.41019100
H	6.26080500	-5.89052900	-1.01153200
H	2.29140800	-7.40616400	-1.63537900
H	4.73756000	-7.56736100	-2.02822700
C	-1.17303100	-0.62914500	4.77330300
C	-0.59718200	-1.68427300	3.84184700
H	-1.69509300	0.15340500	4.21236600
H	-1.88209400	-1.08308000	5.47143600
H	-0.37905800	-0.14799700	5.35021500
H	-0.03612700	-2.43091900	4.41725400
H	-1.38648800	-2.22866000	3.31348200
O	0.28832500	-1.08670400	2.90782100

PRR

C	-0.80757700	-0.31959300	0.25738100
C	-1.14945000	-0.59645300	-1.24031700
H	-0.76778300	-1.28246100	0.77738900
H	-1.80219100	0.19160900	-1.63196500
C	-1.76347400	0.56989000	1.01370800
C	-2.18782600	0.17679600	2.28581700
C	-2.23601400	1.78455200	0.50241700
C	-3.05824800	0.96738900	3.03214800

H	-1.83321000	-0.76682700	2.69308600
C	-3.10598800	2.57792300	1.24490200
H	-1.91639500	2.12231100	-0.48017300
C	-3.52101100	2.17282900	2.51226800
H	-3.37723000	0.63854600	4.01616400
H	-3.46144300	3.51651400	0.83120700
H	-4.20159800	2.79177500	3.08815700
C	-1.90767100	-1.89896600	-1.37297600
O	-1.58870600	-2.84554700	-2.05573000
H	-0.36726000	0.94600600	-3.36694900
C	1.01499800	3.94566600	0.14349100
C	0.97866900	2.62496500	0.57872700
C	0.78414700	1.58114000	-0.32539000
C	0.63925900	1.86144700	-1.69286800
C	0.67993300	3.18990000	-2.12145200
C	0.86088700	4.22871400	-1.21284500
H	1.19494900	0.01179600	1.09930800
H	1.16146100	4.75001200	0.85714500
H	1.08892600	2.39534400	1.63601000
C	0.66763400	0.14588000	0.14912400
C	0.46242300	0.72762000	-2.68511300
H	0.56548300	3.40768800	-3.18074200
H	0.88488600	5.25595900	-1.56257000
C	0.20948800	-0.60618000	-1.96811900
H	1.36042200	0.65036800	-3.31140300
H	0.27594300	-1.44141400	-2.67073200
N	1.14960200	-0.80881500	-0.85329900
C	2.56218500	-0.70904200	-1.18721200
H	2.74193900	-1.38819300	-2.03108300
H	2.85875300	0.30019500	-1.51818700
C	3.42721400	-1.11167900	-0.01237100
C	3.11644600	-2.25271700	0.73383100
C	4.54441600	-0.35599500	0.34248000
C	3.91455700	-2.63358900	1.80758300
H	2.23369400	-2.82681500	0.46793100
C	5.34894200	-0.73772600	1.41565800
H	4.78422100	0.54079000	-0.22312800
C	5.03582700	-1.87751900	2.15058700

H	3.66226000	-3.52066600	2.38035200
H	6.21469900	-0.13922500	1.68132400
H	5.65690800	-2.17327100	2.99009100
C	-4.92229400	-2.86272900	0.38713600
C	-3.80357100	-3.07670100	-0.60768000
H	-5.55705600	-3.75053100	0.42780500
H	-4.51619900	-2.67716300	1.38423600
H	-5.53681500	-2.00763700	0.09730200
H	-3.16738400	-3.92350800	-0.33578200
H	-4.17934700	-3.24897500	-1.62055100
O	-3.00520100	-1.88013400	-0.60760200

