

Supplementary Information for

**DFT study on the mechanism and origin of stereoselectivity of an NHC-catalyzed
activation/transformation of an α -bromo enal**

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Content

Part 1: Supplementary computational details	S2
Part 2 Test results of the different computational methods	S3
Part 3 The deprotonation processes of the pre-NHC	S4
Part 4 Energy profile for the formation of Breslow intermediate via the Si-face addition mode....	S5
Part 5 Energy profile involved in the other three pathways.....	S6
Part 6 Stereoselective addition mode	S7
Part 7 Scanning results for lactamization process.....	S8
Part 8 NCI analysis for stereoselective transition states TS5RR and TS5SS	S9
Part 9 The energies of all the optimized structures.....	S10
Part 10 Cartesian coordinates for all the stationary points	S12

Part 1: Supplementary computational details

In addition, the extent of enantioselectivity, in terms of enantiomeric excess (ee), was also calculated by using the Boltzmann distribution of stereo-selective transition states with the following equation:

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

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

where $\Delta G^{\ddagger}$ is the Gibbs free energy barrier of the competing stereo-selective transition states and $\Delta\Delta G^{\ddagger}$ is the Gibbs free energy barrier difference between the two stereo-selective transition states.

Part 2: Test results of the different computational methods

We have compared the relative Gibbs free energy barriers ($\Delta\Delta G^\ddagger$) between **TS5RS**, **TS5SR**, **TS5RR** and **TS5SS**, which are computed by the Gibbs free energy corrections at the M06-2X/6-31G(d, p)//IEF-PCM_{THF} plus the refined single-point energies at the M06-2X-GD3/6-311++G(2df, 2pd)//IEF-PCM_{THF} level (denoted as L1); and which are computed by the Gibbs free energy corrections at the M06-2X/6-31G(d, p)//IEF-PCM_{THF} plus the refined single-point energies at the M06-2X-GD3/6-311+G(d, p)//IEF-PCM_{THF} level (denoted as L2); B3LYP-D3BJ/6-31G(d, p)//IEF-PCM_{THF} plus the refined single-point energies at the B3LYP-D3BJ/6-311++G(2df, 2pd)//IEF-PCM_{THF} (denoted as L3), the Gibbs free energy corrections at the ω B97X-D/6-31G(d, p)//IEF-PCM_{THF} plus the refined single-point energies at the ω B97X-D/6-311++G(2df, 2pd)//IEF-PCM_{THF} (denoted as L4) levels, respectively. As shown in Table S1, the differences in Gibbs free energy barrier among **TS5RS**, **TS5SR**, **TS5RR** and **TS5SS** remain consistent across various computational method. This finding indicates that the selected method is appropriate and reliable in this kind of reaction system.

Table S1. Test of different methods and basis sets for stereoselective transition states using IEF-PCM solvation model. (unit: kcal/mol).

TS5	L1	L2	L3	L4
TS5SR	0.0	0.0	0.0	0.0
TS5RS	3.1	7.0	4.6	5.1
TS5RR	6.1	6.9	5.7	7.0
TS5SS	4.8	5.2	3.0	4.0

Part 3: The deprotonation processes of the pre-NHC

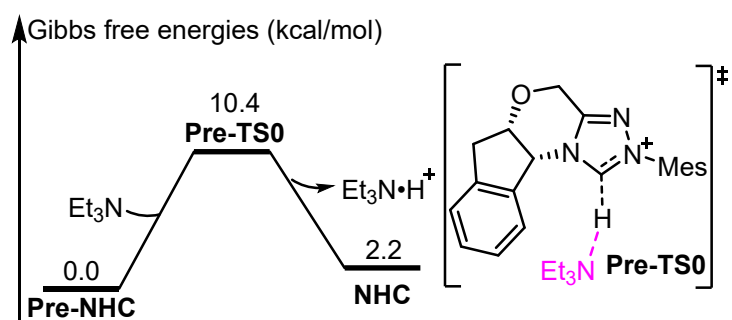


Fig. S1 Relative Gibbs free energy profile for the formation of NHC

The Gibbs free energy barrier for the formation of NHC is only 10.4 kcal/mol, making it easier to happen.

Part 4: Energy profile for the formation of Breslow intermediate via the Si-face addition mode

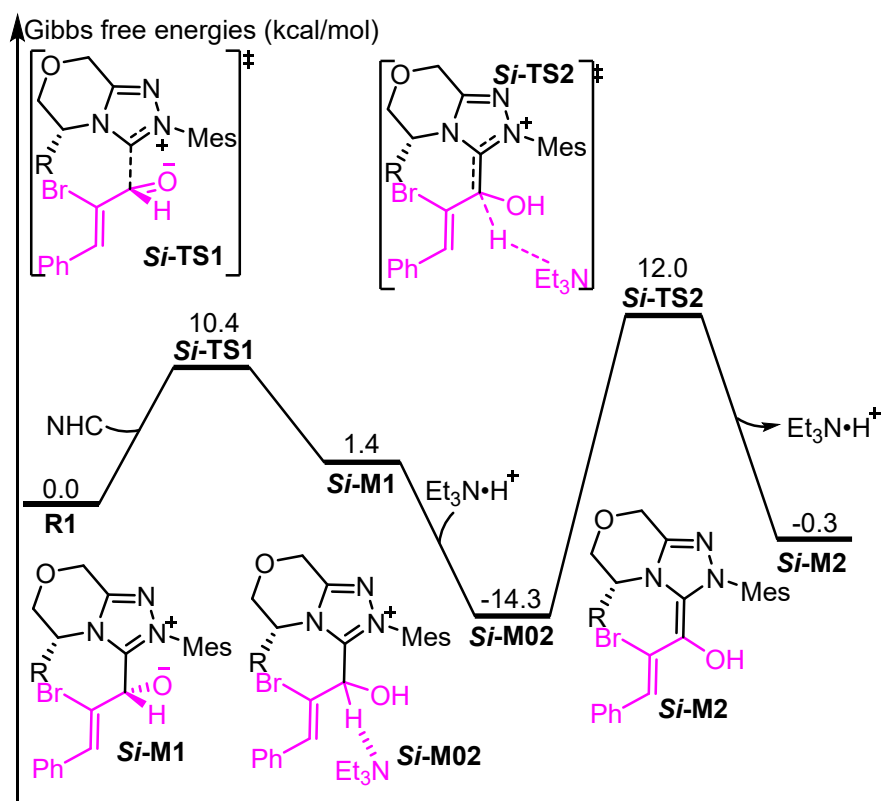


Fig. S2 Relative Gibbs free energy profile for the formation of Breslow intermediate via the Si-face addition mode

Part 5: Energy profile involved in the other three pathways

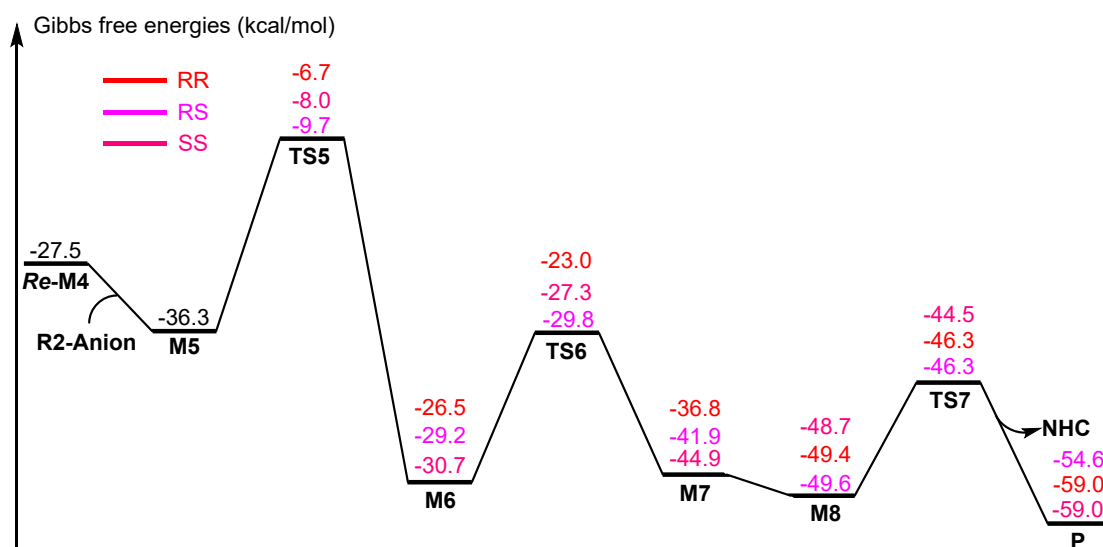
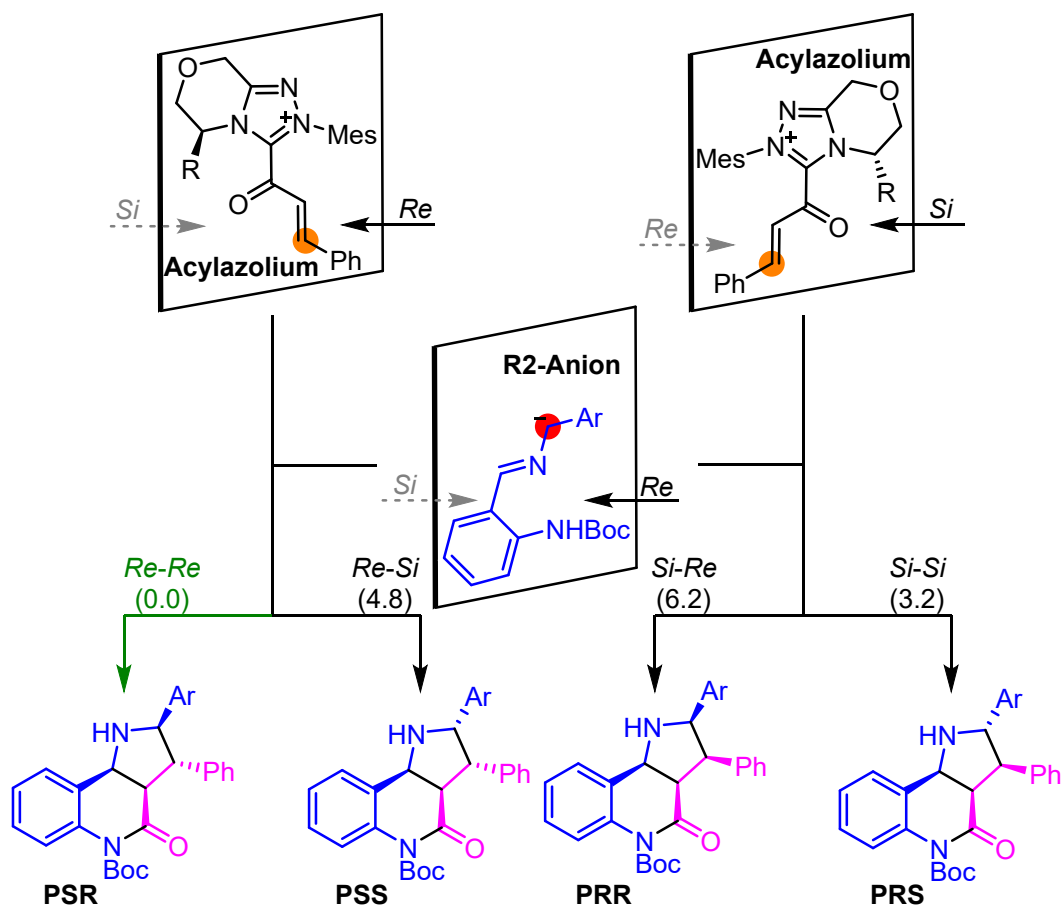


Fig. S3 Energy profile involved in the other three pathways for the reaction between acyl azolium intermediate and **R2-Anion**

Part 6: Stereoselective addition mode



Scheme S1. Possible stereoselective addition modes

Part 7: Scanning results for lactamization process

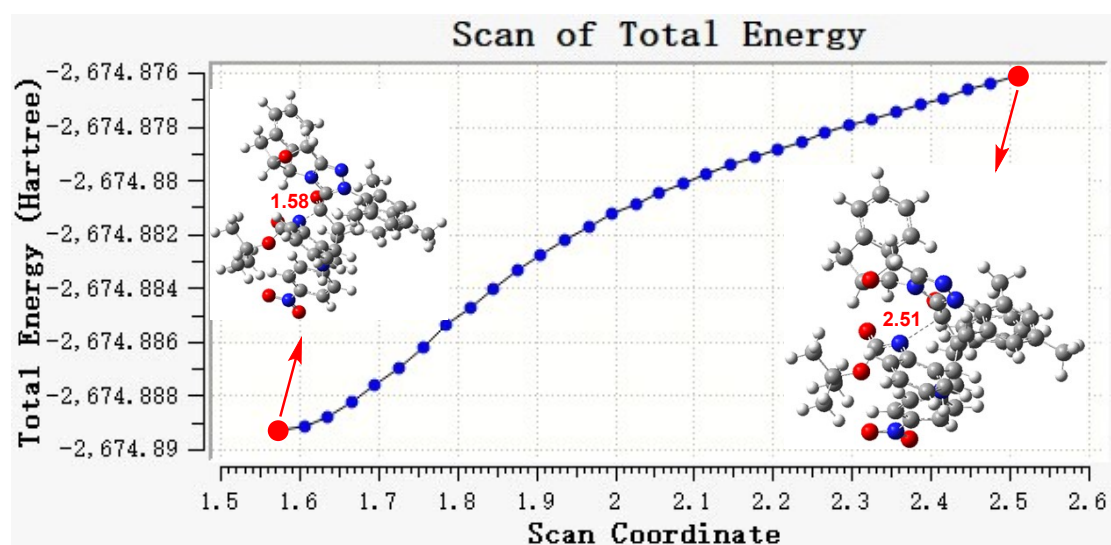


Fig. S4 Scanning results of *SR*-configured pathway involved in the lactamization process

Part 8: NCI analysis for stereoselective transition states TS5RR and TS5SS

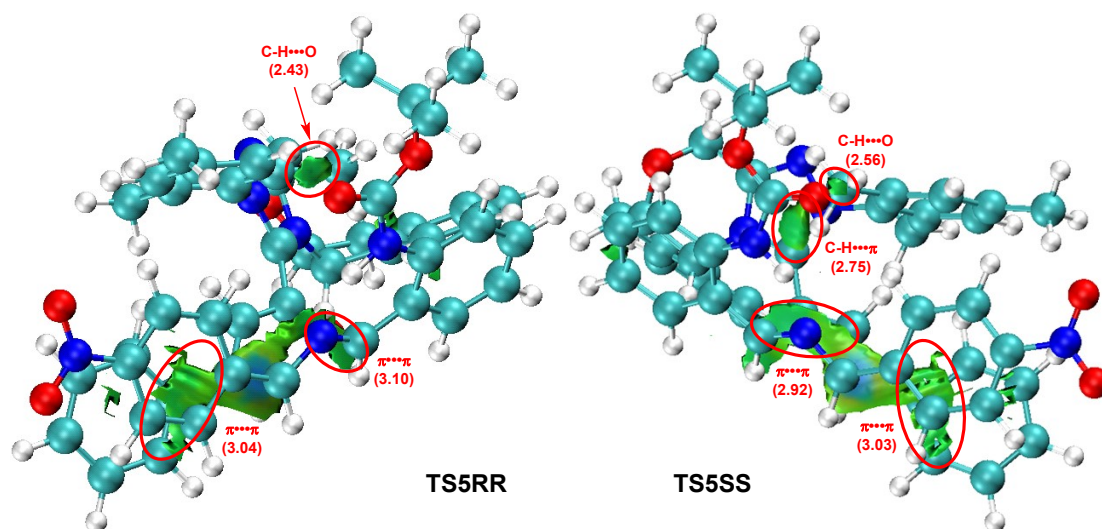


Fig. S5 NCI analysis for stereoselective transition states **TS5RR** and **TS5SS** (distances are given in Å)

Part 9: The energies of all the optimized structures

Table S2. Gibbs free energies (GFE) and Gibbs free energy corrections (GFEC) of the stationary points involved in the NHC-catalyzed activation/transformation of α -bromo enal. (Unit: a.u)

SP	GFE	GFEC	Imaginary Frequencies (cm ⁻¹)
R1	-2993.882159	0.096748	/
R2	-1200.963247	0.325444	/
R2-Anion	-1200.4812	0.313492	/
Et₃N	-292.097112	0.175039	/
Et₃N·H⁺	-292.537596	0.189893	/
Pre-NHC	-1052.041731	0.347185	/
Pre-TS0	-1344.131953	0.541516	1153.93 <i>i</i>
NHC	-1051.583941	0.332179	/
Re-TS1	-4045.458836	0.458028	112.76 <i>i</i>
Re-M1	-4045.467572	0.462279	/
Re-M02	-4338.028822	0.673131	/
Re-TS2	-4338.002605	0.672462	1231.46 <i>i</i>
Re-M2	-4045.472075	0.459096	/
Re-TS3	-4045.472293	0.456752	194.31 <i>i</i>
Re-M3	-4045.5029	0.45932	/
Re-TS4	-4337.998767	0.664879	1331.08 <i>i</i>
Re-M4	-1473.550084	0.462597	/
Si-TS1	-4045.457384	0.458955	108.01 <i>i</i>
Si-M1	-4045.470816	0.458475	/
Si-M02	-4338.039289	0.671182	/
Si-TS2	-4337.999511	0.670057	748.96 <i>i</i>
Si-M2	-4045.465806	0.45786	/
M5	-2674.042692	0.804271	/

TS5RR	-2674.039277	0.804025	114.68 <i>i</i>
TS5RS	-2674.039383	0.802941	24.94 <i>i</i>
TS5SR	-2674.052737	0.803576	37.65 <i>i</i>
TS5SS	-2674.041942	0.803635	113.61 <i>i</i>
M6RR	-2674.075987	0.809185	/
M6RS	-2674.077861	0.805232	/
M6SR	-2674.078991	0.804603	/
M6SS	-2674.081349	0.806973	/
TS6RR	-2674.024812	0.809436	292.31 <i>i</i>
TS6RS	-2674.037058	0.808259	298.72 <i>i</i>
TS6SR	-2674.048979	0.809868	246.02 <i>i</i>
TS6SS	-2674.034011	0.80618	250.28 <i>i</i>
M7RR	-2674.04835	0.813762	/
M7RS	-2674.057799	0.81187	/
M7SR	-2674.066802	0.812045	/
M7SS	-2674.063332	0.816422	/
M8RR	-2674.070497	0.813322	/
M8RS	-2674.070699	0.813834	/
M8SR	-2674.077985	0.811318	/
M8SS	-2674.070821	0.814944	/
TS7RR	-2674.066453	0.813369	156.93 <i>i</i>
TS7RS	-2674.065253	0.812806	156.44 <i>i</i>
TS7SR	-2674.067893	0.81042	136.74 <i>i</i>
TS7SS	-2674.064943	0.814258	150.13 <i>i</i>
PRR	-1622.501552	0.449256	/
PRS	-1622.501763	0.448696	/
PSR	-1622.495466	0.452019	/
PSS	-1622.50156	0.449248	/

Part 10: Cartesian coordinates for all the stationary points

R1

C	-3.93011200	-0.42312800	-0.00000500
C	-2.87693100	-1.33611400	-0.00014300
C	-1.55839900	-0.89686900	-0.00014600
C	-1.27045000	0.47892400	-0.00001400
C	-2.34474100	1.38666400	0.00011100
C	-3.66031500	0.94386500	0.00011900
H	-4.95608600	-0.77623900	0.00000100
H	-3.08281400	-2.40127800	-0.00024900
H	-0.75994500	-1.62538700	-0.00026300
H	-2.13451400	2.45230000	0.00020400
H	-4.47281500	1.66246300	0.00022200
C	0.06682700	1.06706600	0.00000400
H	0.07761300	2.15791600	0.00004900
C	1.31461100	0.57175600	0.00001800
C	2.48249600	1.49568700	0.00004500
H	3.46919500	0.99829400	0.00032400
Br	1.81503600	-1.25141200	0.00004100
O	2.37439600	2.70053200	-0.00020900

R2-Anion

C	4.31226900	-3.50391700	-0.00013900
C	4.81446100	-2.20531200	0.00113000
C	3.95235300	-1.11210200	0.00167300
C	2.56458600	-1.29490100	0.00088900
C	2.03378200	-2.61822000	-0.00023600
C	2.93842400	-3.69201200	-0.00076400

H	4.98149600	-4.35779900	-0.00058600
H	5.88579300	-2.03094600	0.00175300
H	4.35735700	-0.11149700	0.00271700
H	2.53018700	-4.69966800	-0.00168900
N	1.62309300	-0.25603700	0.00144000
C	1.72441400	1.10347700	0.00098700
O	0.73267100	1.81640700	0.00172200
O	2.98833100	1.54846700	-0.00043000
C	3.27492100	2.97843600	-0.00084400
C	2.72551500	3.62699300	-1.26737700
H	1.63618200	3.62600300	-1.26804900
H	3.08190500	4.65942500	-1.32479700
H	3.08654600	3.08948000	-2.14905400
C	2.72948600	3.62662300	1.26756700
H	3.09523000	3.09038700	2.14807800
H	3.08389200	4.65985100	1.32291900
H	1.64015800	3.62335500	1.27260900
C	4.79934800	3.01068500	-0.00328600
H	5.18917700	2.50881600	-0.89323900
H	5.14924100	4.04602900	-0.00350600
H	5.19202400	2.50826800	0.88510800
C	0.61355200	-2.94904900	-0.00080000
H	0.38426900	-4.02292100	-0.00174000
N	-0.35194800	-2.07874300	-0.00020500
C	-4.06078700	-1.97045400	-0.00084400
C	-2.48340900	-0.10176000	0.00040800
C	-5.10948300	-1.09343300	-0.00064200
H	-4.25569400	-3.03960400	-0.00140100
C	-3.53371100	0.77350500	0.00060100
H	-1.46961600	0.28562000	0.00077100

C	-4.86484100	0.29787400	0.00007300
H	-6.13467300	-1.44433500	-0.00102500
H	-3.36461800	1.84394600	0.00115500
N	-5.93744200	1.20293700	0.00024300
O	-5.70332200	2.42222200	0.00083400
O	-7.10056200	0.76725300	-0.00020600
H	0.64971200	-0.59551700	0.00154500
C	-2.69278200	-1.52640200	-0.00035500
C	-1.65417900	-2.45483900	-0.00068400
H	-1.89495100	-3.52194700	-0.00142400
NHC			
C	-4.17689300	0.26160400	-0.15693500
C	-2.92370900	0.50414600	-0.71096500
C	-2.46386800	1.79774700	-0.93277200
C	-3.29379700	2.86397500	-0.59506000
C	-4.55644200	2.62847400	-0.04318800
C	-5.00631100	1.32885500	0.18055800
C	-4.42912000	-1.21747600	-0.01048500
C	-3.07167300	-1.89646300	-0.31725300
C	-2.18309800	-0.78547500	-0.99034600
H	-1.47504400	1.96124400	-1.35378400
H	-5.19052600	3.46916800	0.21992800
H	-5.98438300	1.15294600	0.61870800
H	-4.76950600	-1.50000200	0.99072600
H	-3.19276000	-2.74027900	-0.99740800
H	-5.19262400	-1.55704500	-0.71792500
H	-2.07745700	-0.96559900	-2.06285400
N	-0.84537700	-0.76415200	-0.42632000
O	-2.47853900	-2.46642800	0.84170200

C	0.31437000	-0.35464400	-1.03117000
C	-0.64803200	-1.01516800	0.90426000
N	1.14850200	-0.40950500	0.03093100
N	0.59146600	-0.81931700	1.23026700
C	-1.80741300	-1.54222900	1.68355800
H	-2.47409700	-0.72611900	1.99735100
H	-1.47078300	-2.08199500	2.56866500
C	2.53878200	-0.07075700	0.00495200
C	2.93264400	1.17127100	0.51006000
C	3.45072700	-0.99341400	-0.51217300
C	4.29094500	1.48321400	0.48447300
C	4.79966500	-0.63823200	-0.52094000
C	5.23607400	0.59291400	-0.02942100
H	4.61916500	2.44471600	0.87258900
H	5.52688300	-1.34290500	-0.91743300
C	2.97917500	-2.32273200	-1.03792200
H	2.41153600	-2.86301400	-0.27391600
H	2.31321000	-2.18486800	-1.89452200
C	1.90864600	2.12925000	1.05774100
H	1.10335200	2.28862100	0.33354800
H	1.44843900	1.73031000	1.96656400
H	2.36493500	3.09250200	1.29206200
H	3.82531100	-2.93962400	-1.34494800
C	6.69538900	0.96753400	-0.07628300
H	6.91825100	1.54572900	-0.97897600
H	7.33121400	0.07948300	-0.08703500
H	6.97328700	1.58138000	0.78381700
H	-2.95858100	3.88326200	-0.75706200

NEt₃

N	0.00000000	0.00000000	0.18368700
C	0.40499900	1.32906100	-0.27618500
H	1.41897700	1.51125200	0.08806100
H	0.45294600	1.36364800	-1.38342200
C	-0.48741200	2.45518800	0.23569200
H	-0.65540000	2.34183400	1.31066300
H	0.00000000	3.41797000	0.06317800
H	-1.45797200	2.48597500	-0.26412800
C	-1.35350000	-0.31379100	-0.27618500
H	-2.01827100	0.47324400	0.08806100
H	-1.40742700	-0.28956100	-1.38342200
C	-1.88254900	-1.64970600	0.23569200
H	-1.70038800	-1.73850900	1.31066300
H	-2.96004900	-1.70898500	0.06317800
H	-1.42393200	-2.50562800	-0.26412800
C	0.94850100	-1.01527000	-0.27618500
H	0.59929400	-1.98449600	0.08806100
H	0.95448100	-1.07408700	-1.38342200
C	2.36996100	-0.80548200	0.23569200
H	2.96004900	-1.70898500	0.06317800
H	2.88190400	0.01965300	-0.26412800
H	2.35578700	-0.60332400	1.31066300
NEt ₃ •H ⁺			
N	0.00089300	0.00153700	-0.19955900
C	1.27824500	0.67128500	0.24706200
H	1.27637700	1.66244500	-0.20505100
H	1.19771800	0.78184600	1.33161500
C	2.53001100	-0.08744900	-0.15546400
H	2.53564200	-0.31745200	-1.22448200

H	3.38816500	0.55479800	0.04965300
H	2.66347200	-1.00938200	0.41121700
C	-0.05277400	-1.44402500	0.23297700
H	0.79544100	-1.93395500	-0.24342900
H	0.10671400	-1.44326100	1.31426700
C	-1.34557000	-2.14080900	-0.15092500
H	-1.57481500	-2.00483300	-1.21147500
H	-1.21357300	-3.20954900	0.02519300
H	-2.19574700	-1.80805900	0.44538100
C	-1.21941400	0.76823300	0.24855700
H	-2.07409500	0.26798400	-0.20524200
H	-1.27565200	0.64323200	1.33312700
C	-1.19109100	2.23063100	-0.15827600
H	-2.17997500	2.65079200	0.03224100
H	-0.46649200	2.81263200	0.41219100
H	-0.98398300	2.34480600	-1.22612900
H	-0.00187900	0.01000000	-1.22575500
Re-TS1			
C	5.43464000	-0.82853800	0.10253600
C	4.05964500	-1.04245500	0.07536800
C	3.43693900	-1.92468000	0.95309100
C	4.22995100	-2.59653700	1.88035300
C	5.61142200	-2.38568300	1.91833000
C	6.22419200	-1.50496400	1.02963000
C	5.85325000	0.16213900	-0.95394000
C	4.53443100	0.76658700	-1.49170900
C	3.39185300	-0.18884900	-0.98112100
H	2.36307300	-2.09030900	0.89353300
H	6.21361500	-2.91497900	2.65008300

H	7.29748100	-1.34342200	1.06460200
H	6.49982500	0.95808900	-0.57133400
H	4.52578600	0.81078900	-2.58094000
H	6.39880800	-0.33619300	-1.76165700
H	2.98708100	-0.78788600	-1.80017300
N	2.29233900	0.58168500	-0.40966300
O	4.35732900	2.11731700	-1.08775400
C	0.98069500	0.25433200	-0.30802300
C	2.54269500	1.71593300	0.31751300
N	0.51368900	1.22916600	0.48569400
N	1.46006100	2.15258400	0.88158200
C	3.92271300	2.28183400	0.25163400
H	4.59135500	1.77568600	0.96197100
H	3.91309700	3.34883500	0.47340500
C	-0.82246500	1.34469900	0.99137700
C	-1.59791100	2.43834200	0.60148100
C	-1.28110000	0.36626300	1.88097700
C	-2.88422300	2.54002300	1.13468300
C	-2.57489800	0.50862700	2.37794700
C	-3.38632900	1.58877200	2.02212000
H	-3.50683800	3.38251700	0.84360400
H	-2.95905300	-0.24165500	3.06536100
C	-0.40461000	-0.78819500	2.29362100
H	-0.21710700	-1.47421600	1.45887400
H	0.56876000	-0.43133900	2.64705200
C	-1.06710900	3.45975200	-0.36775500
H	-0.25058000	4.03573000	0.07571700
H	-0.67499200	2.96589600	-1.26227400
H	-1.85856100	4.14836800	-0.66883000
H	-0.87790100	-1.34908000	3.10182300

C	-4.78224900	1.69877200	2.57751300
H	-4.76574500	1.75864000	3.66981800
H	-5.37280200	0.81842800	2.30464800
H	-5.29316400	2.58483900	2.19465300
H	3.77422800	-3.29098300	2.57869500
C	-6.37600000	-1.51058100	-0.12762800
C	-5.60781900	-0.36286700	-0.31712200
C	-4.22860100	-0.45355600	-0.47400400
C	-3.59388100	-1.70343100	-0.44610800
C	-4.37395700	-2.84822000	-0.22869100
C	-5.75342500	-2.75628300	-0.08159200
H	-7.45199600	-1.43347600	-0.00800200
H	-6.08338400	0.61340400	-0.33455200
H	-3.64081100	0.44853800	-0.59351300
H	-3.88728000	-3.81863900	-0.18069500
H	-6.34037600	-3.65530900	0.07666600
C	-2.14091800	-1.87406800	-0.57388800
H	-1.71606900	-2.75676300	-0.09431400
C	-1.21455400	-1.14581100	-1.20059900
C	0.24025300	-1.54951900	-1.20040700
H	0.75189000	-1.23293400	-2.12938700
Br	-1.56843800	0.37314000	-2.27555900
O	0.61874600	-2.52576200	-0.54563100
Re-M1			
C	-5.47158900	0.86006800	-0.10809400
C	-4.10195700	1.07586700	0.02384100
C	-3.57875800	1.90450100	1.01175300
C	-4.47297100	2.51653800	1.88810200
C	-5.84906700	2.30537900	1.76691300

C	-6.35951400	1.48023800	0.76647700
C	-5.76667400	-0.06910700	-1.25835100
C	-4.40429800	-0.70056400	-1.61342400
C	-3.33372800	0.28285800	-1.01492600
H	-2.50292800	2.06260100	1.05773400
H	-6.52922300	2.78793800	2.46189000
H	-7.42922600	1.31618100	0.67710100
H	-6.49119200	-0.85237400	-1.01770000
H	-4.26655500	-0.80724900	-2.68974600
H	-6.15894500	0.48747200	-2.11631800
H	-2.89752700	0.91961700	-1.78737300
N	-2.25128000	-0.48629500	-0.40233900
O	-4.28442500	-2.02675800	-1.11000900
C	-0.93516800	-0.22983700	-0.29712300
C	-2.52907800	-1.59244500	0.34984600
N	-0.47633800	-1.17320900	0.53094200
N	-1.46010500	-2.04330700	0.93248300
C	-3.91845600	-2.13391200	0.25560200
H	-4.60286800	-1.58070300	0.91163000
H	-3.93465500	-3.18928900	0.52573100
C	0.85691000	-1.34741500	1.04258300
C	1.60514500	-2.43550900	0.59198800
C	1.31935100	-0.43505900	1.99603600
C	2.90149200	-2.56658100	1.09119300
C	2.62375700	-0.60468200	2.45326000
C	3.43032100	-1.65272800	2.00337300
H	3.51298500	-3.39797500	0.74964900
H	3.02034000	0.10030900	3.17952700
C	0.43512500	0.66933500	2.50795900
H	0.12423400	1.34595800	1.70126100

H	-0.47557100	0.25105600	2.95221100
C	1.03350000	-3.43681600	-0.37507900
H	0.32622100	-4.10074600	0.13073400
H	0.50084400	-2.93897100	-1.18925300
H	1.83058600	-4.04501500	-0.80639000
H	0.95562700	1.24379200	3.27633000
C	4.85737900	-1.76319800	2.46965000
H	4.94510200	-1.53332100	3.53445000
H	5.48242600	-1.04540900	1.92637100
H	5.26004000	-2.76282000	2.29387000
H	-4.09802800	3.16641000	2.67229300
C	6.32492300	1.98588000	-0.36559100
C	5.70980100	0.73758000	-0.44493400
C	4.32222700	0.63369200	-0.47903200
C	3.52448300	1.78690000	-0.44364600
C	4.15459300	3.03445000	-0.33746800
C	5.54116000	3.13633900	-0.30858800
H	7.40732400	2.06048600	-0.33921200
H	6.31413500	-0.16425600	-0.47425500
H	3.85296400	-0.34327800	-0.51968300
H	3.54348900	3.93142100	-0.28621500
H	6.00920700	4.11283800	-0.23489800
C	2.05442200	1.74914000	-0.45059200
H	1.52966500	2.54005800	0.08660900
C	1.20276300	0.90309000	-1.02283300
C	-0.31821800	1.06350500	-0.90122000
H	-0.67343300	1.00821200	-1.96518000
Br	1.70758100	-0.51953200	-2.18485400
O	-0.73477300	2.09992300	-0.19685600

Re-M02

C	-5.23203200	-0.76962200	0.72544800
C	-3.88710600	-0.61421900	1.05271600
C	-3.41103700	-0.89657200	2.33028600
C	-4.31938600	-1.33764100	3.28935000
C	-5.67106600	-1.48980300	2.97013200
C	-6.13689900	-1.20710900	1.68864100
C	-5.49601500	-0.41115900	-0.71314100
C	-4.10083200	-0.27087700	-1.35858200
C	-3.09966700	-0.13223900	-0.14752800
H	-2.35813100	-0.77914300	2.56770300
H	-6.36450300	-1.83908600	3.72816600
H	-7.18617800	-1.33514400	1.44165700
H	-6.08122200	-1.16387400	-1.24927400
H	-4.03676500	0.60827100	-2.00059400
H	-6.03967400	0.53642000	-0.78570300
H	-2.75135500	0.89974400	-0.04021600
N	-1.91592000	-0.96205500	-0.38849300
O	-3.78272700	-1.35241700	-2.22004200
C	-0.62355400	-0.77239200	-0.08130600
C	-2.02201700	-2.18874000	-0.97800700
N	-0.00181100	-1.88752300	-0.46863300
N	-0.86173500	-2.77443900	-1.04345800
C	-3.34893000	-2.53522400	-1.57094200
H	-4.05421700	-2.87259400	-0.80065500
H	-3.23479500	-3.31362000	-2.32417900
C	1.39529800	-2.23025200	-0.37101200
C	2.13908500	-2.28126200	-1.55144600
C	1.91485600	-2.53118300	0.89051100
C	3.49260800	-2.59554600	-1.42660200

C	3.27240400	-2.82939000	0.95784700
C	4.07623100	-2.85360900	-0.18562100
H	4.10472900	-2.63114200	-2.32394200
H	3.71311300	-3.05100300	1.92630600
C	1.04470200	-2.53225300	2.11907200
H	0.74011300	-1.51910800	2.40016200
H	0.13290800	-3.11532800	1.95446200
C	1.51335100	-2.04093700	-2.89917100
H	0.98909000	-2.93817900	-3.24111100
H	0.79044800	-1.22185200	-2.86937100
H	2.28248000	-1.79107200	-3.63190400
H	1.58264200	-2.96964900	2.96096100
C	5.55323000	-3.11473800	-0.06826300
H	5.76132700	-3.87332200	0.68974700
H	6.06857600	-2.19573300	0.23316900
H	5.97695500	-3.44336500	-1.01922500
H	-3.97376900	-1.56848600	4.29136700
C	6.48208300	1.46989800	1.31057800
C	5.89781900	0.79587400	0.23952400
C	4.52755700	0.55577700	0.22163100
C	3.72279500	0.99389000	1.28186200
C	4.32334300	1.64615000	2.36662100
C	5.69127600	1.89418700	2.37626100
H	7.55102500	1.65588600	1.31828300
H	6.51245000	0.44857200	-0.58506700
H	4.08436700	0.01102200	-0.60424600
H	3.70720100	1.96502900	3.20261400
H	6.14122100	2.40970800	3.21815200
C	2.27408000	0.74571200	1.34123100
H	1.86153300	0.58020200	2.33641200

C	1.37418600	0.71164500	0.35899400
C	-0.10653300	0.49638800	0.56137500
H	-0.62287700	1.32847600	0.04346100
Br	1.73361400	1.10341500	-1.45502200
O	-0.49574400	0.44660900	1.91257300
N	-1.50729500	3.26704200	-0.56555400
C	-2.29588100	3.99385000	0.44185100
H	-1.59964800	4.41821900	1.16820700
H	-2.82071300	4.84510500	-0.02645000
C	-3.28703500	3.11767900	1.19865400
H	-2.77120600	2.28735600	1.69377800
H	-3.78895700	3.70638400	1.97005600
H	-4.06842700	2.70190500	0.55447100
C	-2.32686000	3.00029300	-1.75683900
H	-3.31331400	2.66307400	-1.41988900
H	-2.50281200	3.93674500	-2.31529400
C	-1.73572200	1.94956700	-2.69174500
H	-1.56659700	0.99689600	-2.17675400
H	-2.42485100	1.76341100	-3.52008100
H	-0.78108500	2.26048200	-3.12077200
C	-0.32704800	4.05746800	-0.95743100
H	0.14225700	3.54997300	-1.80231600
H	-0.64474400	5.05317400	-1.31567000
C	0.71869900	4.21016100	0.14035300
H	1.63893200	4.61422200	-0.28911800
H	0.40360400	4.88941500	0.93534900
H	0.96062100	3.24295600	0.58905300
H	-0.51702200	1.35220700	2.25497800

Re-TS2

C	-5.21748700	-0.81961700	1.14365000
C	-3.84115600	-0.66649100	1.28945400
C	-3.14165500	-1.30551000	2.30947000
C	-3.85155200	-2.12268100	3.18560400
C	-5.23195800	-2.28591700	3.04196000
C	-5.92478700	-1.63306500	2.02514000
C	-5.74273100	-0.01604900	-0.01724900
C	-4.48892500	0.47754400	-0.77267100
C	-3.28243800	0.24436700	0.21558900
H	-2.07165600	-1.15833500	2.42184400
H	-5.77040700	-2.92893400	3.73060600
H	-6.99727600	-1.76231200	1.91622900
H	-6.38116700	-0.59442700	-0.69198200
H	-4.56958200	1.53452100	-1.03207700
H	-6.33294900	0.83655000	0.33255300
H	-2.91758500	1.18108000	0.63186800
N	-2.16598500	-0.38632000	-0.49305700
O	-4.31210200	-0.17545400	-2.02026900
C	-0.82306000	-0.33715000	-0.29135000
C	-2.41075000	-1.36626800	-1.41799400
N	-0.33629100	-1.33389000	-1.06067000
N	-1.32019900	-1.95199100	-1.79441000
C	-3.81326800	-1.49766500	-1.91379300
H	-4.41863900	-2.11269700	-1.23524700
H	-3.82079400	-1.94623700	-2.90669300
C	0.94173200	-1.99172400	-0.97643300
C	1.72442200	-2.09246200	-2.12767600
C	1.30829800	-2.55724000	0.25076500
C	2.96132300	-2.72467300	-2.00540800
C	2.55722800	-3.16988500	0.32019300

C	3.40214700	-3.24702800	-0.78930800
H	3.59915000	-2.79742600	-2.88242700
H	2.87635600	-3.60399900	1.26453100
C	0.38636100	-2.54619600	1.44289200
H	0.32726400	-1.55586400	1.90667000
H	-0.62857400	-2.84557200	1.15842300
C	1.26584900	-1.53229700	-3.44588500
H	0.47991900	-2.15617700	-3.88032400
H	0.85858600	-0.52453000	-3.32468800
H	2.10024400	-1.48560000	-4.14759300
H	0.74487600	-3.24744200	2.19786300
C	4.76609700	-3.87077900	-0.65610700
H	4.70414100	-4.85216900	-0.17827300
H	5.40894900	-3.24324600	-0.02983900
H	5.24750900	-3.98876600	-1.62844300
H	-3.32945200	-2.63538000	3.98652200
C	6.36277300	0.59630800	2.12371100
C	5.81267900	-0.06720700	1.02878500
C	4.43426700	-0.09481300	0.84055800
C	3.58406400	0.55517400	1.74648600
C	4.14659500	1.19633400	2.85792400
C	5.52467900	1.22639000	3.04125500
H	7.43830700	0.61399600	2.26650800
H	6.45999500	-0.57460700	0.32017600
H	4.01156900	-0.63134200	-0.00247100
H	3.49263900	1.67970100	3.57859500
H	5.94409400	1.73580700	3.90276200
C	2.11636600	0.52564100	1.61792200
H	1.55948300	0.41504800	2.54781700
C	1.35816200	0.61837500	0.51840100

C	-0.12825600	0.68798700	0.49525500
H	-0.38988500	2.04146900	-0.10203900
Br	2.13306300	0.96440600	-1.18802600
O	-0.70122300	0.68895200	1.79984200
N	-0.68690500	3.21996700	-0.53447000
C	-1.17093500	4.09415400	0.57389800
H	-0.35082400	4.17550300	1.28952200
H	-1.33817700	5.09300800	0.15066200
C	-2.42029100	3.62672700	1.30395900
H	-2.27780200	2.64982500	1.77299300
H	-2.62627200	4.34102400	2.10379000
H	-3.30450100	3.59621500	0.66300700
C	-1.75902900	2.93748000	-1.52583900
H	-2.55828300	2.43433100	-0.98283400
H	-2.16488300	3.88950000	-1.88976900
C	-1.28652900	2.05125900	-2.67724600
H	-0.53799300	1.32901700	-2.33422000
H	-2.13842000	1.50037000	-3.08355600
H	-0.83656100	2.63212700	-3.48425600
C	0.46993600	3.88855900	-1.20194800
H	0.80720200	3.22745000	-1.99743600
H	0.09127500	4.81002100	-1.66363200
C	1.62706000	4.19778700	-0.26156800
H	2.50497300	4.44431700	-0.86243400
H	1.41812900	5.05009400	0.38717900
H	1.88454300	3.33274900	0.35606500
H	-0.47388800	1.52856700	2.22226600
Re-M2			
C	-5.36361600	1.05036000	0.20967500

C	-3.97850700	1.18824000	0.22859400
C	-3.32955600	1.83538400	1.27684800
C	-4.09866700	2.34465300	2.32033500
C	-5.48973200	2.20878800	2.30748800
C	-6.13129900	1.56385900	1.25235400
C	-5.82608800	0.31948700	-1.02431500
C	-4.53618800	-0.20111500	-1.70368900
C	-3.34333800	0.53963300	-0.98366500
H	-2.24881900	1.94404500	1.26647200
H	-6.07547200	2.60832600	3.12941200
H	-7.21209400	1.45691800	1.24692300
H	-6.49388200	-0.51907400	-0.80162300
H	-4.52363300	0.03496900	-2.76801900
H	-6.36857800	0.99028900	-1.69820000
H	-2.90174400	1.28004800	-1.65080200
N	-2.29661100	-0.40238300	-0.61755900
O	-4.44128100	-1.61627600	-1.66007000
C	-0.92551600	-0.23363400	-0.49068300
C	-2.59041800	-1.68918200	-0.24439400
N	-0.49719900	-1.46319100	-0.01576900
N	-1.55280500	-2.36738700	0.10285200
C	-4.00657000	-2.12627100	-0.41133500
H	-4.63124000	-1.75764900	0.41490100
H	-4.06843300	-3.21358500	-0.44754100
C	0.70167700	-1.72178200	0.71215300
C	1.03192900	-0.93032900	1.82004700
C	1.51826400	-2.78055500	0.29060500
C	2.25825100	-1.16684300	2.44565900
C	2.71779200	-2.99340100	0.96318400
C	3.11686000	-2.18189700	2.02837000

H	2.53861100	-0.54677300	3.29446600
H	3.36864700	-3.80004900	0.63338200
C	1.11290800	-3.63623700	-0.87731400
H	0.22637300	-4.23024100	-0.63878100
H	0.85919100	-3.00488200	-1.73411800
C	0.10358400	0.12736500	2.35646600
H	0.24285100	1.08185500	1.83754300
H	-0.94408700	-0.16502300	2.23475100
H	0.29514200	0.28683300	3.41967600
H	1.92348500	-4.31030400	-1.16090200
C	4.42906100	-2.41900500	2.73125800
H	5.16496000	-2.85743100	2.05295800
H	4.30404000	-3.10806300	3.57308700
H	4.83731500	-1.48538500	3.12581700
H	-3.61541400	2.85126100	3.14948900
C	6.25487400	2.47729800	-0.18371500
C	5.72822700	1.19548300	-0.03276400
C	4.35262500	0.99130400	-0.05713300
C	3.47689900	2.07178800	-0.24497100
C	4.01742000	3.35942100	-0.36515500
C	5.39372200	3.56070700	-0.34538800
H	7.32890400	2.63214000	-0.16468100
H	6.39292800	0.35010000	0.11677700
H	3.94511800	-0.00577700	0.07906600
H	3.34597000	4.20547800	-0.48484400
H	5.79432800	4.56379300	-0.45289500
C	2.01559600	1.89868300	-0.22655100
H	1.44626000	2.65794600	0.31013500
C	1.26205100	0.93116900	-0.77769600
C	-0.18551600	0.88992200	-0.74555700

Br	2.06902900	-0.39257000	-1.91638900
O	-0.85551200	2.11631900	-0.70734700
H	-0.66645400	2.59081900	-1.52843400
Si-TS1			
C	2.99523600	2.44415800	-0.12455400
C	1.90856200	1.67327900	0.27885500
C	1.47892900	1.64247800	1.60187800
C	2.20299500	2.37430800	2.54250400
C	3.31991600	3.12004900	2.15420100
C	3.71949500	3.16785500	0.81886500
C	3.19434200	2.35049700	-1.61805700
C	1.91459000	1.66279700	-2.14973300
C	1.30441100	0.94622300	-0.89976800
H	0.60649900	1.05782900	1.89327200
H	3.87216100	3.68343400	2.89975000
H	4.57220400	3.77057600	0.52078500
H	3.32899300	3.32324600	-2.09976000
H	2.14618900	0.93315900	-2.92695500
H	4.07261500	1.74078500	-1.85705000
H	1.57630600	-0.11226800	-0.91125900
N	-0.14592000	1.03438000	-0.89117100
O	1.01781000	2.57071600	-2.77995000
C	-1.05775900	0.17668400	-0.36995100
C	-0.77268400	2.17673400	-1.31312100
N	-2.19694400	0.85865600	-0.53198500
N	-2.05475500	2.09939500	-1.12137900
C	0.08694200	3.22832300	-1.93618100
H	0.59092700	3.81699500	-1.15735300
H	-0.50708500	3.89748500	-2.55835900

C	-3.48854600	0.39523700	-0.12066900
C	-4.03868100	0.92842000	1.04676800
C	-4.11864400	-0.59736400	-0.87538900
C	-5.29278800	0.46195500	1.43788500
C	-5.36717600	-1.03905300	-0.43867200
C	-5.97131000	-0.51370100	0.70546200
H	-5.74245100	0.85993400	2.34423900
H	-5.87981200	-1.81257900	-1.00551400
C	-3.45483400	-1.17504100	-2.09808300
H	-3.15440400	-0.38282200	-2.79083000
H	-2.54719300	-1.72770400	-1.83012400
C	-3.26564800	1.92808500	1.86388300
H	-2.32080900	1.47778800	2.19003400
H	-3.02824400	2.82096400	1.27907200
H	-3.83484600	2.22738500	2.74556000
H	-4.13280900	-1.85351100	-2.61844100
C	-7.33809400	-0.98411500	1.13202600
H	-7.49658700	-0.82013500	2.20004700
H	-7.47348400	-2.04749700	0.92078600
H	-8.11975400	-0.43958100	0.59242100
H	1.89571400	2.36852800	3.58332300
C	5.60547200	-2.35830400	0.17868000
C	4.63100300	-3.31055500	-0.11207700
C	3.30905300	-3.10415900	0.26926200
C	2.94498000	-1.93737900	0.95423800
C	3.93852200	-0.99729800	1.26827800
C	5.25580200	-1.20062900	0.87155900
H	6.63436500	-2.52189600	-0.12548100
H	4.90150300	-4.22219800	-0.63504000
H	2.55829100	-3.85421400	0.04890300

H	3.66567600	-0.09703100	1.81399200
H	6.01024200	-0.45720200	1.10883500
C	1.56353600	-1.63469000	1.36128800
H	1.43497800	-1.09245500	2.29778700
C	0.41694300	-1.81739800	0.70410500
C	-0.89872000	-1.27215400	1.21238300
H	-1.77980600	-1.79468500	0.79898000
Br	0.28573600	-2.64160800	-0.99893500
O	-0.94554200	-0.65128300	2.27716000
Si-M1			
C	-2.70385800	3.04618100	0.11292800
C	-1.83378100	2.06652900	-0.35628500
C	-1.53324000	1.92740000	-1.70919700
C	-2.14945000	2.80283900	-2.60203900
C	-3.03399200	3.78404100	-2.14486600
C	-3.31633100	3.91519600	-0.78660400
C	-2.84381200	2.98737900	1.61256200
C	-1.78422700	1.96369100	2.08791900
C	-1.30061300	1.22833600	0.78098800
H	-0.82051300	1.16641200	-2.03755400
H	-3.50017000	4.45847400	-2.85641900
H	-3.99592800	4.68602100	-0.43555400
H	-2.67128200	3.95318100	2.09830800
H	-2.20994800	1.23278900	2.77551900
H	-3.84587000	2.65654900	1.90255800
H	-1.69213800	0.21182400	0.76416500
N	0.16379500	1.13844900	0.74263800
O	-0.73636600	2.56762500	2.83094100
C	0.99331600	0.23822200	0.17830900