PRs

C	-0.87102300	-0.34384500	0.23885300
C	-1.15688100	-0.63576100	-1.27186000
H	-0.74136200	-1.30449300	0.75074600
H	-1.92059300	0.04597700	-1.65856900
C	-1.92851200	0.43489200	0.98277300
C	-2.32402700	0.00542800	2.25216200
C	-2.51983300	1.59076300	0.45882500
C	-3.28112500	0.70553800	2.98358100
H	-1.87730600	-0.89321800	2.67054200
C	-3.47584900	2.29301600	1.18585300
H	-2.22311500	1.95721800	-0.52057400
C	-3.86104200	1.85325000	2.45106700
H	-3.57571900	0.35063400	3.96617200
H	-3.92082300	3.18785800	0.76214200
H	-4.60977100	2.40038000	3.01495800
C	-1.68908800	-2.04441500	-1.39741000
O	-1.12446600	-2.97106400	-1.93267500
H	-0.55661400	1.09192000	-3.31688600
C	0.46901700	4.09065500	0.30867800
C	0.57716600	2.75854500	0.69424000
C	0.51227200	1.73583600	-0.25138900
C	0.34740400	2.04954200	-1.60865100
C	0.24439300	3.38970800	-1.98767300
C	0.29951200	4.40629900	-1.03856500
H	1.07874700	0.16510700	1.11777400

H	0.51621600	4.87904800	1.05312300
H	0.69806900	2.50168400	1.74407500
C	0.54884500	0.27854400	0.16608100
C	0.29368600	0.94052300	-2.64208900
H	0.11418700	3.63395500	-3.03934000
H	0.21214200	5.44258000	-1.34951300
C	0.19648900	-0.44216900	-1.98095900
H	1.19315800	0.98633100	-3.26954600
H	0.37262100	-1.23333000	-2.71494800
N	1.14263000	-0.57718600	-0.86381500
C	2.53912000	-0.31764200	-1.17426100
H	2.78341000	-0.90387000	-2.06994200
H	2.73972400	0.73889200	-1.41920800
C	3.44111200	-0.73904000	-0.03350300
C	3.18733000	-1.92351400	0.66417600
C	4.54417600	0.03485000	0.32754300
C	4.02622300	-2.32860900	1.69738500
H	2.31691300	-2.51261100	0.39085800
C	5.38942000	-0.37133100	1.35919800
H	4.74076800	0.96471000	-0.20026100
C	5.13234100	-1.55412700	2.04690400
H	3.81782100	-3.24999500	2.23248300
H	6.24374500	0.24118400	1.63001800
H	5.78604500	-1.86920300	2.85400300
C	-2.78747300	-4.23662800	0.44719000
C	-3.43575500	-3.47142400	-0.69040500
H	-2.89835700	-3.68642100	1.38496200
H	-3.26103000	-5.21484700	0.56005200
H	-1.72441000	-4.38731200	0.24649500
H	-3.30144000	-3.98171900	-1.64632600
H	-4.49936100	-3.30950700	-0.51200700
O	-2.87671700	-2.14818000	-0.78495700
PSR			
C	0.50312600	0.83455100	0.73711800
C	1.45957200	0.73440700	-0.48466000
H	1.06193000	0.59226500	1.64472300
H	1.40017200	1.64947400	-1.08162300

C	-0.08644500	2.21951900	0.88986500
C	0.51590700	3.13274800	1.75874900
C	-1.20401300	2.62715300	0.15383900
C	0.01375100	4.42515800	1.89572800
H	1.38591500	2.82368100	2.33316800
C	-1.71004600	3.91672100	0.29353700
H	-1.66974100	1.92681500	-0.53453700
C	-1.10335100	4.82062200	1.16362100
H	0.49084600	5.12065300	2.57933200
H	-2.58215900	4.21609400	-0.27986900
H	-1.50082700	5.82460100	1.27280900
C	2.91100700	0.54359000	-0.11242700
O	3.34952500	0.40606400	1.00653400
H	2.55892300	-1.79568000	-0.99692000
C	-0.07441800	-3.26710800	2.78379300
C	-0.56658900	-2.08669600	2.23420400
C	-0.05299200	-1.59403900	1.03440800
C	0.95766400	-2.29927400	0.36621500
C	1.44385000	-3.48319700	0.92325000
C	0.93776500	-3.96511100	2.12688500
H	-1.52601400	-0.02933800	0.81850800
H	-0.47976400	-3.64310500	3.71778100
H	-1.35825700	-1.53731200	2.73842800
C	-0.52934000	-0.27982500	0.44146300
C	1.46321400	-1.80985000	-0.97617900
H	2.22665800	-4.03125200	0.40428700
H	1.32819400	-4.88567100	2.54891000
C	0.89779200	-0.42705200	-1.34804900
H	1.16486100	-2.53017400	-1.74890900
H	1.06139500	-0.23845600	-2.41333000
N	-0.53024000	-0.31548600	-1.02815400
C	-1.39692400	-1.32578100	-1.62810500
H	-1.18052800	-2.34353000	-1.26493500
H	-1.20945100	-1.31408900	-2.70840900
C	-2.84467000	-0.99562300	-1.34803100
C	-3.58981500	-1.75351800	-0.44520500
C	-3.43866400	0.11509800	-1.95454300
C	-4.91092900	-1.41326700	-0.15506200