C	0.94139900	2.12961400	1.28161400
N	2.21578000	0.71016200	0.41417200
N	2.20598200	1.89050400	1.10617800
C	0.24640200	3.20968700	2.04113100
H	-0.19516000	3.94503000	1.35458100
H	0.94371800	3.71551800	2.70829400
C	3.45596600	0.13568800	-0.02988400
C	3.99469800	0.60217300	-1.22985800
C	4.05640700	-0.84576600	0.76066800
C	5.20889700	0.04895200	-1.63412500
C	5.26653100	-1.36965600	0.30983700
C	5.85332900	-0.93404300	-0.88086900
H	5.65795800	0.39173500	-2.56286300
H	5.76258100	-2.13502900	0.90148500
C	3.40767200	-1.30880700	2.03794400
H	3.25204000	-0.47026100	2.72399000
H	2.42543200	-1.75547000	1.84522000
C	3.26667800	1.63759100	-2.04186000
H	2.27626100	1.24698000	-2.30644000
H	3.13209000	2.56105900	-1.46957000
H	3.82184400	1.87260100	-2.95142600
H	4.03016100	-2.05288200	2.53668500
C	7.14705600	-1.54136500	-1.35807200
H	6.95269700	-2.45447300	-1.92998800
H	7.79049700	-1.81008200	-0.51712800
H	7.69205100	-0.85288900	-2.00726300
H	-1.93672900	2.72603900	-3.66358600
C	-5.56659600	-3.26553500	-0.52954300
C	-4.47194100	-3.93223300	0.01721900
C	-3.18199500	-3.45016200	-0.18165500

C	-2.96986300	-2.28796900	-0.93405500
C	-4.07602600	-1.63745500	-1.49813400
C	-5.36508200	-2.11527300	-1.28987500
H	-6.57056400	-3.64611300	-0.37144100
H	-4.62235200	-4.83870700	0.59508000
H	-2.33433400	-3.98141600	0.23623800
H	-3.91338100	-0.74262100	-2.09367000
H	-6.21113300	-1.59457500	-1.72690000
C	-1.63770200	-1.71675400	-1.18430300
H	-1.46656100	-1.22743000	-2.14384700
C	-0.57398700	-1.61536500	-0.39246500
C	0.70970200	-0.90059500	-0.83462000
H	1.53440800	-1.62947000	-0.63086000
Br	-0.51662800	-2.23254300	1.41539500
O	0.66937100	-0.37797900	-2.04771900

Si-M02

C	-4.09006000	-2.19121200	1.28203200
C	-2.90030700	-1.48087700	1.15354000
C	-2.26328100	-0.90807000	2.25112200
C	-2.85832500	-1.04948500	3.50233700
C	-4.05999400	-1.75007500	3.64014300
C	-4.68248900	-2.32646200	2.53548800
C	-4.56629100	-2.72158200	-0.04568200
C	-3.43329700	-2.40494900	-1.05193200
C	-2.45030400	-1.43944900	-0.28586600
H	-1.31646000	-0.38239400	2.13939700
H	-4.50968600	-1.85266600	4.62239200
H	-5.61110200	-2.87693300	2.65062000
H	-4.76087700	-3.79880900	-0.03042500

H	-3.81270800	-1.89496200	-1.93719200
H	-5.49454900	-2.23324900	-0.35634700
H	-2.50497000	-0.43947200	-0.71441100
N	-1.05782200	-1.90267400	-0.41650400
O	-2.80642900	-3.56801200	-1.56483400
C	0.11258600	-1.24988200	-0.36042400
C	-0.76067600	-3.23673700	-0.51745300
N	1.05256800	-2.18637400	-0.43773700
N	0.52573900	-3.43614900	-0.54242100
C	-1.90266300	-4.18657600	-0.67164100
H	-2.36230700	-4.39833400	0.30359400
H	-1.56065600	-5.11989100	-1.11757400
C	2.47686300	-1.96969500	-0.39881600
C	3.12797700	-2.13886200	0.82365000
C	3.12151400	-1.58951600	-1.58050800
C	4.50695400	-1.92860000	0.83798500
C	4.49529900	-1.36882000	-1.50407300
C	5.20232700	-1.54593900	-0.31040400
H	5.04574000	-2.05579200	1.77329100
H	5.02978300	-1.06854100	-2.40159300
C	2.36051400	-1.44276900	-2.87213000
H	1.85385400	-2.37785800	-3.13052700
H	1.59029400	-0.66498700	-2.81379600
C	2.35947500	-2.50014500	2.06516800
H	1.60652500	-1.73163600	2.27161500
H	1.84332200	-3.45726500	1.94619500
H	3.02983800	-2.57417500	2.92229600
H	3.03805000	-1.18277500	-3.68593600
C	6.69509900	-1.34740300	-0.27931900
H	6.98750600	-0.47479800	-0.86884000

H	7.20316200	-2.21759800	-0.70668400
H	7.05792100	-1.21680500	0.74227100
H	-2.38442800	-0.61670100	4.37699800
C	-4.51092200	4.68848800	-0.69053300
C	-3.50295200	4.51753000	-1.63752100
C	-2.45499800	3.63486900	-1.39840500
C	-2.40408200	2.91308200	-0.19906600
C	-3.40859600	3.11034200	0.75838900
C	-4.46185800	3.98247000	0.50982700
H	-5.32687000	5.37705700	-0.88396800
H	-3.52843000	5.07958600	-2.56520000
H	-1.67097800	3.51758100	-2.13704000
H	-3.36290400	2.56314800	1.69622000
H	-5.23842600	4.11732200	1.25524000
C	-1.32619200	1.97017500	0.13607000
H	-1.06277100	1.89374000	1.19108900
C	-0.64373000	1.13172000	-0.64284400
C	0.43941400	0.20804200	-0.13109500
H	1.33621700	0.38695900	-0.74901600
Br	-0.89143900	0.92748300	-2.51008700
O	0.72137100	0.37956400	1.21241100
N	2.49640400	2.25271500	1.23210100
C	2.26523500	2.76535900	2.59996100
H	1.32567200	3.32746600	2.55925600
H	2.08384200	1.89264600	3.23860100
C	3.35730600	3.63001200	3.22407600
H	3.64272100	4.46317700	2.57623900
H	2.98537000	4.05020900	4.16189600
H	4.24977300	3.04495200	3.45677700
C	2.45244500	3.32588000	0.22129900

H	1.54744800	3.91058000	0.41713700
H	3.30680000	4.00359200	0.35321800
C	2.42989200	2.82787100	-1.22107000
H	1.47022600	2.38162900	-1.49433200
H	2.58993700	3.67492900	-1.89234400
H	3.21998300	2.09723300	-1.42205900
C	3.67048800	1.35816000	1.11238800
H	3.70586500	0.76393300	2.03233100
H	3.46428400	0.64686500	0.30295100
C	5.02790900	2.00490700	0.84545600
H	5.79052300	1.22062900	0.85015800
H	5.05958400	2.48838700	-0.13480800
H	5.30102100	2.74662300	1.59756500
H	1.38378500	1.18965700	1.22821900

Si-TS2

C	-4.44135300	-2.39301900	0.43518300
C	-3.19555900	-1.95105500	0.87404000
C	-2.73043400	-2.22170100	2.15590700
C	-3.54694900	-2.96441000	3.00673000
C	-4.79792000	-3.41357500	2.57548700
C	-5.25600300	-3.12917100	1.29031500
C	-4.70315800	-1.95372300	-0.98424300
C	-3.33143900	-1.48336900	-1.51234300
C	-2.49575100	-1.17623100	-0.21964400
H	-1.75870800	-1.85569400	2.47832500
H	-5.41919700	-3.99472400	3.24926000
H	-6.22673400	-3.48444900	0.95867700
H	-5.09927500	-2.74710400	-1.62397200
H	-3.40038600	-0.58802400	-2.13126100

H	-5.41845300	-1.12475500	-1.00685100
H	-2.47962100	-0.10460900	-0.01551400
N	-1.11573700	-1.62485300	-0.39818900
O	-2.72176000	-2.45145900	-2.35737100
C	0.06140000	-1.07642700	-0.02719100
C	-0.85418100	-2.80240600	-1.03189500
N	0.97537800	-1.96805100	-0.42593500
N	0.42484000	-3.04059600	-1.06341700
C	-2.00488200	-3.48265200	-1.69926000
H	-2.62471000	-4.02278700	-0.97262300
H	-1.64460000	-4.17853100	-2.45613500
C	2.40815600	-1.91016500	-0.31687500
C	3.00058100	-2.28377700	0.89101900
C	3.13615900	-1.59331500	-1.46773700
C	4.39386700	-2.28073400	0.94452400
C	4.52642600	-1.59220100	-1.35771500
C	5.16940700	-1.93133400	-0.16370800
H	4.88405200	-2.55737700	1.87440600
H	5.12070700	-1.32976300	-2.22944700
C	2.45111400	-1.31008100	-2.77904400
H	2.20059200	-2.24971300	-3.28132600
H	1.51806400	-0.75502300	-2.64461800
C	2.16169100	-2.69468500	2.07167300
H	1.44668600	-1.91485800	2.34935000
H	1.58065100	-3.59220700	1.83560900
H	2.79235700	-2.91195000	2.93440500
H	3.10635800	-0.73488800	-3.43589600
C	6.67363000	-1.94529900	-0.08713700
H	7.01854600	-1.86623700	0.94574800
H	7.10312300	-1.12188100	-0.66253400

H	7.06871500	-2.87808600	-0.50148100
H	-3.20988000	-3.19693800	4.01143800
C	-3.65453400	5.56337700	-0.46949500
C	-2.51012500	5.23579400	-1.19310200
C	-1.72747800	4.14591400	-0.82449700
C	-2.08374400	3.35334700	0.27679600
C	-3.22455700	3.71085300	1.01205100
C	-4.00750400	4.79697500	0.63964100
H	-4.26055900	6.41464600	-0.76148900
H	-2.21709100	5.83827100	-2.04696100
H	-0.83588000	3.91516700	-1.39521600
H	-3.49873200	3.11953800	1.88140900
H	-4.89040400	5.04855900	1.21828200
C	-1.30703200	2.19752800	0.75115100
H	-1.36848600	1.99784600	1.82032600
C	-0.57064400	1.29242200	0.08911600
C	0.26045900	0.21449600	0.69988400
H	1.63787100	0.96000400	0.74866100
Br	-0.45615600	1.28506300	-1.81969500
O	-0.15991100	-0.00492900	2.05158000
N	2.50574500	1.77733100	0.97823600
C	2.03921200	2.47222000	2.22249700
H	0.94622400	2.44873400	2.19627900
H	2.36943800	1.85501100	3.06383600
C	2.50116100	3.91208300	2.41056400
H	2.04512400	4.57993600	1.67729800
H	2.18230700	4.24326900	3.40114400
H	3.58581800	4.01652400	2.35228800
C	2.52108800	2.68047300	-0.20669200
H	1.50204800	3.07071400	-0.29850500

H	3.18384500	3.52729700	-0.01115000
C	2.93543100	1.96163500	-1.47934600
H	2.38738600	1.02534200	-1.59512600
H	2.70197500	2.59483800	-2.33774400
H	4.00647000	1.74388300	-1.49614300
C	3.75875700	1.00067500	1.17177100
H	3.56192200	0.30556500	1.99361500
H	3.89160300	0.39508700	0.27382400
C	5.00983800	1.81663500	1.45508800
H	5.86671100	1.13801100	1.46522600
H	5.19245100	2.57033500	0.68385700
H	4.96652100	2.31131600	2.42771500
H	0.58164200	0.16621600	2.64273600

Si-M2

C	3.20699500	2.47877000	-0.24702600
C	2.25811100	1.63289400	0.32899600
C	2.41895900	1.14304300	1.61795400
C	3.57975000	1.47405000	2.31618700
C	4.54683200	2.29374400	1.73313500
C	4.36299900	2.81014700	0.44980600
C	2.75538500	2.91671700	-1.62164600
C	1.24448800	2.62947000	-1.60526800
C	1.12850600	1.40267200	-0.65620600
H	1.65489900	0.52345100	2.07664700
H	5.44297400	2.54635500	2.29076700
H	5.10374000	3.47141300	0.01000200
H	2.94897300	3.97019500	-1.83590200
H	0.84942500	2.39088600	-2.59675900
H	3.24045300	2.31752700	-2.40180100

H	1.30367500	0.49783500	-1.24715800
N	-0.19653300	1.30368500	-0.07356100
O	0.52761800	3.77852600	-1.15228800
C	-1.12898200	0.27625700	-0.15511500
C	-0.88191300	2.46027500	0.20877100
N	-2.31292000	0.90424400	0.17281500
N	-2.14617500	2.27227900	0.36586800
C	-0.09977500	3.72564300	0.12309400
H	0.63957800	3.77256400	0.93254200
H	-0.76604000	4.58553400	0.19013400
C	-3.58836900	0.31977100	0.41873100
C	-3.73141700	-0.63615100	1.43130500
C	-4.67498900	0.74338700	-0.36008600
C	-5.00294900	-1.16764200	1.65128900
C	-5.92574500	0.19180200	-0.09361100
C	-6.11044600	-0.76317300	0.90843300
H	-5.12832600	-1.91428300	2.43195900
H	-6.77673300	0.50610000	-0.69369700
C	-4.49342200	1.74749400	-1.46754400
H	-4.32026500	2.74976100	-1.06713100
H	-3.62391400	1.49658600	-2.08318800
C	-2.56078800	-1.09917700	2.25433600
H	-1.98119800	-1.84908400	1.70451400
H	-1.88654800	-0.27080200	2.49297700
H	-2.90587200	-1.54698400	3.18830400
H	-5.37798000	1.77374600	-2.10643600
C	-7.48042800	-1.32428000	1.19008000
H	-8.05226600	-1.44863800	0.26703300
H	-8.04971100	-0.65161500	1.83999200
H	-7.41630300	-2.29334900	1.68979100

H	3.72830000	1.09404800	3.32170000
C	5.33209300	-2.50889700	1.10113300
C	4.89484100	-2.07270500	-0.14809500
C	3.54649500	-1.81863800	-0.37574800
C	2.60499700	-2.00214300	0.64765300
C	3.06232500	-2.42077100	1.90636000
C	4.40895000	-2.68125800	2.13057200
H	6.38553500	-2.70431400	1.27358200
H	5.61095300	-1.91893400	-0.94914500
H	3.22403400	-1.46764800	-1.34913900
H	2.34532400	-2.54009500	2.71457600
H	4.73940600	-3.01150700	3.11020600
C	1.18002300	-1.67295000	0.51429500
H	0.69368600	-1.37311200	1.44223800
C	0.35038500	-1.64618900	-0.54450900
C	-0.94143600	-1.02333500	-0.56393800
Br	0.85399400	-2.48096600	-2.23596200
O	-2.03514800	-1.80754900	-0.90887700
H	-2.43479100	-1.45406500	-1.71448100
Re-TS3			
C	5.35044900	-0.32719100	0.80331400
C	3.98831800	-0.61491900	0.79064400
C	3.27043100	-0.78369700	1.97209900
C	3.94510200	-0.64840000	3.18243400
C	5.31202500	-0.35685100	3.20246600
C	6.02383400	-0.19727800	2.01604400
C	5.90153300	-0.20840000	-0.59396500
C	4.67147400	-0.27735500	-1.53322400
C	3.45647100	-0.69812600	-0.62188400

H	2.20971000	-1.01874200	1.94784100
H	5.82334500	-0.25336700	4.15420700
H	7.08558700	0.02979200	2.03626900
H	6.44803300	0.72573500	-0.76124900
H	4.80968600	-1.02593000	-2.31301900
H	6.59448400	-1.02601500	-0.81400500
H	3.11386700	-1.69874500	-0.87207300
N	2.31943500	0.21424100	-0.81287000
O	4.46258400	0.93139100	-2.24550700
C	0.98801900	0.06758200	-0.52076400
C	2.53002600	1.54120800	-1.08887200
N	0.47548400	1.31326500	-0.68965100
N	1.43947400	2.23130700	-1.04082700
C	3.91336200	1.96515400	-1.45467800
H	4.51226000	2.14968000	-0.55108900
H	3.88454000	2.87661300	-2.05130400
C	-0.88024300	1.74600100	-0.55193700
C	-1.22411200	2.44855900	0.60564200
C	-1.79767500	1.43378800	-1.55584100
C	-2.55399400	2.83346200	0.75383600
C	-3.11452600	1.85119200	-1.36670800
C	-3.51249700	2.53049500	-0.21510000
H	-2.85269500	3.36553000	1.65389200
H	-3.85509500	1.61183900	-2.12669700
C	-1.39341700	0.62610900	-2.76013400
H	-0.42132900	0.94460900	-3.14732600
H	-1.32257300	-0.43715200	-2.49739000
C	-0.18991000	2.73153500	1.66196400
H	0.31347900	1.80825300	1.97245300
H	0.58386100	3.40631300	1.28454400

H	-0.64966700	3.18586500	2.54094000
H	-2.13501400	0.72794200	-3.55468400
C	-4.96205800	2.86549700	0.01189400
H	-5.44980000	2.03807200	0.54030400
H	-5.48935400	3.01350800	-0.93340500
H	-5.07341000	3.76662600	0.61965300
H	3.40841200	-0.77346300	4.11709400
C	-6.13528200	-0.62913300	1.32342100
C	-5.52167600	-0.85734800	0.09190700
C	-4.13535300	-0.89114500	-0.01394800
C	-3.33337800	-0.71061800	1.12236700
C	-3.96244500	-0.44954000	2.34844900
C	-5.34858700	-0.41590900	2.45336500
H	-7.21782800	-0.60524500	1.39844200
H	-6.12775000	-1.00182900	-0.79725500
H	-3.66915000	-1.05433000	-0.97719700
H	-3.35088100	-0.28201100	3.23139100
H	-5.81310900	-0.22443700	3.41537900
C	-1.86507600	-0.73251300	1.11368700
H	-1.40645800	-0.27105000	1.99026500
C	-0.96695000	-1.21600600	0.26156400
C	0.36270800	-1.11608300	-0.06167200
Br	-1.76594500	-2.90709000	-1.14927200
O	1.13218800	-2.26618200	-0.14829700
H	0.55658600	-2.92369700	-0.58581400
Re-M3			
C	-5.26344000	-0.21488500	0.24813900
C	-3.98564400	-0.52346000	0.70773100
C	-3.74484400	-1.63660900	1.50422300

C	-4.81972400	-2.45867300	1.83546400
C	-6.10472100	-2.15776000	1.37739700
C	-6.33684300	-1.03522400	0.58437200
C	-5.25095500	1.05126000	-0.57333500
C	-3.75754600	1.34325400	-0.84585400
C	-2.99055400	0.51198800	0.24292600
H	-2.74199900	-1.86213900	1.85838600
H	-6.93271000	-2.80779700	1.64116700
H	-7.33784600	-0.80862300	0.22993400
H	-5.79359400	0.96373200	-1.51898800
H	-3.49511600	2.39577000	-0.73690200
H	-5.70037600	1.87827200	-0.01377900
H	-2.67182800	1.16799300	1.04779000
N	-1.79153100	-0.11155400	-0.32900100
O	-3.38911700	1.01990000	-2.17993200
C	-0.53784600	-0.29830600	0.12854000
C	-1.82878700	-0.59263100	-1.60787700
N	0.11659400	-0.89550200	-0.87656700
N	-0.67803700	-1.07416900	-1.97028100
C	-3.06745900	-0.33967400	-2.40050700
H	-3.87886100	-1.01411500	-2.09711400
H	-2.86449100	-0.47343700	-3.46258700
C	1.50734800	-1.25981700	-0.95591200
C	1.89964300	-2.50188600	-0.44790900
C	2.38623600	-0.35367300	-1.54736100
C	3.25153500	-2.81607700	-0.51635100
C	3.73385000	-0.72062200	-1.59485200
C	4.18166700	-1.93255500	-1.07862300
H	3.59280000	-3.76756900	-0.11548100
H	4.44973000	-0.02134300	-2.01918400

C	1.90894600	0.95244700	-2.12090000
H	1.40702000	0.78500800	-3.07995200
H	1.19729400	1.46499100	-1.46416800
C	0.89700500	-3.42405900	0.19105900
H	0.51132500	-2.99224800	1.12232700
H	0.04291300	-3.60191700	-0.46910300
H	1.35549400	-4.38489100	0.42893200
H	2.75776000	1.61786200	-2.29013300
C	5.64398500	-2.29002200	-1.09978100
H	6.00535200	-2.48661700	-0.08561000
H	6.24187800	-1.47913800	-1.52031300
H	5.81893300	-3.19349200	-1.69170500
H	-4.65849800	-3.33642900	2.45244200
C	5.68837600	1.72250100	0.49653300
C	4.39204200	2.23703600	0.43258300
C	3.33124000	1.54014000	0.99688500
C	3.56364500	0.31161200	1.63103900
C	4.86558600	-0.18729600	1.71607900
C	5.92458900	0.51291400	1.14525500
H	6.51222500	2.26843600	0.04794500
H	4.20722800	3.18515100	-0.06247500
H	2.31925800	1.93880000	0.92925500
H	5.04161700	-1.14111100	2.20699100
H	6.93123600	0.11102100	1.20357300
C	2.44700300	-0.51021700	2.14139400
H	2.69194400	-1.38980800	2.73587400
C	1.20333600	-0.26177200	1.82402300
C	-0.00390500	0.09759000	1.44329500
Br	-0.54231400	3.02522300	0.05192200
O	-0.80841300	0.89166000	2.20947700

H	-0.77920100	1.78382100	1.75413500
Re-TS4			
C	-5.43570200	-0.29357600	0.22786100
C	-4.12737600	0.09044300	0.50991300
C	-3.81515200	0.85938900	1.62558000
C	-4.84985100	1.24035900	2.47641700
C	-6.16569000	0.85918400	2.20141200
C	-6.46884800	0.09380500	1.07673300
C	-5.50298700	-1.10431200	-1.04264600
C	-4.03499900	-1.44632400	-1.38852800
C	-3.18568700	-0.42221400	-0.55165400
H	-2.78843700	1.15157700	1.83264400
H	-6.96144500	1.16115600	2.87456300
H	-7.49328700	-0.20085600	0.87074600
H	-6.08529000	-2.02476700	-0.94084900
H	-3.80457000	-1.31371900	-2.44590000
H	-5.95463300	-0.52075300	-1.85118100
H	-2.83618600	0.36348200	-1.21132800
N	-2.00986200	-1.07670200	0.04588000
O	-3.72648300	-2.80592800	-1.12553200
C	-0.73317500	-0.69625100	0.26389600
C	-2.12149100	-2.36674900	0.48077700
N	-0.13946000	-1.76037800	0.81733100
N	-0.99262600	-2.81076700	0.94760600
C	-3.40331200	-3.08527100	0.22122400
H	-4.18796800	-2.75795900	0.91586900
H	-3.25398100	-4.15951000	0.32334600
C	1.24265600	-1.98178000	1.15537500
C	1.70776500	-1.55054500	2.40211900

C	2.01665800	-2.69131000	0.23806500
C	3.04269100	-1.80914900	2.69929200
C	3.34479000	-2.93750800	0.59451900
C	3.87223100	-2.49978500	1.80752100
H	3.44460600	-1.47090100	3.65123800
H	3.98378200	-3.46722100	-0.10732200
C	1.44557000	-3.17539200	-1.06797100
H	0.78816300	-4.03454000	-0.89833800
H	0.85290700	-2.40614200	-1.57761200
C	0.79796800	-0.83191000	3.36169200
H	0.42931700	0.10905700	2.93614100
H	-0.07584300	-1.44452600	3.60328100
H	1.32338500	-0.60265600	4.28950700
H	2.24986700	-3.48769500	-1.73623300
C	5.31381100	-2.75436200	2.15902200
H	5.79368300	-1.83904700	2.51763000
H	5.87122200	-3.11933200	1.29426500
H	5.39207300	-3.49999600	2.95600200
H	-4.63347300	1.83513100	3.35747800
C	5.35257400	-0.79418500	-1.71581400
C	4.03942500	-0.75776800	-2.19346500
C	3.03120400	-0.20896300	-1.41668400
C	3.34252300	0.30769000	-0.14259200
C	4.66895700	0.27705400	0.32518700
C	5.66980900	-0.27583900	-0.45935700
H	6.13476500	-1.22874700	-2.32999300
H	3.80454600	-1.16230200	-3.17207700
H	2.00601300	-0.19221600	-1.78544000
H	4.89612900	0.67352500	1.31164700
H	6.69103800	-0.30829000	-0.09627800

C	2.32414200	0.83142100	0.73312400
H	2.66309100	1.19146000	1.70750900
C	1.03407000	1.06543100	0.37418200
C	-0.17054400	0.64785500	-0.00227100
Br	-0.57080600	-0.32696100	-2.97088400
O	-1.03024900	1.50276400	-0.62187500
H	-1.02179200	1.18667600	-1.57951800
N	0.88995000	3.77403400	-0.02991800
C	2.15576700	4.21190300	0.60465700
H	2.94572800	3.56821700	0.19981800
H	2.38335100	5.23472800	0.28333700
C	2.13310700	4.11623200	2.12396200
H	1.75341400	3.14853600	2.46787900
H	3.14945300	4.23594100	2.50313400
H	1.51464500	4.89591800	2.57321000
C	-0.34204400	4.30931200	0.60459600
H	-1.17642200	3.81592600	0.10362100
H	-0.34759100	3.97826100	1.64551700
C	-0.46039200	5.82528400	0.51448400
H	-0.49506200	6.16428300	-0.52353900
H	-1.38761100	6.13803500	0.99889300
H	0.36731500	6.33214800	1.01772300
C	0.90246700	3.97553500	-1.50437200
H	-0.13657600	3.94451300	-1.84019800
H	1.29078500	4.98079400	-1.70307800
C	1.71381600	2.92511600	-2.25303700
H	1.83585400	3.24815500	-3.28903100
H	2.71444500	2.78607200	-1.83386400
H	1.19379300	1.96199500	-2.27268200
H	0.95432200	2.40431500	0.19404300

Re-M4

C	-5.15916100	0.95711900	0.04957000
C	-3.78843100	1.09028100	0.25415000
C	-3.26934600	1.50020300	1.47892800
C	-4.15896900	1.77515600	2.51353500
C	-5.53647600	1.64463400	2.31646500
C	-6.04610100	1.23866200	1.08579200
C	-5.46770400	0.51247900	-1.35629500
C	-4.10442700	0.12294800	-1.97133900
C	-3.02150500	0.72822200	-0.99843000
H	-2.19863900	1.61139300	1.62065700
H	-6.21682200	1.86170700	3.13347700
H	-7.11670800	1.13679200	0.93783400
H	-6.15405100	-0.33870200	-1.40081600
H	-3.97347000	0.53982500	-2.96925600
H	-5.92334700	1.32437100	-1.93132000
H	-2.51176200	1.58258800	-1.44345600
N	-1.99519200	-0.28664200	-0.69409900
O	-3.97199100	-1.27783700	-2.15763000
C	-0.69134800	-0.18135400	-0.39911300
C	-2.32529800	-1.60519800	-0.56425900
N	-0.28799800	-1.41398800	-0.08664000
N	-1.29538500	-2.31554500	-0.19218200
C	-3.70362300	-2.00837900	-0.97713500
H	-4.42810300	-1.79787100	-0.17935800
H	-3.72957200	-3.07072700	-1.21667800
C	1.01563100	-1.81967300	0.37514600
C	1.80596100	-2.58045700	-0.49246200
C	1.43594800	-1.38908500	1.63604100
C	3.09189400	-2.89406900	-0.05931800
C	2.73350800	-1.73020700	2.01548500

C	3.57312600	-2.47351500	1.18419300
H	3.73582700	-3.47560500	-0.71331400
H	3.09606400	-1.40364900	2.98646100
C	0.55535900	-0.57125500	2.54527400
H	0.59849900	0.49376000	2.28840800
H	-0.48969100	-0.89099100	2.50214400
C	1.30165500	-3.01030500	-1.84420900
H	0.45921400	-3.70030200	-1.74802200
H	0.95830000	-2.15243600	-2.43200300
H	2.09495900	-3.50843500	-2.40228300
H	0.89582400	-0.66710400	3.57707800
C	4.96541800	-2.83383200	1.62838600
H	4.95332200	-3.76846300	2.19786500
H	5.38543100	-2.05849700	2.27253400
H	5.62832300	-2.97524100	0.77228100
H	-3.78093200	2.09628800	3.47820100
C	6.52824500	2.35490800	-0.72049300
C	5.75969200	3.51545300	-0.66314100
C	4.37826200	3.42436200	-0.54099000
C	3.74965600	2.17203200	-0.49595600
C	4.53540600	1.00771700	-0.54154900
C	5.91462700	1.10218500	-0.65292700
H	7.60760600	2.42384200	-0.80788700
H	6.23660500	4.48847800	-0.70893400
H	3.77381400	4.32544600	-0.49200500
H	4.06832300	0.02975300	-0.45902200
H	6.51695700	0.20028700	-0.67849800
C	2.29724000	2.12154600	-0.38947200
C	1.53363200	1.02937800	-0.60036200
C	0.09528700	1.11212500	-0.39216800

O	-0.55010200	2.12843800	-0.20366000
H	1.96090300	0.08362100	-0.91081900
H	1.79094700	3.04580500	-0.11258300
M5			
C	-2.55880800	2.09619000	2.04404800
C	-1.27923800	2.02980900	1.49700100
C	-0.39927000	3.10578800	1.58462400
C	-0.82177100	4.25947700	2.23924300
C	-2.10354300	4.33164500	2.79104700
C	-2.97934500	3.25334300	2.69604600
C	-3.32753200	0.82492000	1.80618200
C	-2.29631400	-0.17724600	1.24192900
C	-1.04040700	0.68319200	0.84631900
H	0.58993700	3.04968800	1.14134600
H	-2.41818200	5.23699000	3.30021600
H	-3.97456700	3.31126300	3.12725200
H	-3.78313300	0.41934000	2.71528200
H	-2.66315100	-0.69304800	0.35959000
H	-4.13966400	0.98780600	1.08841000
H	-0.93611400	0.74154400	-0.23648100
N	0.19081700	0.06592400	1.39034100
O	-2.01810400	-1.22149900	2.16288400
C	1.48067100	0.14108500	1.01737800
C	0.16735300	-0.57030500	2.59797900
N	2.17648500	-0.42492900	2.00959800
N	1.36897300	-0.88417900	2.99632100
C	-1.16048600	-0.85355700	3.21804500
H	-1.52163300	0.02868700	3.76593400
H	-1.07906500	-1.69242900	3.90923300

C	3.60639800	-0.48434200	2.16956400
C	4.29922100	0.71691900	2.35911100
C	4.22721600	-1.73357500	2.10451300
C	5.68821100	0.64095300	2.41767200
C	5.62102400	-1.74849500	2.16406900
C	6.36498200	-0.57586000	2.30101000
H	6.25594000	1.55760700	2.55538100
H	6.13473200	-2.70381300	2.09716400
C	3.43986700	-3.01096200	1.99668100
H	2.53879100	-2.88429500	1.39256700
H	4.05138500	-3.79716900	1.55044900
C	3.59728000	2.04555100	2.47517200
H	3.43692800	2.49567200	1.48866800
H	2.62830800	1.95655000	2.97462500
H	4.21073400	2.73954700	3.05189000
H	3.12499000	-3.34498900	2.99016000
C	7.87006900	-0.60936700	2.30161800
H	8.25394700	-0.30237200	1.32292500
H	8.24601000	-1.61235400	2.51125300
H	8.27836100	0.08021400	3.04416200
H	-0.15199000	5.10933900	2.31787800
C	7.79074900	0.89901600	-3.30390400
C	6.85699400	1.75092300	-3.88813300
C	5.58926900	1.87492100	-3.33029800
C	5.23554200	1.14226400	-2.18978500
C	6.18721300	0.29024900	-1.60583600
C	7.45295900	0.17127600	-2.16055300
H	8.78191000	0.80116600	-3.73492300
H	7.11606900	2.31849500	-4.77557200
H	4.85587200	2.53649100	-3.78263800

H	5.93829300	-0.27350600	-0.71089900
H	8.18174500	-0.49114600	-1.70474800
C	3.89423600	1.30696600	-1.64136700
C	3.34716600	0.55490700	-0.66401500
C	1.99421700	0.84649400	-0.22198400
O	1.22700500	1.64997800	-0.72937300
H	3.86059600	-0.30391500	-0.25046200
H	3.29013800	2.11262300	-2.05497000
C	-7.86614700	-2.99457700	0.22471000
C	-8.10213700	-1.78289100	-0.42152700
C	-7.04416400	-1.03838500	-0.93396500
C	-5.72886500	-1.48908900	-0.79649300
C	-5.46926100	-2.73205700	-0.15410800
C	-6.56332100	-3.45402900	0.34741200
H	-8.69011500	-3.57656300	0.62363500
H	-9.11544200	-1.41227100	-0.53767800
H	-7.23210500	-0.10336800	-1.44357600
H	-6.36738700	-4.40037400	0.84496100
N	-4.61363800	-0.79151200	-1.29372900
C	-4.36328600	0.54437000	-1.41829200
O	-3.22367100	0.96526800	-1.57287500
O	-5.46100200	1.30173200	-1.33904400
C	-5.39434300	2.74757200	-1.55444400
C	-4.57881200	3.40644800	-0.44848800
H	-3.53952000	3.07490200	-0.47139100
H	-4.60585900	4.49198300	-0.58007700
H	-5.00997600	3.17274500	0.53018400
C	-4.83746500	3.04619200	-2.94233200
H	-5.39720900	2.48788500	-3.69819300
H	-4.95334100	4.11371500	-3.14898800

H	-3.78213500	2.78377500	-3.00980600
C	-6.85846400	3.16044700	-1.46355900
H	-7.27329300	2.87496500	-0.49314900
H	-6.94670900	4.24349600	-1.57907000
H	-7.44052800	2.67542300	-2.25203400
C	-4.13654100	-3.29939500	0.04623500
H	-4.09158000	-4.19963700	0.67240900
N	-3.05676000	-2.79828700	-0.46623200
C	0.62109400	-3.25978500	-0.55117200
C	-0.75173600	-1.54985200	-1.64405300
C	1.73296100	-2.76593300	-1.17384200
H	0.71258400	-4.11732100	0.11085300
C	0.36033500	-1.05728800	-2.26471400
H	-1.70425400	-1.05731900	-1.81154700
C	1.62414100	-1.66276800	-2.05618100
H	2.70852900	-3.21395400	-1.02110900
H	0.29872800	-0.19207300	-2.91483600
N	2.74222500	-1.23388300	-2.78358500
O	2.61516900	-0.30897100	-3.60100100
O	3.84428700	-1.76366700	-2.56882500
H	-3.75781200	-1.36207400	-1.26203400
C	-0.69261800	-2.71381400	-0.78912900
C	-1.81786800	-3.30700000	-0.23633800
H	-1.71052100	-4.18464600	0.40608600
TS5RR			
C	4.78175600	-4.46364600	-0.60622100
C	4.13952400	-4.64240300	-1.82867700
C	2.94534400	-3.97839200	-2.09356600
C	2.35936200	-3.13675600	-1.13679000

C	3.02763100	-2.95413000	0.08855500
C	4.22382300	-3.60863400	0.34609100
H	5.71740800	-4.97319800	-0.39977200
H	4.56893500	-5.29816700	-2.57950200
H	2.44916800	-4.11605100	-3.05120800
H	2.62540900	-2.27404400	0.83484000
H	4.73080400	-3.44501600	1.29234800
C	1.08660100	-2.48960400	-1.43723600
C	0.25070400	-1.98362900	-0.46452400
C	-1.13701800	-1.74844000	-0.65059800
O	-1.82809700	-1.81256900	-1.67951900
H	0.63637200	-1.87018800	0.53710000
H	0.66087300	-2.67807800	-2.42152000
C	-3.22076000	2.17101700	-3.10730900
C	-3.03116600	3.41833100	-2.51732800
C	-1.82957700	3.73683000	-1.88897800
C	-0.78732600	2.80578200	-1.83315600
C	-0.96166500	1.53339600	-2.44693100
C	-2.18806700	1.24549000	-3.06535600
H	-4.15400900	1.92633400	-3.60341000
H	-3.81987700	4.16364000	-2.55067900
H	-1.69941500	4.71204700	-1.44398300
H	-2.31105500	0.26469400	-3.51676300
N	0.44865600	3.03521200	-1.21622100
C	0.88704800	4.00722900	-0.36229900
O	2.03991600	4.03380700	0.03741800
O	-0.07652900	4.86026200	0.00737200
C	0.21536500	5.97927100	0.90207600
C	1.23632900	6.90949500	0.25700800
H	2.21064900	6.42784500	0.17700600

H	1.33380300	7.81193400	0.86682400
H	0.89617500	7.20374400	-0.73992100
C	0.67634600	5.46415500	2.26188400
H	-0.04634000	4.74199800	2.65539900
H	0.73274200	6.30385900	2.96026200
H	1.65818800	4.99408200	2.19435200
C	-1.14068800	6.66428700	1.02303100
H	-1.48162600	7.01292100	0.04429900
H	-1.06417400	7.52445200	1.69241700
H	-1.88176900	5.96926600	1.42734800
C	0.06066600	0.50090600	-2.53149200
H	-0.23812100	-0.39034300	-3.09683900
N	1.26992200	0.59908800	-2.07024300
C	4.50556700	-1.16654400	-2.30333000
C	3.68503500	0.27326700	-0.52206500
C	5.69568500	-1.33281300	-1.63429000
H	4.35151000	-1.66338600	-3.25623200
C	4.87667300	0.11218800	0.15210000
H	2.89271400	0.87971300	-0.09131300
C	5.87512100	-0.69903100	-0.39907300
H	6.48648000	-1.95541900	-2.03425600
H	5.05216100	0.59064300	1.10790800
N	7.09339900	-0.90999000	0.32996300
O	7.23172400	-0.35823800	1.41968200
O	7.95249100	-1.64037600	-0.15840900
H	1.14255400	2.29452600	-1.38132500
C	3.45645300	-0.37629700	-1.76494300
C	2.19404500	-0.33707200	-2.41061800
H	2.06130500	-0.90234800	-3.33392500
C	-6.41709900	-1.89052600	-0.34407200

C	-5.09151600	-1.51048700	-0.53292100
C	-4.75028800	-0.25150400	-1.01450500
C	-5.77888600	0.64405400	-1.29651200
C	-7.11334200	0.27208800	-1.11213400
C	-7.44310900	-0.99713900	-0.64156000
C	-6.50977300	-3.29739600	0.18899200
C	-5.06814600	-3.66830700	0.60793100
C	-4.14676300	-2.61152700	-0.10798500
H	-3.70863000	0.02156100	-1.17046400
H	-7.90261100	0.98358100	-1.33290900
H	-8.48137600	-1.27921400	-0.49549000
H	-7.18415800	-3.39488400	1.04513100
H	-4.79647100	-4.67433100	0.28925600
H	-6.86660900	-3.98555700	-0.58384200
H	-3.59956500	-3.04311100	-0.94509400
N	-3.15409900	-2.07646200	0.83520800
O	-4.90682300	-3.69348000	2.01931000
C	-1.90529200	-1.60990800	0.65227400
C	-3.48010800	-1.86768300	2.14618400
N	-1.53231900	-1.13813500	1.84891600
N	-2.50474000	-1.29712700	2.79116700
C	-4.78356000	-2.42007300	2.62330800
H	-5.61378200	-1.75216900	2.35790100
H	-4.76273700	-2.55557600	3.70409300
C	-0.33491700	-0.40659400	2.17339300
C	0.69735200	-1.06572800	2.84346100
C	-0.27455000	0.93073800	1.77698900
C	1.86446300	-0.33835000	3.07966900
C	0.90706600	1.61404000	2.04657500
C	1.98578100	0.99492500	2.68288300

H	2.69519000	-0.82790300	3.58150400
H	1.00156400	2.65445700	1.75201400
C	-1.44448300	1.58898000	1.09772800
H	-1.59721400	1.17520000	0.09399700
H	-2.36740600	1.43643900	1.66685800
C	0.56188400	-2.50945000	3.24884100
H	0.39729700	-3.15262300	2.37608100
H	1.46620000	-2.85086100	3.75434400
H	-0.28849600	-2.65031100	3.92210500
H	-1.27366000	2.66215600	0.98659400
C	3.24066800	1.78491500	2.94361600
H	3.07192100	2.52021500	3.73697600
H	3.53594800	2.33939900	2.04710500
H	4.06550100	1.13970800	3.25324000
H	-5.53809000	1.63907300	-1.65592600
M6RR			
C	-2.77812200	-5.98072000	2.10992000
C	-2.25649400	-5.38024100	3.25443400
C	-1.55194000	-4.18405500	3.15289400
C	-1.35875800	-3.56131700	1.91488700
C	-1.87616200	-4.17953900	0.77461600
C	-2.58047800	-5.37796900	0.87028200
H	-3.32786400	-6.91359200	2.18348500
H	-2.39376500	-5.84557700	4.22565000
H	-1.14568400	-3.72014500	4.04947500
H	-1.73620500	-3.71877000	-0.19871100
H	-2.97868600	-5.83966200	-0.02805600
C	-0.65568100	-2.21289700	1.86897500
C	-0.00852600	-1.88352700	0.55861100

C	1.34036600	-1.65563800	0.52013700
O	2.17883500	-1.64014300	1.48631900
H	-0.60859900	-1.84171100	-0.34204700
H	0.14819500	-2.25661000	2.61215200
C	2.69894000	3.08979000	3.33122100
C	2.05994500	4.24313500	2.88102900
C	0.79218000	4.18325800	2.31408800
C	0.12776000	2.95740000	2.18841500
C	0.75867700	1.78161800	2.66461500
C	2.04524800	1.87131800	3.20857700
H	3.68862100	3.14105800	3.77221100
H	2.54776000	5.20803400	2.97656700
H	0.30693300	5.08760800	1.97443700
H	2.52760600	0.95432600	3.53835600
N	-1.15697100	2.83842600	1.63552400
C	-1.74889300	3.53370500	0.61317300
O	-2.82864500	3.20256200	0.15251700
O	-1.00867800	4.56403100	0.18929900
C	-1.53986800	5.52841300	-0.77381000
C	-2.76629500	6.21396000	-0.18300000
H	-3.58395700	5.50432100	-0.05324800
H	-3.09330200	7.01058400	-0.85673600
H	-2.51832900	6.66041600	0.78420700
C	-1.84428100	4.85380600	-2.10687600
H	-0.98273000	4.26659900	-2.44094800
H	-2.04078900	5.62391900	-2.85812800
H	-2.71767700	4.20616000	-2.03071100
C	-0.38552000	6.51167100	-0.92410100
H	-0.14816600	6.97202400	0.03888400
H	-0.65873800	7.29984200	-1.62978700

H	0.50484900	5.99837200	-1.29715700
C	0.16282200	0.43135900	2.60154400
H	0.89430700	-0.38205400	2.68412300
N	-1.08859800	0.24365400	2.44541200
C	-3.97697000	-1.90690700	1.77051100
C	-3.02168500	-0.10302200	0.48668500
C	-5.13486900	-1.85265400	1.00925400
H	-3.89840400	-2.63678100	2.57099400
C	-4.18091000	-0.01601300	-0.27341800
H	-2.20852500	0.58600000	0.28398800
C	-5.21523100	-0.90052100	-0.00176700
H	-5.96736700	-2.51966100	1.19349000
H	-4.28802400	0.73461700	-1.04615000
N	-6.44139700	-0.81939600	-0.79689300
O	-6.49908300	0.02020800	-1.68178400
O	-7.34576100	-1.59601800	-0.53915900
H	-1.62664000	1.95957500	1.86987800
C	-2.90858300	-1.03565100	1.51976800
C	-1.64980600	-1.09886600	2.36442900
H	-1.95854300	-1.38059100	3.38107200
C	6.41039900	-0.57004200	-0.00363400
C	5.04184800	-0.57289700	0.24979900
C	4.39747200	0.52967200	0.80298600
C	5.15827900	1.66028600	1.08939700
C	6.53360900	1.67285500	0.83791400
C	7.17031000	0.55850800	0.29601000
C	6.85863900	-1.88215300	-0.59498700
C	5.55472400	-2.63712300	-0.94922200
C	4.41093900	-1.87701300	-0.18236300
H	3.33140900	0.48703800	1.01472200

H	7.11164000	2.56257100	1.06692900
H	8.23843800	0.57331000	0.10090100
H	7.47797100	-1.76705100	-1.49017800
H	5.58847200	-3.67647900	-0.62302200
H	7.44381800	-2.45768000	0.12927900
H	4.01934700	-2.44418200	0.65909000
N	3.27649900	-1.60724700	-1.08075600
O	5.34632900	-2.72096500	-2.35265700
C	1.96167600	-1.42649100	-0.83145300
C	3.49124800	-1.31899200	-2.39847600
N	1.44592200	-1.03565200	-2.00576500
N	2.39043300	-0.97583900	-2.99481800
C	4.86667000	-1.52815300	-2.94079200
H	5.51049400	-0.66747200	-2.71262000
H	4.82920600	-1.66949000	-4.02068400
C	0.11233500	-0.61253900	-2.33822800
C	-0.66766400	-1.46979400	-3.12054100
C	-0.31138300	0.65059500	-1.92601800
C	-1.91797500	-1.00706100	-3.51976800
C	-1.57666100	1.06438200	-2.34675600
C	-2.38045600	0.26089700	-3.15595000
H	-2.54450900	-1.64866100	-4.13458500
H	-1.94580500	2.03210900	-2.01525100
C	0.54009200	1.50860900	-1.03073200
H	0.51391900	1.11795400	-0.00555900
H	1.58584400	1.51966700	-1.35413500
C	-0.16629100	-2.83891100	-3.49474600
H	0.71097300	-2.77409300	-4.14499100
H	0.12920100	-3.40000300	-2.60154900
H	-0.94295600	-3.40199700	-4.01381400

H	0.17664000	2.53921000	-1.01056700
C	-3.72563600	0.74011300	-3.63650300
H	-3.75325100	0.77747900	-4.72949100
H	-3.94781200	1.74080300	-3.25700800
H	-4.52559400	0.06933400	-3.30817100
H	4.67683500	2.53644800	1.51204600

TS6RR

C	-3.12773200	2.35218700	4.32016700
C	-2.16441100	3.22704600	3.82618400
C	-1.57330600	2.98896700	2.58631800
C	-1.93371800	1.87703300	1.82144100
C	-2.90884900	1.00802500	2.32635300
C	-3.49897000	1.24070700	3.56416900
H	-3.58734400	2.53279300	5.28657600
H	-1.86900400	4.09591000	4.40589600
H	-0.82021000	3.67270700	2.20194500
H	-3.22082500	0.14634800	1.74096700
H	-4.25160300	0.55368500	3.93884000
C	-1.29405300	1.67450600	0.46360800
C	-0.83970800	0.27521100	0.17290400
C	0.51506900	-0.04997000	0.38573200
O	1.49109600	0.71232700	0.34747700
H	-1.56695300	-0.51393500	0.32209300
H	-0.41038300	2.32048000	0.39509100
C	1.89436500	-0.89957300	-3.97906100
C	2.86298500	0.11385100	-3.91511300
C	2.63053400	1.29469800	-3.23400800
C	1.38803500	1.55131300	-2.59747800
C	0.40680600	0.50943200	-2.66919900

C	0.68071000	-0.68444400	-3.35343700
H	2.08577900	-1.81938100	-4.52117600
H	3.81250000	-0.02126500	-4.42694200
H	3.39053200	2.06529800	-3.19999700
H	-0.10496600	-1.43547600	-3.40397000
N	1.01505800	2.73998100	-2.03664900
C	1.79879000	3.50806500	-1.26296800
O	1.40831000	4.54811100	-0.72956800
O	3.07064800	3.04155700	-1.07645300
C	3.92693200	3.62541100	-0.07086200
C	3.25203900	3.60597700	1.30067100
H	2.47675100	4.36785100	1.36916800
H	4.00140300	3.78084500	2.07923200
H	2.79512200	2.62402900	1.45813000
C	4.34939600	5.03386000	-0.48257200
H	4.83062400	5.00774300	-1.46534100
H	5.06757200	5.43202800	0.24108700
H	3.48060000	5.69016400	-0.52664600
C	5.13443100	2.69092500	-0.06041600
H	4.83566500	1.68904200	0.26200600
H	5.89957600	3.07092200	0.62261300
H	5.56571500	2.61390200	-1.06311800
C	-0.89220200	0.63058400	-2.01950100
H	-1.54082700	-0.23602000	-2.11896700
N	-1.44275400	1.86446600	-1.90127700
C	-4.62783700	2.45777300	-0.15200700
C	-3.97992400	0.29282400	-0.97912400
C	-5.93038900	2.01894500	0.03701600
H	-4.37233900	3.47972700	0.11079900
C	-5.27789400	-0.16771600	-0.79886400

H	-3.24826700	-0.41051300	-1.35554400
C	-6.23012400	0.70360800	-0.28980000
H	-6.69945600	2.67129400	0.43067900
H	-5.55339300	-1.18664400	-1.04172400
N	-7.59613200	0.21334800	-0.08512300
O	-7.82933700	-0.95423200	-0.35019300
O	-8.42521500	0.99710600	0.34317100
H	-0.64326000	2.55166100	-1.98006700
C	-3.63152000	1.61062600	-0.65352300
C	-2.22262400	2.16049400	-0.72102000
H	-2.30261400	3.24956200	-0.65618500
C	5.48784800	-1.41403900	1.19890500
C	4.25112000	-1.06510100	0.66239600
C	4.08639100	-0.80567600	-0.69594700
C	5.20488500	-0.90747500	-1.51895500
C	6.45156200	-1.25220700	-0.99013300
C	6.60385900	-1.50510300	0.37107400
C	5.40286300	-1.63303800	2.68772100
C	3.89342400	-1.60128300	3.02302600
C	3.19699300	-1.00561000	1.74322500
H	3.12180500	-0.49968700	-1.09668200
H	7.31154800	-1.32250800	-1.64860600
H	7.57370800	-1.77425900	0.77852900
H	5.83541700	-2.58546800	3.01052400
H	3.68380900	-0.96260300	3.88076800
H	5.92746900	-0.84089100	3.23063600
H	2.84514100	0.00949500	1.91570100
N	2.02442800	-1.81340600	1.36458000
O	3.39597400	-2.87430400	3.41003700
C	0.87722500	-1.49368400	0.73246000

C	2.02198100	-3.16397800	1.56211500
N	0.23038100	-2.65799200	0.59129300
N	0.93188500	-3.70680000	1.10409300
C	3.15475200	-3.75662500	2.33282900
H	4.03883700	-3.88023100	1.69225400
H	2.86774700	-4.72589800	2.73965500
C	-1.01281400	-2.92451500	-0.08324900
C	-2.20053300	-2.82516500	0.64305600
C	-0.94867900	-3.34206400	-1.41469700
C	-3.38742100	-3.04959200	-0.05468800
C	-2.16328900	-3.54362200	-2.06992500
C	-3.38698400	-3.38247400	-1.41209100
H	-4.33195300	-2.97086800	0.47802700
H	-2.15352700	-3.85638900	-3.11114500
C	0.37368000	-3.65819100	-2.06240000
H	1.11810800	-2.87560900	-1.89059300
H	0.76870000	-4.59163500	-1.64896200
C	-2.18244800	-2.51741100	2.11708800
H	-3.19887400	-2.42187800	2.50251600
H	-1.67904200	-3.31949800	2.66579700
H	-1.64836400	-1.58576300	2.33208200
H	0.25678000	-3.78612700	-3.14023300
C	-4.67943600	-3.57949700	-2.16094200
H	-4.65030500	-4.49380400	-2.75883100
H	-4.85466500	-2.74712300	-2.85110300
H	-5.53071500	-3.64171500	-1.47910900
H	5.10524900	-0.70605800	-2.57975400
M7RR			
C	-2.41599000	2.96822500	3.97802000