H	-3.12663100	-2.60992900	0.03957200
C	-4.75605900	0.45791800	-1.66803600
H	-2.85476200	0.71181400	-2.65108500
C	-5.49548100	-0.30760700	-0.76599500
H	-5.48097500	-2.00997400	0.55003700
H	-5.20858300	1.32025100	-2.14760000
H	-6.52346300	-0.04166200	-0.54105500
C	5.75106900	0.28211500	-2.34985200
C	5.08261600	0.28769400	-0.99407800
H	5.61456700	1.24339400	-2.84996100
H	6.82152400	0.10055200	-2.23239300
H	5.33279100	-0.50422700	-2.98229500
H	5.19788500	-0.66805900	-0.47400800
H	5.47453100	1.07447700	-0.34373800
O	3.67885900	0.52527500	-1.21085000

PSS

C	-0.35466400	-0.04047200	0.71479900
C	-1.29248300	0.79887700	-0.17319200
H	0.13949100	0.64472500	1.41150500
H	-2.21948500	0.26866000	-0.41230300
C	-0.98876700	-1.12990100	1.54606100
C	-0.56186800	-1.30607000	2.86528500
C	-1.96300600	-2.00118700	1.04311800
C	-1.08635800	-2.31869500	3.66466700
H	0.19188500	-0.63514500	3.26996200
C	-2.49217500	-3.01249200	1.83921300
H	-2.30013300	-1.90295200	0.01425500
C	-2.05661400	-3.17584700	3.15311000
H	-0.73943900	-2.43348200	4.68680200
H	-3.24540700	-3.67855600	1.43000200
H	-2.47160600	-3.96473700	3.77232700
C	-1.69891100	2.10751300	0.46628900
O	-1.23468800	2.58466800	1.47822000
H	-2.01643800	0.21443700	-2.78209900
C	-0.00016800	-4.00357600	-1.61802900
C	0.52761500	-2.95837700	-0.86647200
C	0.22223600	-1.63378400	-1.17712100

C	-0.62330700	-1.34924800	-2.25848500
C	-1.15028800	-2.40336900	-3.00623000
C	-0.84498700	-3.72446800	-2.69065400
H	1.66252200	-0.77613700	0.17414700
H	0.24334100	-5.03098200	-1.36702600
H	1.17536900	-3.16861500	-0.01885800
C	0.72804000	-0.49573300	-0.31906900
C	-0.94158200	0.09024800	-2.60813400
H	-1.80757200	-2.18243100	-3.84385300
H	-1.26501400	-4.53339700	-3.28008100
C	-0.47395500	1.03308600	-1.50046500
H	-0.42982300	0.36050200	-3.53880400
H	-0.53566500	2.07123100	-1.83975900
N	0.91567600	0.68467800	-1.17556400
C	1.61755800	1.79660200	-0.51993700
H	1.06124900	2.21369500	0.33388400
H	1.69266800	2.59614800	-1.26702700
C	3.00055200	1.39806200	-0.06539100
C	3.90264800	0.82984800	-0.97064500
C	3.39687100	1.58477100	1.25840700
C	5.18087200	0.46813500	-0.55940900
H	3.58604700	0.66770200	-1.99716400
C	4.67918300	1.22531300	1.67336400
H	2.69648400	2.01629600	1.96943600
C	5.57332800	0.66745400	0.76490000
H	5.87437100	0.03059100	-1.27078100
H	4.97514000	1.37767400	2.70654700
H	6.57104100	0.38473200	1.08516400
C	-4.11922900	4.51478100	-0.75149100
C	-3.07642600	4.00301100	0.21614700
H	-4.97153300	3.83324500	-0.79569600
H	-4.47501000	5.49428800	-0.42481200
H	-3.69805600	4.61506900	-1.75426400
H	-2.20634600	4.66323300	0.27059200
H	-3.47496000	3.88663200	1.22762300
O	-2.64625500	2.71382500	-0.26004500

TS4SS^S-D

Single-Point Energy=	-12324.13054970		
C	-4.51209300	-1.07222600	-0.18185400
C	-5.70210500	-1.45403300	0.42641900
C	-6.80404900	-0.60153000	0.37028900
C	-6.68115100	0.63655900	-0.25593700
C	-5.46857000	0.99385300	-0.84638800
C	-4.37772400	0.13846900	-0.84952800
C	-3.40144300	-2.05287700	0.11038200
C	-4.04881800	-3.11341300	1.07679200
C	-5.56615300	-2.79700900	1.09594600
H	-7.74415100	-0.87853600	0.83600300
H	-7.51536600	1.32840600	-0.27494400
H	-3.45105100	0.42813500	-1.33273700
H	-2.94740400	-2.51189600	-0.76709600
H	-3.84951800	-4.11337400	0.69146700
H	-6.11418100	-3.56572300	0.54384200
C	-2.38957600	-1.05718600	2.15947100
C	-3.37363200	-1.83827200	2.96913100
C	-1.34746500	-0.54720300	0.32141200
H	-4.34142600	-1.31994400	2.99591800
H	-5.94476700	-2.80935100	2.12238200
N	-2.33802400	-1.29883600	0.81484400
N	-1.48977700	-0.18358000	2.51970100
N	-0.85007100	0.12777500	1.36617600
O	-3.46354400	-3.11336200	2.36893300
H	-3.00745700	-1.96230600	3.98774300
C	0.08660800	1.20265900	1.32901800
C	-0.28741300	2.42266500	0.75544800
C	1.37597900	1.03545100	1.83256000
C	0.63243200	3.45661600	0.65024900
C	2.30097500	2.06847700	1.74978900
C	1.91991800	3.25959400	1.14389200
H	0.35765700	4.38984600	0.17488000
H	3.31160800	1.92454900	2.11349300
Br	-5.24964600	2.71306900	-1.60919200
Br	1.92802500	-0.60777800	2.53751400
Br	3.20635300	4.60857300	0.92016600
Br	-2.00644600	2.63521400	0.01296100

C	1.47505200	-0.71106300	-2.18797200
C	0.29393600	0.08250600	-1.58960500
H	1.17563400	-1.29241600	-3.06518000
H	0.59054600	1.02677700	-1.15200800
C	2.55994400	0.25643600	-2.61584600
C	3.17725600	0.11079100	-3.85824000
C	3.03746800	1.23613200	-1.73983000
C	4.25396900	0.92100100	-4.21487300
H	2.82228600	-0.65532000	-4.54297600
C	4.10355700	2.05683900	-2.09488200
H	2.59224200	1.34912300	-0.75503800
C	4.71993900	1.89575900	-3.33512300
H	4.72725400	0.79158000	-5.18280200
H	4.44364600	2.81998500	-1.40070200
H	5.55590100	2.52815600	-3.61493300
C	-0.83908500	-0.56044700	-1.06458100
O	-1.53839500	-1.14881100	-1.97346300
H	-0.68607600	-0.37548500	-2.58166600
C	-0.68557600	-3.99602700	0.31824300
C	0.30803300	-3.02198600	0.22953500
C	1.07444600	-2.88891800	-0.92625900
C	0.93995300	-3.83242000	-1.97030000
C	-0.08182500	-4.79003600	-1.88297400
C	-0.90036400	-4.85538800	-0.76126700
H	2.29844500	-1.25457400	-0.22308800
H	-1.28415900	-4.07815500	1.22217100
H	0.49787100	-2.36188500	1.07097900
C	2.05737700	-1.76415700	-1.16228900
C	1.96723700	-3.86042900	-2.99572300
H	-0.20465200	-5.50797300	-2.68884800
H	-1.68137500	-5.60808900	-0.70793900
C	3.13492500	-3.21004600	-2.75091200
H	1.89361700	-4.54903000	-3.82775000
H	4.02323100	-3.37444300	-3.35456100
N	3.27725000	-2.33809700	-1.70716700
C	4.57924400	-1.80109900	-1.32711900
H	4.75939000	-0.81990700	-1.78315800
H	5.33222400	-2.48973400	-1.72377500