C	-1.44487100	3.67849500	3.27631100
C	-1.10920800	3.30555000	1.97638300
C	-1.74269600	2.22567000	1.35364800
C	-2.71605200	1.51838900	2.07133300
C	-3.04959200	1.88434400	3.37213300
H	-2.67704200	3.25427800	4.99196600
H	-0.94316100	4.52032100	3.74317900
H	-0.33945000	3.84233100	1.42577500
H	-3.23242400	0.68214500	1.60442400
H	-3.80845500	1.32526800	3.91118900
C	-1.32541200	1.85612000	-0.04695100
C	-0.90173000	0.39209300	-0.22294100
C	0.43094100	0.12874100	0.41745400
O	1.25316800	0.98447800	0.64272100
H	-1.64576300	-0.25996000	0.24145900
H	-0.46763200	2.47137500	-0.32890400
C	1.66055000	-1.51459200	-3.97949500
C	2.64273000	-0.52530700	-4.03108700
C	2.47831000	0.68222700	-3.36459400
C	1.31504700	0.95646000	-2.60605600
C	0.33112000	-0.07431700	-2.53485200
C	0.50825900	-1.26356100	-3.24064500
H	1.78017900	-2.45052100	-4.51530100
H	3.54375500	-0.68904700	-4.61794500
H	3.24184200	1.44879800	-3.42660100
H	-0.28915500	-2.00326600	-3.21424600
N	0.98556700	2.15541000	-2.02937100
C	1.82502700	2.96402100	-1.38950400
O	1.47486700	4.02572200	-0.85517900
O	3.13304800	2.52802300	-1.30042800

C	4.11844700	3.30043000	-0.58581000
C	3.76259500	3.38598400	0.89714500
H	2.84214700	3.95062700	1.04051900
H	4.57796400	3.86499800	1.44875700
H	3.62564500	2.37357000	1.29123200
C	4.29801900	4.68271300	-1.21429900
H	4.51225600	4.57508900	-2.28246000
H	5.14538400	5.19237800	-0.74506300
H	3.39921600	5.28387300	-1.09068900
C	5.40568500	2.49558400	-0.75489100
H	5.31561600	1.51596700	-0.27756500
H	6.24437400	3.03257000	-0.30185400
H	5.62116600	2.34246900	-1.81700300
C	-0.97326200	0.13338000	-1.78584500
H	-1.55476900	-0.78934300	-1.90717200
N	-1.74254300	1.27234800	-2.33194500
C	-4.59215400	2.42808400	-0.17613100
C	-4.21515800	0.31592500	-1.27594900
C	-5.86338600	2.02328800	0.20300800
H	-4.23872600	3.41459400	0.10931700
C	-5.48228900	-0.11373100	-0.89923700
H	-3.59138800	-0.33008700	-1.88434700
C	-6.27990700	0.74622200	-0.15694600
H	-6.52209700	2.66934300	0.76958300
H	-5.85828300	-1.09018800	-1.17923000
N	-7.61112200	0.29348900	0.25167400
O	-7.94386500	-0.84368900	-0.04047700
O	-8.31738800	1.07351300	0.86772400
H	-1.03394400	1.89470700	-2.71737400
C	-3.74642700	1.57822600	-0.90121400

C	-2.33941700	2.02732600	-1.22617800
H	-2.37996800	3.08658800	-1.50026800
C	5.41313200	-1.18416300	1.29375000
C	4.16092200	-0.87517000	0.76876200
C	3.93786600	-0.78792300	-0.60173100
C	5.01481900	-1.01633100	-1.45418100
C	6.27883500	-1.31355300	-0.93881600
C	6.48918400	-1.39720600	0.43624700
C	5.38010100	-1.24385100	2.79945800
C	3.88264300	-1.16699400	3.18247400
C	3.15034900	-0.68576500	1.87551400
H	2.96375200	-0.52725000	-1.01084900
H	7.10704200	-1.48465300	-1.61908900
H	7.47144100	-1.63727300	0.83178400
H	5.82035500	-2.16070600	3.20380100
H	3.70720700	-0.44732900	3.98144100
H	5.92449200	-0.40312700	3.24020800
H	2.81769700	0.34366700	1.97433200
N	1.95802500	-1.51227500	1.59886300
O	3.38337200	-2.39036600	3.70011600
C	0.82180100	-1.26944200	0.91200600
C	1.96432600	-2.83747600	1.91292900
N	0.18686700	-2.44703700	0.86515600
N	0.88301100	-3.42866500	1.48653400
C	3.10313700	-3.36685000	2.72028700
H	3.96812100	-3.56979200	2.07365400
H	2.80929400	-4.28692300	3.22459700
C	-1.05645400	-2.79242000	0.22145700
C	-2.25195500	-2.50114900	0.88208000
C	-0.98416800	-3.48169300	-0.99155500

C	-3.43263700	-2.79759000	0.20386400
C	-2.19543800	-3.75951500	-1.62444700
C	-3.42082000	-3.39882200	-1.05798700
H	-4.38209900	-2.56777400	0.68050200
H	-2.18037900	-4.27975200	-2.57889200
C	0.33100400	-3.97191500	-1.53857500
H	1.11142900	-3.20728100	-1.48959800
H	0.66926400	-4.83782000	-0.96105000
C	-2.25512400	-1.94021200	2.28007200
H	-3.27651400	-1.74193800	2.60918400
H	-1.80288400	-2.65550700	2.97415700
H	-1.69304300	-1.00421800	2.36170700
H	0.22353000	-4.27557500	-2.58130900
C	-4.70556900	-3.66521700	-1.79646300
H	-4.85586200	-2.91532500	-2.58088600
H	-5.56628000	-3.63229200	-1.12490800
H	-4.68350300	-4.64268100	-2.28412300
H	4.86459500	-0.94606500	-2.52597100

M8RR

C	-2.70037400	3.95677600	3.17112900
C	-1.94955800	4.56872000	2.17150800
C	-1.51817600	3.82904500	1.07239200
C	-1.82825200	2.47339200	0.94636200
C	-2.58319100	1.87070100	1.95809300
C	-3.01226200	2.60247700	3.06017000
H	-3.03531500	4.52698600	4.03178300
H	-1.69362800	5.62107000	2.24753900
H	-0.92445900	4.30932000	0.29795400
H	-2.85319400	0.82046200	1.88236700

H	-3.59518500	2.11398600	3.83506700
C	-1.42096100	1.74678100	-0.31003000
C	-0.95803600	0.28439300	-0.18554100
C	0.47088000	0.26345500	0.42622100
O	0.56569000	0.96440800	1.49354000
H	-1.61483700	-0.23071100	0.51790200
H	-0.60059900	2.30970400	-0.77686200
C	1.11020700	-1.55773700	-4.33903200
C	2.32913300	-0.98034800	-3.97769000
C	2.43341700	-0.23469100	-2.81362900
C	1.31679400	-0.02873600	-1.98343200
C	0.09164600	-0.59292100	-2.35528900
C	0.00586900	-1.35548600	-3.52640100
H	1.02894500	-2.15254000	-5.24258900
H	3.20642100	-1.11769900	-4.60186300
H	3.38051600	0.22241600	-2.54794200
H	-0.95764500	-1.78881000	-3.78585200
N	1.43697700	0.67458600	-0.75727300
C	2.17190700	1.84183900	-0.67273500
O	2.65015600	2.30493600	0.34349200
O	2.28846400	2.42334800	-1.88545400
C	3.27403900	3.47234100	-2.10642100
C	4.66821900	2.98878800	-1.71372100
H	4.74058500	2.80597300	-0.64137300
H	5.40218900	3.74979900	-1.99369200
H	4.91590600	2.06655900	-2.24959000
C	2.86957600	4.73864400	-1.35766600
H	1.83875600	5.00441700	-1.61049300
H	3.52092500	5.56371400	-1.66036000
H	2.94701400	4.59690000	-0.28028000

C	3.19273100	3.69136400	-3.61311900
H	3.42843300	2.76467700	-4.14404300
H	3.90315600	4.46376600	-3.91846000
H	2.18580700	4.00891800	-3.89669300
C	-1.17428400	-0.30507800	-1.59727000
H	-1.74002300	-1.23949100	-1.51952900
N	-1.99873600	0.66990300	-2.36770800
C	-4.69008000	2.22442300	-0.27029400
C	-4.35183900	-0.05787200	-0.96896600
C	-5.92424500	1.89378600	0.26831000
H	-4.33668800	3.24941600	-0.20302200
C	-5.58149000	-0.41405600	-0.42694200
H	-3.75849800	-0.80681400	-1.48177100
C	-6.34346600	0.57066700	0.18660600
H	-6.55435400	2.63343700	0.74573100
H	-5.95707800	-1.42871500	-0.48513400
N	-7.64071900	0.20397400	0.75911900
O	-7.99033800	-0.96258000	0.68605600
O	-8.30513900	1.08290600	1.28197300
H	-1.38419800	1.15478900	-3.01615100
C	-3.88412200	1.25684000	-0.88380100
C	-2.52198000	1.65225500	-1.41763500
H	-2.62730700	2.62351000	-1.91203700
C	5.53706600	-0.26185500	2.00112800
C	4.44858500	-0.44681200	1.15114600
C	4.61598800	-0.75930200	-0.18934200
C	5.91289700	-0.83888700	-0.69633600
C	7.00944000	-0.61815700	0.13908800
C	6.83045800	-0.33797000	1.49496400
C	5.06088900	-0.01724800	3.41422300

C	3.58537700	-0.46845100	3.39909600
C	3.15642000	-0.27910500	1.91310900
H	3.75265800	-0.96464100	-0.81532100
H	8.01392800	-0.68650600	-0.26613400
H	7.68871600	-0.19857800	2.14563000
H	5.62217600	-0.57139500	4.17074700
H	2.96048100	0.13284900	4.06093300
H	5.11959600	1.04745700	3.66681800
H	2.70402100	0.70478200	1.75482900
N	2.16241000	-1.27793400	1.53660000
O	3.43408400	-1.80899100	3.87184900
C	1.02620400	-1.18586400	0.81650700
C	2.29486700	-2.56261900	1.96906100
N	0.52996600	-2.42701700	0.84274600
N	1.30252100	-3.30047100	1.56669100
C	3.42692200	-2.84358800	2.90312000
H	4.37418700	-2.90193700	2.35234200
H	3.25730900	-3.78423600	3.42682600
C	-0.66359600	-2.91674600	0.21661100
C	-1.88350200	-2.72033800	0.86753600
C	-0.53297500	-3.59559500	-0.99739300
C	-3.03024100	-3.14908100	0.20061900
C	-1.70946200	-4.01300000	-1.61842300
C	-2.96284000	-3.77612700	-1.04667500
H	-3.99875600	-2.99613100	0.67053700
H	-1.64494600	-4.52900400	-2.57326800
C	0.82455400	-3.87780300	-1.58400900
H	1.44274800	-2.97389400	-1.61912700
H	1.35203000	-4.62031300	-0.97692900
C	-1.95331900	-2.10890800	2.24417400

H	-2.97949200	-1.81770200	2.47815100
H	-1.62693600	-2.83645100	2.99451700
H	-1.31181200	-1.22766400	2.34884800
H	0.72903900	-4.26141700	-2.60079900
C	-4.22389400	-4.17330400	-1.76883900
H	-4.54651900	-3.37177400	-2.44252600
H	-5.03798800	-4.36405400	-1.06599000
H	-4.06859100	-5.06896100	-2.37435200
H	6.07058900	-1.08298900	-1.74246800
TS7RR			
C	2.82548800	4.26013900	-3.12231000
C	2.35909000	4.90628900	-1.97999400
C	1.88290600	4.16016300	-0.90530900
C	1.87029700	2.76233600	-0.94372800
C	2.32607300	2.12732800	-2.10134700
C	2.80028200	2.86840800	-3.17995600
H	3.19640600	4.83597300	-3.96416500
H	2.36235600	5.99045200	-1.92574300
H	1.52274000	4.66845900	-0.01349500
H	2.31689900	1.04428200	-2.16775300
H	3.15135800	2.35538100	-4.06998500
C	1.47031400	2.02135200	0.30754500
C	0.93285700	0.58249400	0.18258500
C	-0.51123900	0.64204000	-0.33602700
O	-0.69789600	1.25549100	-1.39589900
H	1.51330000	0.03404000	-0.56318400
H	0.69221200	2.61344200	0.81106800
C	-1.01138100	-1.48036600	4.29497400
C	-2.27180900	-1.01003100	3.92339500

C	-2.42394000	-0.23624000	2.78293700
C	-1.31419900	0.10537600	1.98970000
C	-0.05525200	-0.38254500	2.35023100
C	0.08067000	-1.16557300	3.50165600
H	-0.88984300	-2.08990500	5.18407500
H	-3.14528200	-1.25340000	4.51965500
H	-3.40788800	0.12477400	2.50693100
H	1.07289400	-1.52960000	3.75737000
N	-1.46745100	0.86598400	0.79922600
C	-2.44393800	1.85434000	0.69252100
O	-2.97719200	2.20794000	-0.33617300
O	-2.70202500	2.38900300	1.89777300
C	-3.87486400	3.23553800	2.09254200
C	-5.14425000	2.50041100	1.66868500
H	-5.15961600	2.30673400	0.59579300
H	-6.01154300	3.11350000	1.92901300
H	-5.23233100	1.54887100	2.20306600
C	-3.69528000	4.55563900	1.35018200
H	-2.73930500	5.00958900	1.62648500
H	-4.49739800	5.24202900	1.63633900
H	-3.72131900	4.40557800	0.27138800
C	-3.87038600	3.46040100	3.60032000
H	-3.93698600	2.50329000	4.12544200
H	-4.72272200	4.08094500	3.88760000
H	-2.94983300	3.96352900	3.90763000
C	1.18503000	-0.03258600	1.57930400
H	1.77110800	-0.95039900	1.46157600
N	2.00524600	0.93685100	2.35736600
C	4.70916100	2.12952000	0.01234000
C	4.36350300	0.04699600	1.17463000

C	5.91182000	1.66054000	-0.49548000
H	4.39004200	3.13656200	-0.23641700
C	5.56545800	-0.44244600	0.67547800
H	3.78223000	-0.56239500	1.85687400
C	6.31433200	0.37277700	-0.16031600
H	6.53421300	2.27326500	-1.13519600
H	5.92593100	-1.43091000	0.93461300
N	7.58041100	-0.13468400	-0.69413100
O	7.91458400	-1.26876300	-0.39330900
O	8.23526800	0.60109400	-1.41303400
H	1.37666100	1.47005800	2.95350000
C	3.90893300	1.32583700	0.83899000
C	2.59298900	1.85742100	1.38407300
H	2.79172600	2.82285700	1.86182600
C	-5.44795800	-0.62965700	-2.06697000
C	-4.33992200	-0.71772800	-1.22873400
C	-4.46514200	-1.04518100	0.11365400
C	-5.74305200	-1.24854600	0.63243900
C	-6.86362600	-1.13067800	-0.19325700
C	-6.72422200	-0.83002700	-1.54885900
C	-5.01816500	-0.31334300	-3.47977800
C	-3.48744400	-0.53317100	-3.48540600
C	-3.07218700	-0.40626200	-1.98532300
H	-3.57967000	-1.15917700	0.73392600
H	-7.85366900	-1.29160600	0.22140300
H	-7.59876700	-0.76638600	-2.18961700
H	-5.49385400	-0.94706000	-4.23350900
H	-2.97271600	0.21751900	-4.08667200
H	-5.24658200	0.72806500	-3.73160600
H	-2.71586700	0.60456800	-1.76854800

N	-1.99844400	-1.33339900	-1.65442000
O	-3.12211000	-1.77635700	-4.08212400
C	-0.95719500	-1.20400100	-0.79722700
C	-1.99104600	-2.58793900	-2.19403700
N	-0.36733600	-2.40466300	-0.88855000
N	-0.98475400	-3.28124300	-1.75242000
C	-3.03794600	-2.89401300	-3.21492700
H	-3.99854900	-3.10494900	-2.72560700
H	-2.74744500	-3.75692200	-3.81399100
C	0.79652500	-2.82955600	-0.17002100
C	2.05644700	-2.60678200	-0.72926900
C	0.60762800	-3.45250100	1.06746300
C	3.16640800	-2.98527000	0.02700700
C	1.74739000	-3.80645600	1.78737400
C	3.03133100	-3.56722900	1.28876300
H	4.15982500	-2.82043900	-0.38328700
H	1.62966600	-4.27886100	2.75973300
C	-0.78041500	-3.73066000	1.57811100
H	-1.37554100	-2.81172400	1.62107900
H	-1.29787900	-4.43067600	0.91433200
C	2.22502500	-2.00854600	-2.10191700
H	3.17775100	-1.47660300	-2.16900900
H	2.22372000	-2.79455200	-2.86400200
H	1.41783800	-1.31394200	-2.35112800
H	-0.74296600	-4.15872100	2.58097800
C	4.25067400	-3.90819900	2.10592100
H	4.53981500	-3.06027500	2.73721600
H	5.10154900	-4.15027200	1.46464900
H	4.06147500	-4.75753200	2.76606900
H	-5.86749800	-1.50551900	1.68014100

PRR

C	1.66545600	3.57338200	1.71747400
C	1.18526600	2.72049800	2.70934500
C	0.74562500	1.44420000	2.37304400
C	0.78796900	0.99448100	1.04927500
C	1.26103700	1.86086300	0.06076900
C	1.69583700	3.14167400	0.39419400
H	2.00671500	4.57101800	1.97418900
H	1.14879000	3.05028800	3.74275500
H	0.37024900	0.77872000	3.14726000
H	1.28661800	1.54603300	-0.97759700
H	2.05964300	3.80391100	-0.38488200
C	0.38648800	-0.43022300	0.76513900
C	-0.07860100	-0.77610400	-0.66043700
C	-1.34441000	-0.05335400	-1.02722600
O	-1.35118000	0.93875500	-1.72738600
H	0.67667200	-0.47316300	-1.38993300
H	-0.42649500	-0.70037500	1.45207600
C	-2.83824700	-4.52674400	0.96737100
C	-3.91136100	-3.64733000	1.07749600
C	-3.80191900	-2.34430200	0.61146900
C	-2.61080500	-1.90302300	0.02474300
C	-1.50522600	-2.76178400	-0.04562400
C	-1.64933500	-4.07306800	0.41140200
H	-2.92466100	-5.55094000	1.31249200
H	-4.84518300	-3.97342500	1.52288500
H	-4.65051700	-1.67661100	0.69039400
H	-0.81013900	-4.75828100	0.31841900
N	-2.51570200	-0.57122000	-0.47531600

C	-3.70871600	0.19631700	-0.69308600
O	-4.68306100	-0.25203900	-1.24131800
O	-3.55494200	1.39744600	-0.17537200
C	-4.49661800	2.47755700	-0.49802200
C	-5.85429200	2.17747800	0.12431700
H	-6.32008500	1.31086700	-0.34540000
H	-6.50634500	3.04504100	-0.00952200
H	-5.74418100	1.99231200	1.19651400
C	-4.56400700	2.65290100	-2.01066700
H	-3.55231600	2.73784700	-2.41580700
H	-5.11308100	3.57024000	-2.23824800
H	-5.07238000	1.81482200	-2.48895500
C	-3.84398900	3.68563200	0.15951800
H	-3.75089800	3.52971100	1.23728900
H	-4.45378800	4.57508600	-0.01579700
H	-2.84789000	3.84903200	-0.25951500
C	-0.17096300	-2.30470200	-0.60750900
H	-0.04519300	-2.73329000	-1.60918200
N	0.98416200	-2.68624700	0.23634000
C	3.64490700	-0.22705300	1.23571100
C	3.29235600	-1.43384100	-0.82314000
C	4.86141800	0.24590100	0.76742900
H	3.30611800	0.06494900	2.22544200
C	4.50722700	-0.96843700	-1.31390700
H	2.68824100	-2.11134300	-1.41690800
C	5.26789500	-0.13371400	-0.50709200
H	5.48940600	0.89278500	1.36667000
H	4.86717000	-1.24621000	-2.29652200
N	6.55192000	0.35862000	-1.01300800
O	6.89389700	0.01995600	-2.13361400

O	7.21344200	1.08223400	-0.28763100
H	0.73514900	-3.42467400	0.88329200
C	2.84423200	-1.06219000	0.44592800
C	1.49082200	-1.51626400	0.96424800
H	1.59221700	-1.73572500	2.03205900

TS5RS

C	-5.25055100	0.58252700	-2.97940600
C	-4.82289700	-0.69830700	-2.63770700
C	-3.62777400	-0.87303600	-1.94928900
C	-2.83769900	0.23095900	-1.59029800
C	-3.28658400	1.51872600	-1.92949900
C	-4.47870100	1.68951900	-2.62041300
H	-6.18679500	0.72115100	-3.51061000
H	-5.42417100	-1.56288800	-2.90169600
H	-3.28493900	-1.86894300	-1.68169700
H	-2.70916200	2.39209400	-1.63493300
H	-4.81469400	2.68985200	-2.87494200
C	-1.59076200	-0.01752300	-0.88003200
C	-0.55888000	0.88283500	-0.76144700
C	0.77065900	0.48369200	-0.44333600
O	1.23024400	-0.64687200	-0.22834800
H	-0.71634800	1.91969700	-1.02660900
H	-1.38165300	-1.05875000	-0.63499900
C	2.57700000	-1.32827200	4.11017400
C	2.77914200	-2.57121800	3.50788300
C	1.86635500	-3.05455300	2.57901100
C	0.73634200	-2.30879800	2.23288900
C	0.51317800	-1.04361900	2.83545100
C	1.45970900	-0.58183000	3.76680500

H	3.27977700	-0.95115900	4.84646700
H	3.64341600	-3.17334200	3.77037700
H	2.01056500	-4.02505700	2.12044200
H	1.28575200	0.37980500	4.24239200
N	-0.23505000	-2.82538600	1.35465600
C	-0.03636500	-3.34331000	0.10191900
O	-0.96206500	-3.50024000	-0.68007900
O	1.23546700	-3.66956000	-0.12989100
C	1.67239300	-4.05304300	-1.46445700
C	1.19470900	-3.05418800	-2.51809400
H	0.14584900	-3.20542200	-2.76921100
H	1.80078400	-3.17456700	-3.42102800
H	1.31458000	-2.03675800	-2.13491500
C	1.19263400	-5.46890100	-1.75978500
H	1.55899100	-6.16074200	-0.99610500
H	1.57449700	-5.79240100	-2.73247300
H	0.10196400	-5.50101800	-1.78112700
C	3.19013300	-3.99391400	-1.33388600
H	3.50137500	-2.97578400	-1.07689200
H	3.66164800	-4.28802000	-2.27517700
H	3.53228700	-4.66703900	-0.54301600
C	-0.61684500	-0.18469500	2.50187700
H	-0.51501700	0.88397400	2.73319500
N	-1.71735500	-0.64116300	1.97935800
C	-4.96162500	0.66620200	0.78248200
C	-4.31397800	-1.64800300	1.14627100
C	-6.20122500	0.25959200	0.34719500
H	-4.71980000	1.72506600	0.80121000
C	-5.55634000	-2.06188300	0.71948200
H	-3.57569600	-2.38214500	1.45080500

C	-6.49883900	-1.10809700	0.31462100
H	-6.94612700	0.97320100	0.01710300
H	-5.81585600	-3.11302900	0.68225300
N	-7.77628100	-1.53866500	-0.17133800
O	-8.02446200	-2.74282300	-0.19133200
O	-8.57838500	-0.68944500	-0.55638300
H	-1.13764300	-2.35565300	1.43703100
C	-3.96966900	-0.26944500	1.18095700
C	-2.67469000	0.19354600	1.52759900
H	-2.50913100	1.27584500	1.57861100
C	5.94588900	-0.53927600	-0.84290900
C	4.64516200	-0.35366600	-0.37869700
C	4.29223600	-0.62189800	0.94179700
C	5.29545400	-1.05191700	1.80801300
C	6.60508400	-1.22802000	1.35498400
C	6.93910100	-0.98402700	0.02511200
C	6.05709000	-0.21839400	-2.31074000
C	4.73309200	0.48960200	-2.67312100
C	3.75129500	0.16173400	-1.48484700
H	3.26275900	-0.51347400	1.28147200
H	7.37014900	-1.56360500	2.04789800
H	7.95589200	-1.12879100	-0.32695400
H	6.90556000	0.42787500	-2.55474200
H	4.31561900	0.12020600	-3.60961700
H	6.16795400	-1.13469000	-2.89969900
H	2.99095700	-0.56265500	-1.77762400
N	3.04955400	1.38287300	-1.06170600
O	4.91117500	1.88152100	-2.89488900
C	1.80901100	1.57934600	-0.58551600
C	3.67639300	2.59781400	-1.07485600

N	1.73636300	2.88832600	-0.32483500
N	2.89445500	3.53921700	-0.62953400
C	5.02298000	2.65890000	-1.71745600
H	5.80033400	2.28025400	-1.04074300
H	5.25994000	3.68280400	-2.00400000
C	0.64068200	3.58261200	0.29790000
C	-0.22686100	4.32210400	-0.50650700
C	0.49337700	3.44628000	1.67886100
C	-1.32849900	4.90141000	0.12165800
C	-0.62561000	4.04138400	2.25776300
C	-1.55317500	4.75378100	1.49261500
H	-2.02949000	5.47763100	-0.47650600
H	-0.77401900	3.94993600	3.33087900
C	1.52462500	2.71115800	2.49160700
H	1.59035200	1.65552600	2.20422200
H	2.51593700	3.15377100	2.35184500
C	0.01238300	4.46016900	-1.98655300
H	0.97352600	4.94368600	-2.18286700
H	0.03447000	3.48251800	-2.48207300
H	-0.77698200	5.05501800	-2.44753500
H	1.27457200	2.75501100	3.55311900
C	-2.78098000	5.33971900	2.13804700
H	-3.20319600	6.14293400	1.53127600
H	-2.55392000	5.73421000	3.13105500
H	-3.55025700	4.56993000	2.25813200
H	5.05244400	-1.25579300	2.84444700
M6RS			
C	5.77513600	-2.16861600	-2.51749600
C	5.22706400	-1.00874300	-3.05927500