C	4.74061000	-1.69539400	0.17518600
C	5.21478800	-0.51576700	0.74984500
C	4.44287700	-2.78314400	1.00145800
C	5.44880200	-0.44151400	2.12322400
H	5.42136000	0.34158900	0.11271200
C	4.66468000	-2.70693500	2.37331800
H	4.04112200	-3.69185000	0.55971100
C	5.18452300	-1.54009700	2.93557900
H	5.83683900	0.47560400	2.55622700
H	4.44069800	-3.56166400	3.00393800
H	5.36496600	-1.48444500	4.00430100

TS4SS^S-A

Single-Point Energy=			-12553.31600370
C	-3.63071800	-2.48735000	-0.41199900
C	-4.66158000	-3.35634800	-0.07190400
C	-5.97201800	-3.04421100	-0.43217000
C	-6.23504300	-1.84846400	-1.09694700
C	-5.17824500	-0.99802900	-1.42047100
C	-3.86362400	-1.31270400	-1.11535700
C	-2.31016400	-2.93429600	0.17421100
C	-2.67322200	-4.19816700	1.04106900
C	-4.13937000	-4.54971800	0.68396900
H	-6.79057200	-3.70920400	-0.17666400
H	-7.25149600	-1.57225800	-1.35331600
H	-3.05070000	-0.65622900	-1.39662600
H	-1.53497000	-3.14306400	-0.56311700
H	-1.99078600	-5.01029600	0.79111600
H	-4.16866600	-5.44827600	0.06078000
C	-2.28257600	-1.67591100	2.31985200
C	-3.05286400	-2.80195900	2.92973200
C	-1.09809000	-0.75505000	0.74563600
H	-4.11952500	-2.71367500	2.68238500
H	-4.70728600	-4.77178100	1.59249200
N	-1.81070200	-1.84538900	1.04336900
N	-1.91515300	-0.53078500	2.81616500
N	-1.17873400	0.03337100	1.81977400
O	-2.48306700	-3.99414100	2.43179000

H	-2.93720200	-2.79234900	4.01314900
C	-0.78116100	1.39869600	1.88709400
C	-1.38673800	2.33859900	1.04669900
C	0.22867600	1.79595000	2.76133600
C	-0.96111200	3.65870900	1.05302300
C	0.65558900	3.11684400	2.78855400
C	0.05774600	4.02890700	1.92556200
H	-1.41734300	4.38474700	0.39183400
H	1.44549900	3.42332000	3.46249200
Br	-5.50827900	0.67338800	-2.25154300
Br	1.04392300	0.52806600	3.87596000
Br	0.63926800	5.81680800	1.94090900
Br	-2.78004300	1.83003300	-0.11603300
C	1.90588500	-0.16137900	-1.49929600
C	0.82755800	0.25906600	-0.51070300
H	1.43336100	-0.79443900	-2.25854500
H	1.17574200	0.58614700	0.46718900
C	2.61706100	0.96992400	-2.20700200
C	2.88075200	0.87380400	-3.57572900
C	3.04421800	2.10765600	-1.51449900
C	3.55921100	1.89336800	-4.24277800
H	2.54930000	-0.00841300	-4.11901200
C	3.71935000	3.12751200	-2.17816800
H	2.83519600	2.20472100	-0.45106100
C	3.97898700	3.02255700	-3.54469800
H	3.75532400	1.80507800	-5.30676100
H	4.03932500	4.00792000	-1.62982100
H	4.50337600	3.81961100	-4.06144100
C	-0.32942500	-0.53125200	-0.52144600
O	-0.83898100	-1.06471200	-1.54655100
H	-0.66130400	-0.11816500	-2.66959300
C	1.21412700	-2.81871700	2.14428500
C	2.01016700	-1.93258700	1.42296600
C	2.25107000	-2.13621000	0.06596600
C	1.75166300	-3.28068700	-0.58440500
C	0.95701600	-4.17456100	0.15576400
C	0.68341900	-3.94036800	1.49990700
H	3.60432400	-0.48515700	-0.15861000

H	1.00066000	-2.63123900	3.19266900
H	2.42328200	-1.05249700	1.90902400
C	2.94815300	-1.10227200	-0.78331500
C	2.18923300	-3.53932500	-1.94646600
H	0.57623400	-5.06986500	-0.33048600
H	0.06500000	-4.63684200	2.05832600
C	3.24694000	-2.84348500	-2.43568900
H	1.79620000	-4.38579400	-2.49538700
H	3.75599500	-3.13484900	-3.35106100
N	3.75697100	-1.73861900	-1.81119800
C	5.13202300	-1.31581800	-1.99297700
H	5.16742300	-0.22210400	-2.06968800
H	5.47647700	-1.71358700	-2.95552800
C	6.05321700	-1.78008600	-0.87519200
C	7.22015200	-1.06525100	-0.59030700
C	5.75539000	-2.92087500	-0.12724100
C	8.08371100	-1.49051200	0.41660200
H	7.45236700	-0.16796000	-1.15927100
C	6.61669800	-3.34526300	0.88260000
H	4.84144300	-3.47500100	-0.33008900
C	7.78314800	-2.63284300	1.15664600
H	8.98721300	-0.92576800	0.62946000
H	6.37268900	-4.23289100	1.45801800
H	8.45211000	-2.96249800	1.94551300
C	-0.33279700	1.77877200	-3.15816200
O	-0.53668700	0.54571700	-3.45726400
O	-0.16192000	2.19717700	-1.98124700
H	0.18800400	1.37370300	-1.22180900
C	-0.30854300	2.73477000	-4.29944500
H	0.03681900	3.71080000	-3.96925400
H	0.34669700	2.33130400	-5.07431200
H	-1.31530000	2.80550000	-4.71952900

TS5SS^s

Single-Point Energy=			-12324.20255170
C	3.91053900	-2.09857200	-0.66702500
C	5.24358400	-2.46198200	-0.82309800
C	5.99456200	-2.81945900	0.29605500

C	5.40763700	-2.77294100	1.55868000
C	4.06983000	-2.39795000	1.68026900
C	3.29249600	-2.08333200	0.57685000
C	3.31084500	-1.61959200	-1.97142200
C	4.52515800	-1.59392500	-2.97305500
C	5.66143000	-2.37535100	-2.26821500
H	7.03667600	-3.10554800	0.19687900
H	5.98525300	-3.01348700	2.44377300
H	2.24695300	-1.82152400	0.67922800
H	2.48064600	-2.22999700	-2.32295400
H	4.23587200	-2.06005300	-3.91423000
H	5.75695800	-3.37377900	-2.70545200
C	3.65735300	0.81771600	-1.71195900
C	5.03528400	0.62104500	-2.25716300
C	1.62121700	0.16738200	-1.27174200
H	5.70648100	0.24487900	-1.47317600
H	6.61805800	-1.86586900	-2.41650700
N	2.80044400	-0.24979000	-1.75448400
N	3.07690300	1.87315200	-1.22324300
N	1.81276400	1.44907100	-0.93738900
O	4.91358800	-0.27896300	-3.33907000
H	5.42825700	1.56297700	-2.63871900
C	0.95354100	2.32645600	-0.20953100
C	0.66315700	2.08771600	1.13715800
C	0.44464000	3.46539700	-0.83171500
C	-0.08154600	3.00225800	1.86798500
C	-0.30508600	4.38824400	-0.11590400
C	-0.54021800	4.15091100	1.23291500
H	-0.30945600	2.81505300	2.90985100
H	-0.69579900	5.27320800	-0.60215800
Br	3.27411900	-2.24116200	3.39476000
Br	0.73173100	3.72250700	-2.66709900
Br	-1.52231700	5.41354100	2.21744100
Br	1.24708000	0.50844100	1.97958600
C	-1.82573500	-0.59695200	0.08203100
C	-0.84671600	-0.05201800	-0.97975200
H	-1.21120100	-1.21825000	0.74973200
H	-0.87856500	1.01793000	-1.15546300