C	4.07777300	-0.45249800	-2.50235500
C	3.45585800	-1.04502900	-1.40164300
C	4.01450100	-2.21084800	-0.86562000
C	5.16465200	-2.76855500	-1.41757100
H	6.67162400	-2.60263400	-2.94850600
H	5.69586800	-0.53354300	-3.91533800
H	3.66036200	0.46077500	-2.91865700
H	3.54684700	-2.68798900	-0.00622300
H	5.58487300	-3.67333000	-0.98905400
C	2.23812000	-0.40626800	-0.76546400
C	1.12143500	-1.38468300	-0.57911800
C	-0.17926700	-0.97560400	-0.69650900
O	-0.64695400	0.19365400	-0.88833900
H	1.36544200	-2.42614000	-0.42809600
H	1.87587800	0.40983500	-1.40466000
C	-1.62231600	1.14138500	4.78758000
C	-2.39443500	2.15168200	4.21974000
C	-2.13384100	2.62679900	2.93976700
C	-1.08205800	2.09628900	2.17360400
C	-0.26643300	1.09157000	2.76251800
C	-0.56672500	0.62972900	4.04942600
H	-1.83221500	0.77097400	5.78454900
H	-3.21757300	2.58698400	4.77837300
H	-2.74951000	3.41109000	2.52609600
H	0.06627400	-0.14695200	4.47219000
N	-0.77294300	2.51277500	0.88091000
C	-1.47521800	3.24314600	-0.04741500
O	-1.03381800	3.42508800	-1.16652300
O	-2.63169100	3.72825500	0.41652900
C	-3.50979300	4.50902600	-0.44992000

C	-3.97329000	3.66063900	-1.62976500
H	-3.13693700	3.41033700	-2.28262300
H	-4.71555400	4.22494500	-2.20230100
H	-4.43969600	2.73931700	-1.26781300
C	-2.80784300	5.78999500	-0.88941100
H	-2.42948900	6.32727500	-0.01470600
H	-3.52686000	6.43457300	-1.40301400
H	-1.97921700	5.57287600	-1.56274900
C	-4.68220000	4.82855400	0.47012100
H	-5.14031300	3.90130200	0.82559900
H	-5.43402400	5.40793700	-0.07184700
H	-4.34512100	5.41218500	1.33166500
C	0.92215100	0.49502900	2.12610900
H	1.29929800	-0.41606900	2.61819800
N	1.51548500	0.98813400	1.11614400
C	5.10720000	0.92402500	0.57405700
C	3.49144700	2.51932600	-0.25074500
C	6.14355800	1.79315800	0.26060200
H	5.33254200	-0.04543500	1.00846500
C	4.51338600	3.40132100	-0.57291700
H	2.45776000	2.79316300	-0.43706600
C	5.82383300	3.01862500	-0.30986000
H	7.17854700	1.53815300	0.44967100
H	4.31270800	4.36771600	-1.01800900
N	6.90912700	3.94367000	-0.64292900
O	6.61526000	5.01398600	-1.14891300
O	8.05313200	3.59721900	-0.39822500
H	-0.00849900	1.99768100	0.44066500
C	3.77826900	1.27496500	0.32189400
C	2.66100700	0.28935300	0.58328000

H	3.01559000	-0.49888400	1.26819600
C	-5.24845100	0.02497400	-1.50796400
C	-3.95162900	-0.08037100	-1.01026000
C	-3.60060700	0.43851000	0.23295900
C	-4.59731600	1.04463400	0.99518900
C	-5.90614900	1.13697300	0.51192900
C	-6.23952800	0.63922800	-0.74632000
C	-5.35578200	-0.57314100	-2.88688800
C	-4.03192400	-1.34339900	-3.10104500
C	-3.05800000	-0.82414300	-1.97812100
H	-2.56907600	0.37958000	0.57513700
H	-6.67039400	1.60910700	1.12209300
H	-7.25463600	0.72232500	-1.12304100
H	-6.20662100	-1.25158100	-3.00403900
H	-3.60146300	-1.14622300	-4.08259600
H	-5.46319200	0.21203900	-3.64210900
H	-2.25875600	-0.19317200	-2.36417400
N	-2.41362200	-1.96079700	-1.30090300
O	-4.22671100	-2.75202200	-3.08354100
C	-1.21554800	-2.06782200	-0.69247900
C	-3.08461900	-3.13482100	-1.10040100
N	-1.21984400	-3.29325500	-0.14971800
N	-2.37814000	-3.97514300	-0.40540700
C	-4.39798300	-3.29918800	-1.79025900
H	-5.20061700	-2.79737400	-1.23302500
H	-4.64142200	-4.35613300	-1.89534500
C	-0.22606700	-3.88186300	0.70443100
C	0.67830700	-4.79134400	0.15086000
C	-0.20338700	-3.48806200	2.04097500
C	1.65652700	-5.30662400	0.99675500

C	0.79833300	-4.02906700	2.84744500
C	1.73395100	-4.93294300	2.34258800
H	2.38115000	-6.01093500	0.59537100
H	0.84486600	-3.73824900	3.89383900
C	-1.21076100	-2.50322100	2.56835900
H	-1.06072300	-1.51397400	2.12033000
H	-2.23253400	-2.81820800	2.33396900
C	0.61830800	-5.13888200	-1.31207300
H	-0.37285100	-5.50646700	-1.59177200
H	0.82608000	-4.25264800	-1.92309100
H	1.35693500	-5.90323200	-1.55685900
H	-1.12126600	-2.39830100	3.65098500
C	2.80640200	-5.51467700	3.22634100
H	2.64831500	-6.58778300	3.36999200
H	2.81313500	-5.03839300	4.20845700
H	3.79413300	-5.38829200	2.77472700
H	-4.35016400	1.45352700	1.96977600

TS6RS

C	-4.07257700	3.70777500	-2.72260900
C	-3.81774200	2.43211500	-3.21752000
C	-3.17210800	1.48717500	-2.42147100
C	-2.76683400	1.80459300	-1.12415100
C	-3.03716000	3.08792000	-0.63187300
C	-3.68248800	4.03272400	-1.42328000
H	-4.57418300	4.44421600	-3.34198500
H	-4.12172800	2.16857500	-4.22566100
H	-2.97651300	0.49156600	-2.81088400
H	-2.72582500	3.35779100	0.37578000
H	-3.88075600	5.02389000	-1.02610800

C	-2.04586800	0.79039800	-0.26512000
C	-0.69176900	1.27639800	0.17151500
C	0.43807800	0.60631100	-0.34915000
O	0.51950100	-0.59722400	-0.62664800
H	-0.60707200	2.33909200	0.35144000
H	-1.90691700	-0.14211200	-0.82469900
C	2.37558500	-0.08786300	3.90178000
C	2.55180700	-1.46802200	3.73652300
C	1.64182000	-2.23375300	3.02820900
C	0.47500000	-1.66370700	2.45636900
C	0.29003700	-0.25910200	2.66335000
C	1.23971600	0.49370000	3.36725600
H	3.09620500	0.50452100	4.45532300
H	3.41461800	-1.95419300	4.18490600
H	1.80295900	-3.29841400	2.91235800
H	1.05294900	1.55798300	3.50094100
N	-0.53486000	-2.36206800	1.84807700
C	-0.38412200	-3.42600300	1.04767000
O	-1.33810200	-4.01818000	0.53365800
O	0.90723500	-3.79981900	0.79541100
C	1.19689400	-4.88468300	-0.11664200
C	0.69513900	-4.55589200	-1.52145800
H	-0.39326300	-4.54260500	-1.55450100
H	1.07094600	-5.30196300	-2.22861000
H	1.07350900	-3.57352000	-1.82196600
C	0.62243600	-6.20010900	0.40676300
H	0.98289500	-6.38120200	1.42432500
H	0.95951300	-7.02537100	-0.22795700
H	-0.46622600	-6.17085700	0.41313600
C	2.72180500	-4.94659400	-0.11841700

H	3.14452000	-4.02041200	-0.51754100
H	3.06051700	-5.78526200	-0.73367400
H	3.09868800	-5.08403900	0.89981000
C	-0.88693400	0.45243500	2.16636000
H	-1.00751100	1.48337600	2.50224800
N	-2.00675100	-0.24285100	1.90029500
C	-5.32654000	0.14113100	0.37350600
C	-3.92385400	-1.83063600	0.39613800
C	-6.40767100	-0.61356800	-0.06165000
H	-5.44638300	1.20934500	0.52891700
C	-4.99776600	-2.60010900	-0.03245400
H	-2.96669400	-2.32852700	0.55099000
C	-6.21967800	-1.97594800	-0.25344700
H	-7.37680200	-0.16794100	-0.24635400
H	-4.89347100	-3.66498900	-0.19910000
N	-7.35301100	-2.78424800	-0.71258100
O	-7.17240000	-3.97775700	-0.88434600
O	-8.41855600	-2.22109700	-0.90131700
H	-1.74614700	-1.26105700	1.75217100
C	-4.08491400	-0.45564800	0.61070700
C	-2.91396400	0.40637900	1.00517700
H	-3.27772700	1.33975100	1.45587500
C	4.93830500	-1.77796000	-1.67962600
C	3.84827400	-1.23030500	-1.00749900
C	3.65435900	-1.41840600	0.35684300
C	4.59689800	-2.17393600	1.05005300
C	5.69205600	-2.73182000	0.38600500
C	5.86893000	-2.54444700	-0.98338700
C	4.91423000	-1.42005000	-3.14390400
C	3.80998800	-0.34526200	-3.28470800

C	2.97834000	-0.43730100	-1.95330700
H	2.78361800	-1.00633500	0.86397600
H	6.41335900	-3.32007000	0.94442800
H	6.72239700	-2.97871000	-1.49527800
H	5.86699900	-1.02550600	-3.51018800
H	3.15945500	-0.54474600	-4.13608800
H	4.66891400	-2.29344600	-3.75627500
H	2.01247700	-0.90634300	-2.11990100
N	2.71710600	0.90457300	-1.40130200
O	4.33908000	0.94629900	-3.54621800
C	1.70597100	1.40283300	-0.65863700
C	3.64920800	1.89148200	-1.54062700
N	2.06365400	2.66971000	-0.40616100
N	3.27097800	2.98654800	-0.94776900
C	4.83490500	1.61655600	-2.40486800
H	5.58158200	1.01921100	-1.86427100
H	5.28929000	2.55283400	-2.72753600
C	1.35435800	3.68328500	0.32933800
C	0.36325900	4.40674500	-0.33735200
C	1.71667400	3.90180300	1.66020900
C	-0.34898900	5.33895900	0.41610200
C	0.96967000	4.84193200	2.36829500
C	-0.07166100	5.55525800	1.76776500
H	-1.14165800	5.90469000	-0.06697500
H	1.21305700	5.02923100	3.41138300
C	2.90365800	3.20355700	2.26908500
H	2.89803300	3.31227600	3.35540500
H	2.92173200	2.13569700	2.03382600
C	0.05649000	4.15611300	-1.78945600
H	0.96358400	4.21987400	-2.39811700

H	-0.37839700	3.15989200	-1.93339300
H	-0.66638400	4.88564300	-2.15749000
H	3.83024200	3.64307300	1.88642100
C	-0.85619400	6.56339400	2.56582900
H	-1.73165600	6.91029500	2.01398400
H	-0.23698200	7.43380900	2.80280700
H	-1.19200600	6.13392700	3.51325500
H	4.46804300	-2.34143800	2.11319100

M7RS

C	3.26242100	-2.88673400	-3.62011500
C	2.84199000	-1.57026200	-3.79235500
C	2.48455800	-0.80057700	-2.68683000
C	2.53572500	-1.33524400	-1.39665100
C	2.95934900	-2.65974200	-1.23460000
C	3.32293500	-3.42862400	-2.33698500
H	3.54327900	-3.48709600	-4.47947500
H	2.79256900	-1.14005000	-4.78773200
H	2.15032100	0.22615300	-2.81437900
H	2.99245500	-3.10456300	-0.24198400
H	3.65439800	-4.45321800	-2.19461100
C	2.07594500	-0.50053600	-0.22876900
C	0.75978400	-0.99062900	0.38048800
C	-0.40808400	-0.56194500	-0.45690700
O	-0.38165100	0.27502700	-1.32803000
H	0.76236100	-2.08523400	0.38409300
H	1.91853100	0.53133000	-0.55558700
C	-1.87404800	1.04297100	4.10721700
C	-1.97806400	2.31134100	3.53220700
C	-1.24068100	2.64776300	2.40632100

C	-0.33711700	1.73315700	1.81751600
C	-0.24835800	0.43630500	2.40002000
C	-1.00331300	0.12029600	3.53224100
H	-2.44521300	0.78463100	4.99281100
H	-2.64683300	3.04909100	3.96795400
H	-1.32206600	3.63925400	1.97479900
H	-0.87769600	-0.85984800	3.98815600
N	0.57690100	2.03172100	0.83692000
C	0.34147000	2.80279000	-0.21635000
O	1.21046400	3.16572100	-1.01964700
O	-0.99003800	3.13256300	-0.41816500
C	-1.36485200	4.09967400	-1.41984500
C	-1.13526800	3.53367400	-2.81979400
H	-0.07341100	3.35214100	-2.98303100
H	-1.50925300	4.23382600	-3.57330700
H	-1.67435300	2.58654400	-2.93458400
C	-0.63235500	5.42545800	-1.21451500
H	-0.76679400	5.76411700	-0.18206300
H	-1.05478200	6.18328300	-1.88137700
H	0.43178300	5.31836600	-1.41726700
C	-2.85641500	4.30128100	-1.16608100
H	-3.39096800	3.35233800	-1.26134100
H	-3.27551900	5.01147900	-1.88444100
H	-3.02432000	4.67911100	-0.15324900
C	0.80155500	-0.53831700	1.90575800
H	0.70436100	-1.46119100	2.49152600
N	2.15576700	0.00882000	2.11373200
C	5.49754700	-0.13186700	0.97591400
C	4.06201600	1.73909000	0.43465900
C	6.62494500	0.65732100	0.78370600

H	5.61601500	-1.17293400	1.26019600
C	5.17776200	2.54233900	0.24385700
H	3.06729200	2.15745500	0.27500900
C	6.43921500	1.98472600	0.42343600
H	7.62548600	0.26339900	0.90886100
H	5.08401600	3.58129600	-0.04642500
N	7.61956000	2.82945200	0.22014500
O	7.44275400	3.99553100	-0.08949100
O	8.71955100	2.32372700	0.37181900
H	2.05585700	1.01409100	1.96440200
C	4.21564200	0.39584400	0.80893700
C	2.99791400	-0.47296300	1.01137000
H	3.32819200	-1.49477700	1.24425500
C	-5.41981300	1.63605600	-0.44795800
C	-4.25420600	1.06850600	0.06350000
C	-4.01448100	0.98302100	1.42688700
C	-4.98169900	1.48859500	2.29415400
C	-6.14939300	2.06779000	1.79419800
C	-6.37772500	2.14889200	0.42022000
C	-5.43010700	1.57631500	-1.95501800
C	-4.30963100	0.57764800	-2.31009700
C	-3.36263100	0.58073400	-1.05644800
H	-3.09774300	0.54185800	1.81253000
H	-6.89172700	2.45578300	2.48424700
H	-7.29195000	2.59121100	0.03668000
H	-6.38003000	1.23388100	-2.37444200
H	-3.76268500	0.86026000	-3.21031000
H	-5.21446300	2.55819000	-2.39105800
H	-2.47915600	1.21170500	-1.19184500
N	-2.90825000	-0.79028400	-0.78673100

O	-4.82815600	-0.71652900	-2.59705200
C	-1.73939100	-1.30069500	-0.36852700
C	-3.80311500	-1.81908200	-0.83811700
N	-1.97136200	-2.60037900	-0.16846600
N	-3.25163100	-2.94190500	-0.46837300
C	-5.12550100	-1.52958300	-1.47474600
H	-5.81381900	-1.04508300	-0.77213500
H	-5.57072600	-2.45457200	-1.84006500
C	-1.03959000	-3.62118500	0.23962600
C	-0.19008000	-4.16444700	-0.72696700
C	-1.02811900	-3.98421100	1.58737800
C	0.72943200	-5.11396500	-0.28622000
C	-0.08595000	-4.93546700	1.97308700
C	0.79714400	-5.50663100	1.05301800
H	1.41885600	-5.54592700	-1.00713200
H	-0.03948000	-5.23470700	3.01677300
C	-1.99451500	-3.36963100	2.56380300
H	-1.74040500	-3.65450100	3.58571800
H	-1.98723100	-2.27582300	2.50281300
C	-0.22670600	-3.69803600	-2.15754200
H	-1.25186200	-3.64755400	-2.53544800
H	0.22754000	-2.70335600	-2.26238800
H	0.34669900	-4.37626800	-2.79088300
H	-3.01676700	-3.70108500	2.35663700
C	1.79035100	-6.54955200	1.49189100
H	1.36612300	-7.55169100	1.37403200
H	2.05746900	-6.42272400	2.54286800
H	2.70140600	-6.50348800	0.89119500
H	-4.81499700	1.43464100	3.36511100

M8RS

C	-2.91344300	2.78118900	-4.44620200
C	-2.99317500	1.39918000	-4.29199600
C	-2.62081300	0.80661500	-3.08790400
C	-2.16137300	1.57982000	-2.02081400
C	-2.09401600	2.96817200	-2.18407500
C	-2.46173000	3.56525600	-3.38649400
H	-3.19954100	3.24438900	-5.38516200
H	-3.34193800	0.77955800	-5.11235900
H	-2.67440600	-0.27257300	-2.97142000
H	-1.74493900	3.59275000	-1.36245400
H	-2.39640800	4.64365100	-3.49583400
C	-1.81650900	0.94115600	-0.69982200
C	-0.45590200	1.34410700	-0.09926500
C	0.59844500	0.30337700	-0.57593900
O	0.45716400	-0.03386400	-1.80715700
H	-0.16792500	2.30539300	-0.51670200
H	-1.82771600	-0.14825100	-0.82743400
C	0.95758300	0.13158700	4.53591900
C	1.38853800	-1.11331700	4.07361300
C	1.22793700	-1.45897400	2.73875200
C	0.62011600	-0.56828400	1.84104300
C	0.16110100	0.66650000	2.30993500
C	0.33694400	1.00549100	3.65342300
H	1.09292300	0.40653900	5.57657600
H	1.85668400	-1.81649200	4.75497000
H	1.55716700	-2.42939000	2.37954400
H	-0.03469800	1.96750100	3.99818600
N	0.51692400	-0.88283400	0.46352500
C	0.02826100	-2.10732000	0.05495900

O	0.31867800	-2.67319400	-0.97859000
O	-0.84737300	-2.59636300	0.96554900
C	-1.28616400	-3.98478600	0.90445400
C	-0.08207700	-4.91689200	1.00346400
H	0.57765300	-4.80367900	0.14248700
H	-0.43010400	-5.95267600	1.04443600
H	0.48042000	-4.70956600	1.91905200
C	-2.10539100	-4.23570500	-0.35832900
H	-2.88936200	-3.47786900	-0.45731200
H	-2.58576000	-5.21578800	-0.28576600
H	-1.47783900	-4.20764500	-1.24793100
C	-2.16096400	-4.11108000	2.14653400
H	-1.58628100	-3.85607900	3.04096300
H	-2.53068900	-5.13488000	2.24208500
H	-3.02053000	-3.43644900	2.08356000
C	-0.71158000	1.50560100	1.42287300
H	-0.60028300	2.56455800	1.69284700
N	-2.11669200	1.10547300	1.68354300
C	-5.30919400	1.08586100	-0.00250500
C	-4.04578200	-0.90208900	0.52014000
C	-6.46841800	0.32806800	-0.12726100
H	-5.34965900	2.15821000	-0.16531600
C	-5.19111400	-1.67571400	0.40857900
H	-3.09795700	-1.38849700	0.74642600
C	-6.38563600	-1.04017700	0.08689400
H	-7.41944400	0.77885900	-0.38149300
H	-5.17390200	-2.74885000	0.55786600
N	-7.60257900	-1.84811500	-0.03631300
O	-7.51523500	-3.04720100	0.16712000
O	-8.63850800	-1.27884300	-0.33475600

H	-2.11120700	0.11021400	1.90733700
C	-4.09307500	0.48554600	0.32648500
C	-2.82774200	1.30133700	0.41963500
H	-3.08485700	2.36591800	0.33414600
C	4.61023700	-3.10796600	-1.54694600
C	3.82485100	-2.28269200	-0.74371900
C	3.80227500	-2.41897000	0.63606800
C	4.55418400	-3.44092700	1.21535500
C	5.31634800	-4.29473200	0.41562100
C	5.35709900	-4.12913100	-0.96985200
C	4.50433200	-2.68436200	-2.99317300
C	3.90319900	-1.26569500	-2.92284000
C	3.08924000	-1.27474700	-1.59458600
H	3.23150800	-1.72539000	1.24643000
H	5.89957900	-5.08406800	0.87899500
H	5.97598800	-4.77680400	-1.58358100
H	5.46202300	-2.66821200	-3.51948600
H	3.25583900	-1.04242200	-3.77215700
H	3.82880000	-3.34701800	-3.54602300
H	2.04579500	-1.55231700	-1.77215200
N	3.08865300	0.05410100	-0.99404800
O	4.91834600	-0.26030700	-2.96190900
C	2.10447500	0.78482600	-0.43547600
C	4.22926600	0.79915800	-0.99244200
N	2.70236300	1.93375900	-0.10469200
N	4.02918000	1.96628900	-0.45486800
C	5.40263800	0.23007100	-1.72210500
H	5.88718000	-0.55319700	-1.12652600
H	6.12617600	1.01555100	-1.93971800
C	2.13505500	3.07735700	0.55258100

C	1.46959900	4.02699200	-0.22859200
C	2.32145500	3.19992000	1.92968700
C	0.88298000	5.09699000	0.44288800
C	1.72252400	4.29588100	2.55332100
C	0.99108600	5.23982400	1.83071100
H	0.33804500	5.84326200	-0.13012000
H	1.83303900	4.41305100	3.62864000
C	3.17406500	2.21782600	2.68829100
H	3.05079200	2.35561700	3.76348200
H	2.91206900	1.18188900	2.44812400
C	1.41221400	3.89713300	-1.73007200
H	2.40912800	4.04232800	-2.15848300
H	1.06128900	2.91011200	-2.05310500
H	0.74301400	4.64808600	-2.15375000
H	4.22898600	2.36564300	2.43555300
C	0.36499800	6.42196900	2.52357400
H	1.03149800	7.28923500	2.47853000
H	0.17012700	6.20582900	3.57586900
H	-0.57590800	6.70473000	2.04626100
H	4.55443100	-3.56679700	2.29351500

TS7RS

C	-3.27704400	2.66854900	-4.30606500
C	-3.26904200	1.27707500	-4.25943500
C	-2.87755800	0.61790900	-3.09597500
C	-2.48772100	1.33569000	-1.96478000
C	-2.50578700	2.73426200	-2.02037600
C	-2.89369300	3.39689400	-3.18067800
H	-3.57746400	3.18394600	-5.21267200
H	-3.56367200	0.70159500	-5.13138500

H	-2.86552600	-0.46824400	-3.06409400
H	-2.20680600	3.31310200	-1.14692100
H	-2.89636100	4.48235300	-3.20717600
C	-2.10739000	0.62516600	-0.69164000
C	-0.75051300	1.04682000	-0.07791400
C	0.32085800	0.05741600	-0.56624000
O	0.32170900	-0.22295500	-1.77182000
H	-0.47199300	2.02352400	-0.46784100
H	-2.08133500	-0.45399000	-0.88626900
C	0.89940500	0.00194000	4.50990100
C	1.58942500	-1.09994700	4.00299000
C	1.47138700	-1.44856300	2.66477800
C	0.64236000	-0.71120500	1.80479600
C	-0.03468400	0.40238100	2.30743400
C	0.09595300	0.74343000	3.65586400
H	0.99196600	0.27634200	5.55526900
H	2.22830500	-1.69183200	4.65042500
H	2.00710900	-2.31103600	2.28358100
H	-0.45263500	1.60791200	4.02170100
N	0.52739200	-1.04019900	0.42639400
C	0.57870500	-2.36515900	-0.00136300
O	0.98939100	-2.74327500	-1.07667700
O	0.07551200	-3.17523000	0.94498600
C	0.24941600	-4.62149100	0.84826900
C	1.72931700	-4.97709600	0.72993600
H	2.15438800	-4.61998500	-0.20810800
H	1.83665800	-6.06445200	0.77396100
H	2.29322400	-4.54879800	1.56493700
C	-0.57141700	-5.16790200	-0.31515800
H	-1.60812700	-4.82906000	-0.23011100