C	-2.39984600	0.52698400	0.92093300
C	-2.35934800	0.43065800	2.31375400
C	-2.97512000	1.66270000	0.33885200
C	-2.88716700	1.44280800	3.11318800
H	-1.89864800	-0.43930300	2.77517500
C	-3.50313300	2.67423300	1.13527600
H	-3.01694700	1.75300000	-0.74431100
C	-3.46283500	2.56571800	2.52490500
H	-2.84374400	1.35445500	4.19419900
H	-3.93593900	3.55630600	0.67299100
H	-3.86219600	3.36254300	3.14375300
C	0.40988200	-0.68071900	-1.01122100
O	0.61412700	-1.90362600	-0.87089400
H	-1.28484700	-0.68275400	-2.23000900
C	-5.84017800	0.24923000	-2.14748900
C	-5.09718600	-0.38912600	-1.15637700
C	-3.84943600	-0.92107800	-1.46547700
C	-3.35343600	-0.85499300	-2.77214400
C	-4.09849900	-0.21560900	-3.76194000
C	-5.33523200	0.34065100	-3.44394900
H	-3.52650000	-1.88523800	0.42858900
H	-6.80776500	0.67727800	-1.90849300
H	-5.47487300	-0.45563900	-0.13971900
C	-2.94166000	-1.54027600	-0.43003200
C	-2.03810400	-1.50351700	-3.01456400
H	-3.71564500	-0.16418900	-4.77682200
H	-5.91293700	0.83851800	-4.21597700
C	-1.80459600	-2.66433700	-2.23189400
H	-1.66949300	-1.53295600	-4.03465800
H	-1.18227300	-3.48673500	-2.57290800
N	-2.28481200	-2.74157900	-1.01326600
C	-2.04734500	-3.88249500	-0.13620000
H	-1.49394600	-3.53638700	0.74311600
H	-1.39805500	-4.58004100	-0.67293400
C	-3.33590600	-4.55856500	0.28565100
C	-4.46133900	-4.55825600	-0.54040800
C	-3.38743100	-5.22233800	1.51234100
C	-5.62093700	-5.22095000	-0.14578000

H	-4.43666100	-4.03167600	-1.49090100
C	-4.54328800	-5.89286700	1.90207100
H	-2.51748800	-5.21635400	2.16374900
C	-5.66339400	-5.89270000	1.07336100
H	-6.49219400	-5.21132000	-0.79247100
H	-4.57189000	-6.40831100	2.85655800
H	-6.56697400	-6.40970400	1.37924800