H	-0.56347400	-6.26101900	-0.28037600
H	-0.16502900	-4.83798700	-1.27081400
C	-0.30963100	-5.11013900	2.17942800
H	0.24476800	-4.66360100	3.00960100
H	-0.22477800	-6.19778900	2.24246900
H	-1.36312800	-4.83406000	2.27475700
C	-1.01430000	1.14182200	1.44598600
H	-1.01502500	2.20225100	1.73261500
N	-2.37150300	0.60486500	1.69895000
C	-5.58205700	0.65196700	0.01419500
C	-4.31107400	-1.35357900	0.43958400
C	-6.73513000	-0.10302700	-0.16403500
H	-5.62718200	1.73154100	-0.08937100
C	-5.45101400	-2.12583900	0.27415900
H	-3.36789500	-1.85147900	0.65114900
C	-6.64552000	-1.48069900	-0.02458800
H	-7.68622600	0.35640900	-0.40174300
H	-5.42696100	-3.20426700	0.36519900
N	-7.85623500	-2.28784900	-0.20389400
O	-7.76582400	-3.49449500	-0.05434300
O	-8.89014200	-1.70988800	-0.49245900
H	-2.28228400	-0.40414400	1.82150200
C	-4.36452200	0.04146400	0.32241800
C	-3.11233700	0.86895100	0.46522500
H	-3.39124400	1.93123700	0.46673700
C	5.16036400	-2.14185300	-1.67304600
C	4.21049600	-1.52043700	-0.86695700
C	4.19367100	-1.69924800	0.50917900
C	5.13433600	-2.55483400	1.08089700
C	6.07470100	-3.20341500	0.27694000

C	6.09982400	-2.99590800	-1.10260300
C	4.98006600	-1.73367500	-3.11559100
C	4.00918700	-0.53068700	-3.06783900
C	3.27470200	-0.67399300	-1.69491200
H	3.47610200	-1.15997500	1.12232300
H	6.80465400	-3.86500500	0.73242900
H	6.84917100	-3.48523500	-1.71784100
H	5.91333600	-1.44672900	-3.60847500
H	3.28968700	-0.55772800	-3.88736700
H	4.53675700	-2.54901200	-3.69767400
H	2.30293800	-1.15759500	-1.82675600
N	3.04053700	0.62856900	-1.08653400
O	4.68436200	0.71431400	-3.23178400
C	2.00310200	1.06808500	-0.33531100
C	3.98161300	1.61403100	-1.18830800
N	2.38494800	2.31828700	-0.03467700
N	3.60589900	2.68570600	-0.55679200
C	5.16772300	1.32953600	-2.05011900
H	5.88456700	0.68870100	-1.51890900
H	5.66404400	2.25622400	-2.33825900
C	1.63443800	3.25696100	0.74572200
C	0.77541300	4.13658300	0.07977900
C	1.79442600	3.24587300	2.13157600
C	-0.00871300	4.98046800	0.86443000
C	0.99448300	4.11626200	2.87448600
C	0.08219400	4.97584400	2.26033800
H	-0.69980000	5.66382600	0.37631200
H	1.08747000	4.12016900	3.95803900
C	2.81442700	2.34606700	2.77587600
H	2.76957600	2.42975900	3.86275700

H	2.64493200	1.29801900	2.50693000
C	0.72749900	4.17528700	-1.42619800
H	1.68290700	4.53006900	-1.82516100
H	0.54794200	3.18531300	-1.86073900
H	-0.06180900	4.84604000	-1.77081200
H	3.82161100	2.61638000	2.44268900
C	-0.76131300	5.91548800	3.08272300
H	-0.27391200	6.89163500	3.17265900
H	-0.91509600	5.52674700	4.09159500
H	-1.73768500	6.07591800	2.61989600
H	5.14181700	-2.71053100	2.15532300
PRS			
C	3.43598600	-4.84011700	-1.49609500
C	3.21058400	-3.79984800	-2.39305600
C	2.47385400	-2.68451400	-1.99872800
C	1.95851900	-2.58776700	-0.70390500
C	2.18483000	-3.64344900	0.18610400
C	2.91693000	-4.76030000	-0.20495600
H	4.00958700	-5.70957500	-1.80011500
H	3.60437100	-3.85577500	-3.40287900
H	2.28891600	-1.87940200	-2.70590000
H	1.77968300	-3.59943500	1.19481900
H	3.08208100	-5.56902100	0.49974200
C	1.14611400	-1.38051800	-0.29124900
C	-0.32692700	-1.71831700	0.06398700
C	-1.27982900	-0.94428100	-0.83457900
O	-1.01175400	-0.65721200	-1.98568600
H	-0.55303600	-2.77733400	-0.10648000
H	1.13869000	-0.67204200	-1.12449300

C	-3.49485400	-0.93658700	3.79152400
C	-4.47283400	-0.60945800	2.85425800
C	-4.15052600	-0.50308000	1.50759000
C	-2.83319200	-0.70962800	1.08987500
C	-1.84940100	-1.06638900	2.01512700
C	-2.19480400	-1.17215700	3.36179400
H	-3.74738300	-1.02056100	4.84258600
H	-5.49799800	-0.44433600	3.16827600
H	-4.92425100	-0.26940600	0.78367500
H	-1.42119000	-1.44821200	4.07314200
N	-2.49813200	-0.58493400	-0.28330900
C	-3.41640400	0.07691100	-1.17741000
O	-3.93194800	-0.48416600	-2.10476200
O	-3.57143300	1.33192800	-0.79548800
C	-4.52059900	2.21560800	-1.49178600
C	-5.93272800	1.66203600	-1.34330800
H	-6.03674700	0.69580600	-1.83875500
H	-6.63784500	2.36338500	-1.79692900
H	-6.19029300	1.56040100	-0.28488000
C	-4.10106100	2.37394700	-2.94803300
H	-3.04873200	2.66532600	-3.00447800
H	-4.70254600	3.16460500	-3.40436200
H	-4.24795800	1.45084900	-3.50808300
C	-4.36769900	3.52715300	-0.73443000
H	-4.59566400	3.38394200	0.32484500
H	-5.05612200	4.26933400	-1.14517000
H	-3.34679800	3.90583000	-0.82753700
C	-0.44875200	-1.35154000	1.55782900
H	-0.06028200	-2.19566600	2.14165700
N	0.48525500	-0.23901100	1.76652000

C	3.53581800	0.43274600	-0.30940300
C	2.63526900	1.59864200	1.60281200
C	4.43889000	1.46408400	-0.52703500
H	3.54851300	-0.42768500	-0.97019400
C	3.52971100	2.64157700	1.39881400
H	1.94029800	1.64103600	2.43405400
C	4.41572700	2.55375600	0.33364900
H	5.14777600	1.43347400	-1.34466900
H	3.54804800	3.50845700	2.04708900
N	5.36188100	3.65104100	0.11105100
O	5.33583800	4.59366500	0.88399200
O	6.12625300	3.56360600	-0.83475700
H	0.08970100	0.60142200	1.33826600
C	2.62298500	0.48872900	0.75019100
C	1.66430100	-0.65222300	0.99700800
H	2.19104900	-1.39775600	1.61102200

TS5SR

C	4.99060900	-0.81982800	1.91504300
C	3.65386300	-0.49763500	1.68898300
C	2.81767900	-0.11864700	2.73823600
C	3.34840700	-0.05291000	4.02352300
C	4.68991800	-0.37050200	4.25357000
C	5.51659500	-0.76120000	3.20419600
C	5.69018300	-1.22263600	0.64543500
C	4.65328600	-1.00611100	-0.48346900
C	3.29444800	-0.62521500	0.22198600
H	1.76951600	0.09574100	2.55629900
H	5.08920400	-0.31553000	5.26120800
H	6.55720400	-1.01257500	3.38592100

H	6.59130600	-0.63158900	0.45007900
H	4.48712200	-1.91888700	-1.05649100
H	6.00461600	-2.27054600	0.67963000
H	2.52780700	-1.37832900	0.04028900
N	2.77777400	0.66995500	-0.28441200
O	5.10073600	-0.06415200	-1.44298300
C	1.56509700	1.25513600	-0.15913600
C	3.63852700	1.62613900	-0.74044900
N	1.75541300	2.53438600	-0.52582600
N	3.04480000	2.77200400	-0.89822100
C	5.06601300	1.26587500	-0.98490800
H	5.64661500	1.39982000	-0.06043000
H	5.48480100	1.90972300	-1.75858000
C	0.90234900	3.67807200	-0.30416200
C	0.71807300	4.08356400	1.02597200
C	0.33240000	4.34343600	-1.38879700
C	-0.12798700	5.16317700	1.25302400
C	-0.50711900	5.42345200	-1.10315400
C	-0.76126500	5.83585000	0.20285200
H	-0.29437800	5.49237700	2.27558000
H	-0.96766400	5.95571100	-1.93133700
C	0.58108200	3.93770500	-2.81640400
H	1.57419500	3.50453900	-2.94611600
H	-0.16204600	3.20595500	-3.15252900
C	1.37477500	3.36272900	2.17375600
H	0.81938300	2.45265900	2.42799800
H	2.40520700	3.07628700	1.94135900
H	1.38988100	3.99954400	3.05925800
H	0.49828900	4.80784100	-3.47019000
C	-1.69811000	6.97878900	0.49091200

H	-2.63133000	6.60660200	0.92506300
H	-1.94406300	7.53029600	-0.41812300
H	-1.25843800	7.67337000	1.21111000
H	2.71380600	0.23920900	4.85361400
C	-5.70992400	2.73515900	1.71615700
C	-5.55004500	1.38782400	2.02208900
C	-4.35470000	0.74157900	1.71954600
C	-3.29195700	1.43122900	1.11744300
C	-3.46579300	2.79524100	0.81861600
C	-4.66289900	3.43417900	1.10928300
H	-6.64169900	3.24197100	1.94522200
H	-6.35862900	0.83296800	2.48748900
H	-4.23655400	-0.31626400	1.94200600
H	-2.66023500	3.36236500	0.35823700
H	-4.78468000	4.48535700	0.86733100
C	-2.05150300	0.70900100	0.83630300
C	-0.89446800	1.28255500	0.38469000
C	0.31640000	0.52615200	0.30241000
O	0.48775600	-0.64762000	0.66326000
H	-0.89646400	2.30511200	0.03746300
H	-2.00570100	-0.32943500	1.15971400
C	2.84282700	-0.04966900	-3.71329800
C	3.22788400	-1.35737600	-3.41711400
C	2.35510200	-2.20272200	-2.74408900
C	1.09433600	-1.75581700	-2.33531100
C	0.67502800	-0.43882100	-2.65343700
C	1.58067400	0.38724400	-3.34469400
H	3.52087700	0.61861300	-4.23436200
H	4.20971700	-1.71740200	-3.70708000
H	2.63940500	-3.22494800	-2.52121800

H	1.27464800	1.39901700	-3.59309600
N	0.18426800	-2.61821400	-1.69833900
C	0.40107900	-3.42774600	-0.61889500
O	-0.51972000	-3.97158100	-0.03361100
O	1.70065500	-3.56314500	-0.30998400
C	2.09466600	-4.39519900	0.82367100
C	1.49093600	-3.84668400	2.11282700
H	0.41494900	-4.01238900	2.14711300
H	1.96064700	-4.34190000	2.96769200
H	1.68732000	-2.77140600	2.18129900
C	1.71307000	-5.84843300	0.56217600
H	2.14014500	-6.18389200	-0.38757100
H	2.11804900	-6.47521600	1.36156700
H	0.63058500	-5.96777400	0.53204800
C	3.61040500	-4.23890300	0.84840600
H	3.87898200	-3.21253800	1.11524400
H	4.04041200	-4.90523900	1.60039400
H	4.03974300	-4.48536400	-0.12749500
C	-0.62188700	0.11402000	-2.27770900
H	-0.78721300	1.17405800	-2.50465200
N	-1.61235200	-0.63011400	-1.83866000
C	-5.17867200	-0.38072700	-0.98874900
C	-3.69847700	-2.28037500	-0.67561200
C	-6.25123400	-1.12919000	-0.54329600
H	-5.32906300	0.65891300	-1.26657400
C	-4.76295700	-3.03376000	-0.22736500
H	-2.70429300	-2.71736500	-0.68852900
C	-6.03589500	-2.45486500	-0.16965200
H	-7.24566500	-0.70624100	-0.47142800
H	-4.63032500	-4.06109800	0.08893600

N	-7.14921300	-3.24511900	0.30320600
O	-6.94458300	-4.41328900	0.61200000
O	-8.25242900	-2.71551200	0.37672100
H	-0.77221100	-2.24947400	-1.70638000
C	-3.88102500	-0.93336200	-1.07659300
C	-2.79305400	-0.10711200	-1.51896500
H	-3.00835800	0.94349900	-1.73954900

M6SR

C	5.18048900	-0.05831500	-0.81201100
C	3.86382800	-0.42592400	-1.07994100
C	3.40964100	-0.64779000	-2.37398500
C	4.32137700	-0.51509000	-3.42063200
C	5.64589800	-0.15066400	-3.16446200
C	6.08409200	0.08823300	-1.86143300
C	5.38563400	0.13554400	0.67161900
C	4.16642300	-0.54464700	1.32767900
C	3.07877900	-0.54624000	0.20407800
H	2.36599700	-0.89732800	-2.54555200
H	6.34337700	-0.05076900	-3.99004300
H	7.11504400	0.37142100	-1.66940400
H	6.31690900	-0.29060700	1.05388100
H	3.80896900	0.00600700	2.19860300
H	5.37672600	1.20396100	0.92261400
H	2.36539300	0.27120500	0.31233000
N	2.31921000	-1.79546300	0.24352700
O	4.47838500	-1.84182800	1.83305700
C	1.02085000	-2.04633700	0.00790700
C	2.93173600	-2.98468800	0.51906400
N	0.90080300	-3.37352900	0.14419000

N	2.08704700	-3.97295600	0.47576000
C	4.36880200	-2.91901900	0.92021100
H	5.01033600	-2.78280200	0.03960100
H	4.66159700	-3.83036900	1.44103600
C	-0.29153500	-4.15762800	-0.02159300
C	-0.78898700	-4.35048900	-1.31252800
C	-0.93214400	-4.62246100	1.12735200
C	-1.99379900	-5.03801300	-1.43080300
C	-2.13337400	-5.31010900	0.95464600
C	-2.68077300	-5.51710900	-0.31253600
H	-2.41466200	-5.19195600	-2.42133000
H	-2.66007900	-5.67601000	1.83233100
C	-0.36920300	-4.33495100	2.49364100
H	0.61612500	-4.79141200	2.62139000
H	-0.24949400	-3.25507300	2.64146400
C	-0.07876100	-3.79177500	-2.51541200
H	-0.23387100	-2.70869100	-2.57837200
H	0.99871600	-3.97443100	-2.46597500
H	-0.46491600	-4.24267800	-3.43068000
H	-1.03365700	-4.71545500	3.27043900
C	-3.99132700	-6.23970600	-0.48418000
H	-4.67269000	-5.65719400	-1.11061200
H	-4.47450900	-6.41816700	0.47848200
H	-3.84137700	-7.20688900	-0.97338600
H	3.99934900	-0.68741400	-4.44243600
C	-6.13574600	-1.74306900	-1.51252200
C	-5.58889200	-0.61947900	-2.12761000
C	-4.35041500	-0.13355600	-1.71767600
C	-3.63512900	-0.75604600	-0.69081700
C	-4.19432300	-1.88353800	-0.08026500

C	-5.43381200	-2.37323100	-0.48665300
H	-7.10021600	-2.12577200	-1.83084400
H	-6.12522300	-0.12063300	-2.92885000
H	-3.93034200	0.74860300	-2.19461700
H	-3.65885100	-2.39371700	0.71678800
H	-5.85156900	-3.24990700	-0.00031800
C	-2.30597100	-0.18172100	-0.24094100
C	-1.26152400	-1.21542900	0.00978200
C	0.03078400	-0.98020900	-0.37113500
O	0.54315500	0.02166500	-0.96675400
H	-1.52403300	-2.11847300	0.54485400
H	-1.92974500	0.49819500	-1.01477000
C	2.55102600	1.20396000	4.37301200
C	3.28557500	2.13118200	3.63541800
C	2.82920600	2.59375200	2.40615700
C	1.60412000	2.14829300	1.88527100
C	0.82545700	1.24327700	2.65355900
C	1.33049700	0.77332000	3.87164200
H	2.91802900	0.83444700	5.32366200
H	4.23285400	2.50098000	4.01552600
H	3.41398700	3.31030600	1.84686400
H	0.72964000	0.06676900	4.43859600
N	1.08651800	2.58045300	0.66681900
C	1.70318400	3.07936100	-0.45533200
O	1.05687900	3.43597000	-1.42091500
O	3.03789800	3.11657000	-0.35121800
C	3.83115500	3.82900200	-1.35392200
C	3.72264400	3.13181400	-2.70416300
H	2.72623000	3.24809800	-3.12907900
H	4.45860800	3.56303100	-3.38947300

H	3.94157000	2.06676900	-2.58677300
C	3.40048100	5.29115700	-1.40857900
H	3.45814500	5.73800400	-0.41128400
H	4.07848200	5.83877800	-2.06898700
H	2.38398700	5.38928800	-1.78901200
C	5.25032100	3.71251200	-0.81186000
H	5.55950700	2.66423700	-0.78757100
H	5.93776300	4.26035200	-1.46147200
H	5.31575300	4.13183700	0.19651400
C	-0.52088500	0.77986400	2.26848100
H	-0.90098500	-0.07083600	2.85290900
N	-1.23211700	1.32561400	1.36409000
C	-4.86122800	1.60022400	1.19441400
C	-3.20987100	2.92676900	0.03344200
C	-5.84677500	2.52500400	0.87889800
H	-5.12249700	0.71126600	1.76058000
C	-4.18084700	3.86347200	-0.29214600
H	-2.18488500	3.07553900	-0.29201000
C	-5.48437900	3.64297000	0.13796800
H	-6.87422000	2.39327800	1.19348600
H	-3.94523500	4.74943700	-0.86812800
N	-6.51502100	4.62579900	-0.20214500
O	-6.18396900	5.60253400	-0.85351400
O	-7.65398700	4.41814700	0.18303000
H	0.13006900	2.26708300	0.48385500
C	-3.54112200	1.78752200	0.77633900
C	-2.50538000	0.72211400	1.04373000
H	-2.85686500	0.06111200	1.85293500

TS6SR

C	4.79584300	-1.15617300	2.01744100
C	3.48943600	-0.74717400	1.75582300
C	2.59990400	-0.46717900	2.79213300
C	3.04816700	-0.59126900	4.10452800
C	4.35844400	-0.99681800	4.37201500
C	5.23747400	-1.28746900	3.33251900
C	5.55754500	-1.43297200	0.74961800
C	4.61609100	-0.99740600	-0.39852300
C	3.22504100	-0.66406500	0.26544400
H	1.57585400	-0.18383300	2.56976000
H	4.69235300	-1.09047800	5.40042800
H	6.25355500	-1.60823300	3.54231700
H	6.50503200	-0.88706800	0.69153800
H	4.46655300	-1.79702200	-1.12367000
H	5.80142800	-2.49622500	0.65930100
H	2.44244800	-1.34802500	-0.07025500
N	2.80692900	0.71264400	-0.08921800
O	5.15851200	0.07271800	-1.15651900
C	1.60394600	1.31493200	-0.03386600
C	3.73326400	1.69818800	-0.28103000
N	1.85469800	2.62383900	-0.14731800
N	3.18118000	2.87640100	-0.31822300
C	5.16069100	1.30338100	-0.46759400
H	5.66766000	1.23265500	0.50515600
H	5.67603200	2.04234100	-1.08121900
C	0.93132200	3.71414100	0.02474400
C	0.72899900	4.58894400	-1.04729700
C	0.24703900	3.81988300	1.24157700
C	-0.24465000	5.57421400	-0.88862800
C	-0.71761100	4.81992900	1.34102300

C	-0.98507600	5.69537500	0.28849500
H	-0.43592400	6.25653900	-1.71303600
H	-1.28684600	4.90378400	2.26371500
C	0.47612800	2.88340600	2.39944900
H	-0.20430000	2.02554900	2.34230300
H	1.50142200	2.50400600	2.43476600
C	1.52185700	4.48033300	-2.32236600
H	2.49393500	4.97002100	-2.21183600
H	1.71946300	3.43937700	-2.58893900
H	0.98835300	4.95989400	-3.14457500
H	0.27518800	3.40098600	3.33907800
C	-2.03833900	6.76166100	0.43255800
H	-1.60430900	7.68044700	0.83987200
H	-2.83041900	6.43501300	1.11055000
H	-2.48626100	7.00608700	-0.53356700
H	2.37184000	-0.37901500	4.92604900
C	-4.74558200	3.72804000	1.67547600
C	-4.43744200	2.58295900	2.40525700
C	-3.62324600	1.59654400	1.85075800
C	-3.09884500	1.74314500	0.56502600
C	-3.41860200	2.89663000	-0.16122900
C	-4.23541100	3.88054300	0.38623900
H	-5.38274400	4.49484100	2.10453600
H	-4.83440800	2.45326100	3.40715300
H	-3.38769000	0.70189300	2.42102500
H	-3.01456900	3.03458500	-1.16259200
H	-4.47301100	4.76826000	-0.19230200
C	-2.19881000	0.68491800	-0.03064400
C	-0.85881100	1.22528000	-0.41404300
C	0.27707400	0.59870300	0.12537000

O	0.34615100	-0.52299800	0.65473600
H	-0.79342300	2.26337600	-0.71196500
H	-2.04035700	-0.11779900	0.69809600
C	2.68025200	0.39333400	-3.63027400
C	3.12294400	-0.89987300	-3.32432500
C	2.28037100	-1.83831600	-2.75149800
C	0.93571400	-1.52778600	-2.41962400
C	0.49360100	-0.21154700	-2.75592500
C	1.36150700	0.71171300	-3.35791700
H	3.34686800	1.11605700	-4.08781900
H	4.14900000	-1.17906500	-3.54852400
H	2.64522000	-2.83696100	-2.54401900
H	0.96898200	1.69397800	-3.61333300
N	0.00741700	-2.39401800	-1.90241700
C	0.24774100	-3.37961100	-1.02812000
O	-0.63620400	-4.11812400	-0.58843000
O	1.54822200	-3.49969400	-0.60633500
C	1.92181500	-4.52541500	0.34528800
C	1.22969000	-4.29275800	1.68619500
H	0.15472900	-4.44291600	1.59618300
H	1.63296000	-4.98630000	2.43055800
H	1.42274500	-3.26987400	2.02723400
C	1.64472800	-5.91672300	-0.22103100
H	2.12899800	-6.02318100	-1.19688400
H	2.06021900	-6.67233500	0.45238300
H	0.57491000	-6.08465400	-0.33427000
C	3.42569100	-4.32039400	0.49865800
H	3.62456700	-3.34332800	0.94822500
H	3.84890800	-5.08625700	1.15436300
H	3.92221000	-4.37780000	-0.47557700

C	-0.83594100	0.26920200	-2.38665600
H	-1.12415500	1.24552800	-2.77662800
N	-1.82201100	-0.57956400	-2.07502700
C	-5.23450400	-0.60604100	-0.68020000
C	-3.54340500	-2.33166300	-0.53971300
C	-6.19573100	-1.48763500	-0.20452700
H	-5.51313200	0.41687300	-0.91647500
C	-4.49562000	-3.22675800	-0.06904100
H	-2.51865600	-2.68651900	-0.64628400
C	-5.80410900	-2.78729700	0.08920300
H	-7.22613100	-1.18696400	-0.06436900
H	-4.23317500	-4.24820200	0.17662200
N	-6.81144500	-3.72708600	0.58921300
O	-6.45197700	-4.85844500	0.86674000
O	-7.95857400	-3.32785700	0.70394000
H	-1.40151500	-1.52797700	-1.85848100
C	-3.91014700	-1.01739800	-0.85805700
C	-2.88313500	-0.00923900	-1.29907000
H	-3.37060900	0.78583000	-1.87854600

M7SR

C	-2.59889500	-3.55186100	2.87092400
C	-1.59194200	-2.60372800	2.69828000
C	-0.96477000	-2.00354100	3.78453100
C	-1.36002600	-2.37892900	5.06716900
C	-2.36773100	-3.32905400	5.24820200
C	-2.99664400	-3.91917400	4.15286900
C	-3.12273200	-4.02928100	1.53862200
C	-2.08730400	-3.53587800	0.50675300
C	-1.34506400	-2.36115100	1.22524000

H	-0.19395500	-1.25373000	3.63311300
H	-2.66295700	-3.61167500	6.25359500
H	-3.77783300	-4.65914600	4.29807900
H	-3.23725800	-5.11487300	1.47254700
H	-2.55549600	-3.16987100	-0.40872600
H	-4.09937500	-3.57986100	1.32791900
H	-1.73831800	-1.40264300	0.87837900
N	0.08271600	-2.41807400	0.91193000
O	-1.21653700	-4.58111500	0.07880700
C	0.97490400	-1.45751100	0.64781900
C	0.73972100	-3.60897300	0.86377300
N	2.14599600	-2.08638200	0.51013400
N	2.01092300	-3.43771800	0.62908900
C	-0.10689400	-4.84028500	0.91987000
H	-0.40750200	-5.06360600	1.95153000
H	0.43701900	-5.69042400	0.50908400
C	3.45166100	-1.51546300	0.31058500
C	4.12483100	-1.82912500	-0.87598000
C	3.98565300	-0.68776200	1.30314800
C	5.34839500	-1.20003900	-1.09145900
C	5.21607900	-0.08683200	1.03395100
C	5.89781400	-0.31290900	-0.16152200
H	5.88731000	-1.41047700	-2.01181200
H	5.64447400	0.57938200	1.77828800
C	3.27040500	-0.40360600	2.59906100
H	2.60615200	0.46563600	2.51275500
H	2.67475100	-1.25632800	2.93524900
C	3.57380000	-2.83058500	-1.85250000
H	3.76335600	-3.84627800	-1.49248100
H	2.49406300	-2.71701300	-1.98214100