M4SS^s

Single-Point Energy=			-12324.24168350
C	-4.35708000	0.02260600	0.87167900
C	-5.70416700	0.36299000	0.82899300
C	-6.46017500	0.03380800	-0.29544100
C	-5.84368000	-0.58888400	-1.37820800
C	-4.48417200	-0.89523300	-1.31337100
C	-3.72665700	-0.62303700	-0.18490600
C	-3.68596700	0.58868100	2.10331300
C	-4.78452800	1.50053300	2.76590300
C	-6.11284200	1.11185300	2.07082900
H	-7.51349300	0.28881100	-0.34848900
H	-6.40788800	-0.81895300	-2.27457400
H	-2.67290200	-0.87398700	-0.15259800
H	-3.30244800	-0.16158900	2.79169600
H	-4.81705500	1.31375600	3.83814700
H	-6.70968800	0.47704200	2.73218300
C	-2.76913300	2.65295400	1.10566800
C	-4.08922100	3.30270900	1.37339300
C	-1.29607400	1.06184200	1.29874100
H	-4.81249600	3.02599800	0.59426700
H	-6.70463300	2.00745100	1.86026100
N	-2.54786800	1.40994400	1.63070400
N	-1.72266200	3.08560200	0.46271900
N	-0.81728400	2.08076000	0.58486400
O	-4.48930000	2.88288200	2.65937100
H	-3.97639300	4.38645500	1.38517200
C	0.39469800	2.20678300	-0.16031600
C	0.54814000	1.54728500	-1.38079300
C	1.35921000	3.11833800	0.26909200

C	1.61948000	1.85669000	-2.20852500
C	2.44235100	3.42549500	-0.53752800
C	2.53759100	2.80938300	-1.78218100
H	1.74206600	1.35567200	-3.16058400
H	3.19342200	4.13102400	-0.20495000
Br	-3.60964100	-1.64411700	-2.82053000
Br	1.19278100	3.88077100	1.97326300
Br	3.98145700	3.25238800	-2.89610300
Br	-0.67660700	0.21256500	-1.90349900
C	1.36940700	-1.32078400	0.67846900
C	0.86013200	-0.33050700	1.76400300
H	0.52647100	-1.56955200	0.02346300
H	1.30872200	0.65948200	1.66634700
C	2.45507100	-0.76755700	-0.21585500
C	2.56231800	-1.29564200	-1.50880800
C	3.40563900	0.16022300	0.21489700
C	3.60063000	-0.90701900	-2.35004000
H	1.82480100	-2.02059300	-1.85296600
C	4.44713000	0.54765800	-0.62641500
H	3.36115100	0.56843200	1.22184300
C	4.54910100	0.01488300	-1.90885500
H	3.66951500	-1.32519400	-3.34950500
H	5.17682500	1.27362800	-0.27987200
H	5.35498800	0.32715300	-2.56469900
C	-0.63329100	-0.24055200	1.69751200
O	-1.38442800	-1.15665800	1.94276700
H	1.09909800	-0.69991500	2.76672300
C	5.27137500	-2.19449700	2.83599600
C	4.26209100	-2.39662900	1.89790500
C	2.93830600	-2.57552100	2.30056300
C	2.62538200	-2.61018000	3.67387100
C	3.64857000	-2.39615200	4.60869900
C	4.95647400	-2.17919000	4.19481900
H	2.24827700	-3.22890400	0.40016700
H	6.29521200	-2.04996400	2.50772000
H	4.50194200	-2.40770900	0.83777500
C	1.83642700	-2.70204200	1.26546400
C	1.26845100	-2.95521200	4.06891400

H	3.40679900	-2.42182300	5.66775300
H	5.73634200	-2.01781200	4.93243700
C	0.41604000	-3.40914200	3.12694100
H	0.98054500	-2.94788900	5.11259400
H	-0.57437000	-3.77353000	3.38548600
N	0.72998800	-3.49530600	1.78944300
C	-0.35538400	-3.94744100	0.90690800
H	-1.20841600	-3.25891700	0.97464000
H	-0.69364900	-4.91860000	1.28700900
C	0.02431800	-4.08828700	-0.54728800
C	1.09143400	-4.89219100	-0.95883600
C	-0.72189400	-3.41243000	-1.51336300
C	1.42592900	-4.98216600	-2.30700800
H	1.66679400	-5.43795700	-0.21464400
C	-0.39858900	-3.50738700	-2.86499400
H	-1.58463500	-2.82623600	-1.20653000
C	0.68696100	-4.28361500	-3.26302400
H	2.26357300	-5.59995300	-2.61368500
H	-0.99324700	-2.97396000	-3.60123900
H	0.95092900	-4.35538300	-4.31304400