H	4.04737200	-2.70985300	-2.82723100
H	3.99788100	-0.17056800	3.37821000
C	7.19554900	0.39218300	-0.45495800
H	7.91936000	-0.28845700	-0.90962700
H	7.63336900	0.81066200	0.45327100
H	7.03070100	1.21395700	-1.15962400
H	-0.88392000	-1.92761600	5.93139800
C	4.48616900	5.00291700	1.38950900
C	3.20030600	5.28315200	1.84892800
C	2.14458400	4.43823800	1.52272100
C	2.34532500	3.30184000	0.73037900
C	3.63686500	3.03935500	0.26453000
C	4.69926900	3.87927800	0.59722100
H	5.31433100	5.65442300	1.64854600
H	3.02034900	6.15578500	2.46895300
H	1.14395600	4.65427500	1.89080300
H	3.83881300	2.17222200	-0.35926100
H	5.69606300	3.64929400	0.23246500
C	1.13843400	2.45305700	0.38685200
C	1.45505000	1.02323900	-0.07618100
C	0.62494200	0.02170100	0.70046500
O	-0.17736300	0.30601000	1.56524600
H	2.49221900	0.75886500	0.13786400
H	0.49949800	2.41131100	1.27146500
C	1.93552700	-1.45349700	-4.34840700
C	0.85336500	-2.31510600	-4.16943800
C	-0.07492300	-2.08518900	-3.16077500
C	0.03163200	-0.96111900	-2.31784500
C	1.16270300	-0.12623800	-2.46718100
C	2.08805800	-0.37727100	-3.48140800

H	2.65894000	-1.62958200	-5.13767800
H	0.73090300	-3.17559600	-4.82111300
H	-0.92031800	-2.75218900	-3.02672600
H	2.93420600	0.29644600	-3.59718800
N	-0.85188300	-0.65050400	-1.29124600
C	-2.17739700	-0.69633700	-1.43311300
O	-2.97790500	-0.50536300	-0.50033800
O	-2.62469100	-0.93107200	-2.70438300
C	-4.03763500	-0.94644800	-3.01020600
C	-4.74226100	-2.07701800	-2.26197300
H	-4.75068200	-1.88555700	-1.18894000
H	-5.77264300	-2.16754000	-2.61896900
H	-4.22980500	-3.02529800	-2.45734000
C	-4.66825800	0.41453300	-2.72154100
H	-4.09450700	1.20035100	-3.22271800
H	-5.69085400	0.43481200	-3.11044800
H	-4.68531600	0.61573600	-1.65095400
C	-4.05460900	-1.22475000	-4.51098000
H	-3.56302700	-2.17832200	-4.72431100
H	-5.08411800	-1.27076800	-4.87601700
H	-3.52514800	-0.43363000	-5.04853000
C	1.30245400	1.12285400	-1.63492900
H	2.22927000	1.62274900	-1.94903700
N	0.20889000	2.06322700	-1.85849500
C	-1.36825400	4.89750100	-0.26825700
C	-2.04026000	2.59251200	0.00970600
C	-2.61671600	5.32622000	0.16854200
H	-0.61836000	5.63027700	-0.55106600
C	-3.29412400	3.00132200	0.43930700
H	-1.83206500	1.52502200	-0.03273400

C	-3.55756300	4.36496700	0.51156600
H	-2.86619700	6.37751200	0.23710400
H	-4.05340300	2.28055900	0.71659000
N	-4.87916900	4.80595900	0.96665800
O	-5.69518300	3.95122500	1.26707500
O	-5.09523700	6.00532800	1.02268700
H	-0.65549300	1.53481100	-1.76004400
C	-1.06926300	3.53599200	-0.35452200
C	0.29718000	3.07601100	-0.80651700
H	0.85275400	3.94186400	-1.18672300

M8SR

C	3.96701200	3.13336000	-2.58941300
C	3.11791900	2.06711200	-2.29886700
C	2.68012100	1.19174500	-3.28731400
C	3.12316000	1.40274200	-4.59201600
C	3.97428500	2.46914100	-4.89275900
C	4.39964600	3.34456200	-3.89502400
C	4.28289200	3.92627300	-1.34558700
C	3.84138200	3.01307300	-0.18418000
C	2.79166900	2.03814000	-0.81844000
H	1.99709700	0.38919300	-3.02512900
H	4.30991800	2.61651100	-5.91453000
H	5.06354000	4.17091000	-4.13103800
H	5.34076100	4.18357100	-1.24148900
H	3.39983100	3.57672700	0.63919100
H	3.71214800	4.86110300	-1.32683000
H	1.76445400	2.34606500	-0.62467400
N	2.97628600	0.69632300	-0.25805000
O	4.94568800	2.33107400	0.40468300

C	2.09979400	-0.28643700	0.03004600
C	4.23602900	0.18329200	-0.14355100
N	2.86576800	-1.35650400	0.25971800
N	4.20821900	-1.07595600	0.17104700
C	5.36810400	1.15312500	-0.26168300
H	5.62096900	1.33847900	-1.31291700
H	6.24733000	0.77247800	0.25792600
C	2.46522100	-2.70196300	0.56393200
C	2.60385700	-3.15071700	1.87608500
C	1.96246100	-3.49136600	-0.47798400
C	2.15055300	-4.44251400	2.15535300
C	1.53050500	-4.77140700	-0.14664900
C	1.60613800	-5.25707400	1.16362100
H	2.22822200	-4.81657800	3.17303700
H	1.11072100	-5.40044800	-0.92810300
C	1.84443500	-2.94928500	-1.87857800
H	1.17464200	-2.07994000	-1.92181400
H	2.82207800	-2.62650300	-2.25263600
C	3.25524200	-2.29641300	2.92981500
H	4.34462700	-2.36966500	2.84891100
H	2.98464900	-1.24177500	2.82584800
H	2.96137500	-2.62596800	3.92788900
H	1.44757600	-3.71447800	-2.54834800
C	1.12199200	-6.64829000	1.47999600
H	1.04488900	-6.80729900	2.55724800
H	1.81000900	-7.39718900	1.07576300
H	0.14125400	-6.83056000	1.03188200
H	2.80069200	0.73431400	-5.38391900
C	-1.92224000	-4.26982000	-3.48524300
C	-2.09063800	-2.93280400	-3.83547200

C	-2.02165200	-1.93952500	-2.86007900
C	-1.78495100	-2.26423600	-1.52365600
C	-1.61994300	-3.61221100	-1.18283900
C	-1.68649100	-4.60773600	-2.15284400
H	-1.97433600	-5.04434200	-4.24394700
H	-2.27200000	-2.66073300	-4.87069800
H	-2.13386100	-0.89427400	-3.13382300
H	-1.41971200	-3.88502800	-0.14759500
H	-1.55351000	-5.64801500	-1.86955000
C	-1.67818600	-1.18298200	-0.47700200
C	-0.35118200	-1.22068800	0.31822200
C	0.55642100	-0.03770000	-0.16675100
O	0.42951400	0.28338400	-1.40960100
H	0.15835900	-2.15795500	0.11610500
H	-1.73758000	-0.20997900	-0.97199500
C	1.31802300	-0.08343300	4.78858300
C	1.87647600	1.08848400	4.27862600
C	1.57227200	1.50374900	2.98473000
C	0.68694700	0.75573400	2.21103100
C	0.14723700	-0.43533400	2.70340800
C	0.46543700	-0.84809800	3.99556700
H	1.56051900	-0.40745500	5.79545700
H	2.55293200	1.67874400	4.88816800
H	1.99151300	2.41792600	2.57451100
H	0.04539500	-1.77592600	4.37664300
N	0.34655700	1.12457400	0.87786300
C	-0.55816800	2.13428200	0.66024100
O	-1.03071100	2.44913500	-0.41699900
O	-0.82931600	2.77985900	1.81592200
C	-1.50802000	4.06504600	1.80489800

C	-0.70110200	5.07321000	0.99158600
H	-0.69325600	4.80521600	-0.06515800
H	-1.14315300	6.06732700	1.10193600
H	0.32832800	5.11242300	1.36209800
C	-2.93868900	3.92588600	1.29224000
H	-3.44688400	3.11468200	1.82279300
H	-3.48180100	4.85640800	1.48233000
H	-2.95135700	3.71739700	0.22193000
C	-1.50931400	4.44866600	3.28098400
H	-0.48490800	4.49459400	3.66038800
H	-1.97934700	5.42614600	3.41510700
H	-2.06340100	3.70813800	3.86372600
C	-0.78407200	-1.19686600	1.80334700
H	-0.85254200	-2.23933200	2.16251900
N	-2.10953800	-0.56713700	1.73036900
C	-5.22915700	-1.30132600	0.03671000
C	-4.06030600	0.81223400	-0.01715900
C	-6.40651700	-0.67254900	-0.35437200
H	-5.22528000	-2.37330400	0.20951000
C	-5.22516000	1.45954900	-0.39915500
H	-3.13622600	1.37172100	0.09812400
C	-6.38015600	0.69976400	-0.55964000
H	-7.32872100	-1.22194900	-0.49456000
H	-5.25085300	2.52790800	-0.57678600
N	-7.61729400	1.37289000	-0.96375000
O	-7.58730300	2.58244600	-1.11729600
O	-8.61533200	0.69021300	-1.12573200
H	-2.62277300	-0.67635400	2.60209900
C	-4.05443200	-0.56915800	0.21167400
C	-2.77080300	-1.24693400	0.61816700

H	-2.98693200	-2.30497800	0.85055000
TS7SR			
C	-1.20877400	-4.73955600	-2.43059300
C	-1.18651400	-3.37495100	-2.15486400
C	-1.33203000	-2.42428100	-3.15912000
C	-1.50973500	-2.86922900	-4.46730700
C	-1.53418000	-4.23699300	-4.75363700
C	-1.38141700	-5.18140600	-3.73980000
C	-1.02149000	-5.54682700	-1.16999000
C	-1.20019100	-4.53262500	-0.01692900
C	-0.99875900	-3.12190800	-0.67449800
H	-1.28687300	-1.36632500	-2.91543300
H	-1.67548300	-4.56795300	-5.77774100
H	-1.40438100	-6.24310100	-3.96727200
H	-1.73913900	-6.36583900	-1.06305900
H	-0.47060700	-4.68978500	0.77927900
H	-0.01839800	-5.98505300	-1.13505800
H	-0.00579400	-2.71671700	-0.47321100
N	-2.00069200	-2.18133900	-0.17615700
O	-2.46109300	-4.67322100	0.62801600
C	-1.93159300	-0.83945300	-0.00143000
C	-3.29665300	-2.59485000	-0.01482000
N	-3.21083800	-0.52166700	0.24006700
N	-4.07811400	-1.59354600	0.25141700
C	-3.55015500	-4.06708500	-0.04885900
H	-3.64188200	-4.42981800	-1.08147600
H	-4.46131000	-4.31173500	0.49689300
C	-3.72602800	0.80181000	0.42757900
C	-4.09902600	1.20027600	1.71319900

C	-3.83801000	1.63274500	-0.69068200
C	-4.56061500	2.50650000	1.87170400
C	-4.31832800	2.92581500	-0.48347100
C	-4.66836900	3.38213200	0.78855300
H	-4.84804600	2.84570500	2.86410300
H	-4.40645100	3.59546100	-1.33573500
C	-3.42215900	1.15841400	-2.05918300
H	-2.33017900	1.07613600	-2.13677400
H	-3.83685500	0.16941400	-2.27735900
C	-4.03316300	0.23144600	2.86134200
H	-4.87068500	-0.47174300	2.81114700
H	-3.10972600	-0.35411300	2.83141400
H	-4.07804200	0.75795800	3.81637100
H	-3.76156800	1.85810500	-2.82458700
C	-5.12724000	4.80279800	0.99393200
H	-5.90155000	4.86321800	1.76238500
H	-5.52308300	5.22752000	0.06872900
H	-4.29209900	5.43219700	1.31981400
H	-1.62750300	-2.14946700	-5.27084200
C	-1.20769900	5.89165700	-2.68340300
C	-0.07563600	5.30074400	-3.24208900
C	0.47217900	4.15894000	-2.66561200
C	-0.09288500	3.58372300	-1.52144200
C	-1.22217600	4.19143100	-0.96638600
C	-1.77841700	5.33137800	-1.54479800
H	-1.64117900	6.77853300	-3.13408000
H	0.37667100	5.72508600	-4.13298100
H	1.35001800	3.69667900	-3.11136600
H	-1.69544200	3.77560600	-0.08164300
H	-2.66231300	5.77956600	-1.09955000

C	0.57262600	2.36108300	-0.91902200
C	-0.34841800	1.49925100	-0.03450300
C	-0.06294000	-0.01306300	-0.27538700
O	0.28710700	-0.39979700	-1.39177500
H	-1.39312800	1.67745700	-0.27727800
H	0.93800000	1.75304800	-1.74874400
C	-1.12151800	0.33986000	4.65369400
C	-0.82361500	-0.99346500	4.36931100
C	-0.29603100	-1.34474900	3.13126000
C	-0.03273500	-0.34972900	2.19009600
C	-0.35436200	0.98068900	2.45428400
C	-0.90165600	1.31958300	3.69024200
H	-1.53842400	0.61034900	5.61821800
H	-1.01102000	-1.76343200	5.11036700
H	-0.06712300	-2.37972300	2.89334000
H	-1.14406000	2.35889800	3.89483400
N	0.53267300	-0.66438500	0.91964100
C	1.71654600	-1.39111800	0.83760400
O	2.10793500	-1.99259900	-0.14064900
O	2.37642500	-1.30667000	2.00259000
C	3.51965900	-2.17188900	2.28533100
C	3.11864700	-3.63620100	2.13702900
H	2.89397000	-3.88313100	1.09921100
H	3.94317100	-4.26814200	2.47775700
H	2.24426700	-3.85200100	2.75925300
C	4.69255800	-1.79574600	1.38770000
H	4.88654600	-0.72106300	1.45974400
H	5.58663300	-2.33263800	1.71712800
H	4.48713100	-2.05082100	0.34781800
C	3.82464200	-1.84475900	3.74214400

H	2.95764100	-2.06867900	4.36974700
H	4.67438800	-2.43945200	4.08612800
H	4.07014800	-0.78510300	3.85038400
C	-0.01426400	1.98222700	1.39136500
H	-0.55013500	2.91991500	1.58594400
N	1.43099900	2.26934400	1.38434400
C	4.25891600	3.00695700	-0.05351000
C	3.28194800	0.98015600	-0.93418200
C	5.53484400	2.51292700	-0.29311500
H	4.13927900	3.98947000	0.39240500
C	4.54951700	0.46960400	-1.18116600
H	2.41787300	0.37265700	-1.19148800
C	5.65255600	1.24433800	-0.84694300
H	6.42283100	3.08252200	-0.04993300
H	4.68587300	-0.51271500	-1.61615500
N	6.99227100	0.69258900	-1.06693900
O	7.07839900	-0.47013400	-1.42446800
O	7.95062900	1.42137900	-0.87284300
H	1.93041900	1.39506900	1.54699100
C	3.12452700	2.25041500	-0.36480700
C	1.75829200	2.76744900	0.03156900
H	1.80426700	3.86254800	0.07042600
PSR			
C	6.60463500	1.04031600	0.32168100
C	5.69874600	2.05931200	0.61251000
C	4.33915500	1.77988300	0.69053800
C	3.85531300	0.48304300	0.48133300
C	4.77076300	-0.52797500	0.18547800
C	6.13588500	-0.25167200	0.10890600

H	7.66716100	1.25271400	0.26454400
H	6.05257100	3.07092500	0.78438100
H	3.63529700	2.57669500	0.92120700
H	4.43429600	-1.54651200	0.01591700
H	6.83193100	-1.05336200	-0.11669200
C	2.35378500	0.27647000	0.53984400
C	1.89161800	-1.19374700	0.64668600
C	0.63076300	-1.23697200	1.50941600
O	0.61140400	-0.75267200	2.61407400
H	2.63619500	-1.82370400	1.14237100
H	1.98762800	0.83957400	1.40204400
C	0.08662500	-4.90614100	-1.87372600
C	-0.99004000	-4.97037100	-0.99025900
C	-1.21054600	-3.95119500	-0.07125800
C	-0.35955400	-2.84700600	-0.05732800
C	0.73069200	-2.77932000	-0.92514900
C	0.94799800	-3.81588900	-1.83028800
H	0.25751900	-5.70664300	-2.58513500
H	-1.65712000	-5.82557000	-1.00580000
H	-2.03946500	-4.00401900	0.62501500
H	1.79948200	-3.75834500	-2.50184100
N	-0.52711100	-1.79213800	0.90440600
C	-1.78519500	-1.20011900	1.17034900
O	-1.98387600	-0.40973900	2.06028800
O	-2.66308500	-1.59074700	0.25285700
C	-4.04302300	-1.09095200	0.27692200
C	-4.72835900	-1.52915400	1.56520900
H	-4.28184000	-1.04643700	2.43461200
H	-5.78565500	-1.25525900	1.51539500
H	-4.66016600	-2.61509700	1.67819100

C	-4.05231700	0.42307500	0.09474700
H	-3.43602400	0.70304000	-0.76514600
H	-5.07778100	0.75099100	-0.09641800
H	-3.68063900	0.93332500	0.98316800
C	-4.65847200	-1.78565500	-0.93091900
H	-4.58714100	-2.87116000	-0.82188300
H	-5.71176800	-1.50910600	-1.01812500
H	-4.13974400	-1.49005900	-1.84637200
C	1.63091500	-1.58552500	-0.81748400
H	2.58834300	-1.79386000	-1.30913200
N	1.04141500	-0.38939400	-1.43673100
C	0.44716500	2.81431200	-1.63166300
C	-0.27243800	1.85139200	0.46050800
C	-0.59176300	3.73539500	-1.57838100
H	1.13009100	2.82553400	-2.47532300
C	-1.32060900	2.75916600	0.52984100
H	-0.16498600	1.14073000	1.27364600
C	-1.46353000	3.68069900	-0.49871100
H	-0.73764700	4.47527900	-2.35523000
H	-2.01314600	2.75553300	1.36205700
N	-2.58360600	4.62573400	-0.44704000
O	-3.39446800	4.49817200	0.45416000
O	-2.64856500	5.48301900	-1.31120400
H	0.03988300	-0.38446300	-1.24825400
C	0.61572700	1.86200600	-0.62135000
C	1.66524600	0.78311800	-0.78683600
H	2.45145100	1.16661700	-1.44673600
TS5SS			
C	6.01396500	-2.59316000	-0.06068600

C	4.63386000	-2.58589000	-0.24438200
C	3.87962300	-3.75119200	-0.13510800
C	4.53655200	-4.93789400	0.17787200
C	5.92125200	-4.95206200	0.36872000
C	6.66899900	-3.78382700	0.24628600
C	6.60430000	-1.22097400	-0.25340200
C	5.39465600	-0.26535200	-0.39176400
C	4.13088700	-1.19350200	-0.55201400
H	2.80757800	-3.73077300	-0.30686300
H	6.41904500	-5.88511400	0.61261900
H	7.74474800	-3.79949000	0.39280900
H	7.23944700	-0.90457500	0.58048600
H	5.48012300	0.37013900	-1.27147400
H	7.22211300	-1.18346100	-1.15555600
H	3.69453300	-1.11326100	-1.54428300
N	3.07747800	-0.80985700	0.41158300
O	5.30078300	0.65142200	0.68647400
C	1.74202800	-1.02093200	0.41642000
C	3.41605900	-0.31814900	1.63971100
N	1.34238200	-0.64719500	1.64460000
N	2.37475100	-0.19702400	2.40843900
C	4.83741900	0.06495200	1.88331800
H	5.43094200	-0.81450800	2.16926100
H	4.89534900	0.80753400	2.67878500
C	0.02981700	-0.68223400	2.23907700
C	-0.76938900	0.45566000	2.11949900
C	-0.38872100	-1.86087800	2.85406100
C	-2.06076600	0.38183000	2.63209600
C	-1.69399100	-1.88633900	3.34859600
C	-2.54482300	-0.78459100	3.23330800

H	-2.70995800	1.24991500	2.54431000
H	-2.05963900	-2.79813800	3.81347100
C	0.50615200	-3.06945000	2.89903900
H	0.61156900	-3.50238300	1.89706900
H	1.50722200	-2.81277800	3.25707500
C	-0.27057800	1.65047900	1.36164100
H	0.68115400	2.02063600	1.75692500
H	-0.10702600	1.37047600	0.31319700
H	-1.00104400	2.46237700	1.38189800
H	0.08778000	-3.83427900	3.55429500
C	-3.97261400	-0.84639300	3.70856900
H	-4.66399100	-0.65354400	2.87991300
H	-4.16284000	-0.08579800	4.47142200
H	-4.20821800	-1.82438500	4.13261800
H	3.97119300	-5.85941800	0.26950400
C	-5.14249600	-3.88772100	-0.84145200
C	-4.50801800	-4.07044600	-2.06790400
C	-3.24724400	-3.52493500	-2.28893900
C	-2.58961600	-2.79392200	-1.28821300
C	-3.24534400	-2.61319900	-0.05671900
C	-4.50552200	-3.15312600	0.16024000
H	-6.12753400	-4.30885100	-0.66742000
H	-4.99554200	-4.63712400	-2.85489400
H	-2.75575800	-3.66677200	-3.24850900
H	-2.76874200	-2.05027000	0.74029300
H	-4.99584400	-2.99935300	1.11760200
C	-1.25247500	-2.27116200	-1.55116400
C	-0.42956700	-1.73670500	-0.58349400
C	0.97228100	-1.60956400	-0.75067500
O	1.66835500	-2.00832500	-1.70504000

H	-0.87639100	-1.39001900	0.33471900
H	-0.78976500	-2.58082000	-2.48749900
C	3.72692400	1.70860000	-2.78310200
C	3.67838500	2.96743100	-2.18835900
C	2.47723700	3.48305900	-1.71142300
C	1.29489500	2.73813300	-1.79794600
C	1.33583900	1.43893200	-2.37629400
C	2.56134100	0.96172300	-2.86972700
H	4.65384700	1.32759300	-3.19983700
H	4.57645200	3.57251800	-2.11641300
H	2.45147000	4.47525400	-1.28614500
H	2.56867900	-0.01837300	-3.33992600
N	0.03962200	3.21478000	-1.39809400
C	-0.33379200	4.21143800	-0.53633100
O	-1.50455500	4.38379000	-0.24050800
O	0.69741500	4.92091400	-0.06955200
C	0.48359700	6.02412000	0.86475500
C	-0.12791300	5.50116800	2.16001000
H	0.48147900	4.68480700	2.55914300
H	-0.14641500	6.30771400	2.89830800
H	-1.14539100	5.14554100	1.99786600
C	1.90093900	6.53017900	1.10584400
H	2.34499400	6.88031600	0.16971200
H	1.88340100	7.36057300	1.81587800
H	2.52546600	5.73127300	1.51459100
C	-0.36993200	7.10585400	0.21225600
H	-1.38886200	6.75644000	0.04775500
H	-0.39414200	7.98331200	0.86437900
H	0.06896700	7.40155900	-0.74497800
C	0.18780600	0.55699200	-2.55534500

H	0.40984500	-0.37424300	-3.09115700
N	-1.03245200	0.81930400	-2.18953000
C	-4.44461400	-0.56747600	-2.41182000
C	-3.41999800	0.73131800	-0.63110000
C	-5.62150900	-0.63087900	-1.69899200
H	-4.37723000	-1.05098800	-3.38132100
C	-4.59317300	0.66702800	0.09117700
H	-2.55829300	1.25491900	-0.22734100
C	-5.68291000	-0.03076500	-0.43766700
H	-6.48658800	-1.15954500	-2.07975100
H	-4.68567100	1.13578100	1.06401100
N	-6.87298900	-0.17995500	0.35590500
O	-6.86971300	0.25404000	1.50623800
O	-7.84328400	-0.74396700	-0.13946700
H	-0.73577200	2.58227400	-1.62044200
C	-3.30211500	0.08859500	-1.89020900
C	-2.04208800	-0.00992900	-2.54776300
H	-1.96392400	-0.59511200	-3.46459700

M6SS

C	5.28542500	2.26619100	0.42668100
C	3.91898600	2.37094500	0.66942300
C	3.34109300	3.55919500	1.10647000
C	4.16795200	4.66594400	1.28147900
C	5.54043500	4.57332600	1.03138800
C	6.10989500	3.37420600	0.60886800
C	5.66082200	0.86960500	0.00115600
C	4.31703900	0.14109800	-0.23660300
C	3.21301400	1.06236300	0.39420700
H	2.27634200	3.58614500	1.32331200

H	6.17067500	5.44604000	1.17175400
H	7.17738500	3.30639900	0.42111400
H	6.26892100	0.84081900	-0.90861100
H	4.29357700	-0.83717200	0.24504200
H	6.23210100	0.36370600	0.78583600
H	2.77223400	0.63304100	1.29414600
N	2.11659800	1.26094000	-0.56125800
O	4.09655700	-0.14654600	-1.61037900
C	0.81143400	1.49268500	-0.34937300
C	2.33080700	1.33663500	-1.90827100
N	0.29943600	1.74034900	-1.55983600
N	1.23955400	1.63127200	-2.54984300
C	3.69166000	0.96185600	-2.39346100
H	4.39104500	1.80412700	-2.30122500
H	3.65089500	0.64183500	-3.43500000
C	-1.02933400	2.20379200	-1.85612400
C	-1.88484900	1.37027100	-2.58289400
C	-1.41381100	3.45696000	-1.37042200
C	-3.18254500	1.82586500	-2.80601900
C	-2.72294600	3.86611800	-1.62437900
C	-3.61898200	3.06646000	-2.33451300
H	-3.87178700	1.18971900	-3.35614500
H	-3.05047100	4.83297500	-1.25088100
C	-0.47322900	4.32202900	-0.57364100
H	-0.38302800	3.95147800	0.45379800
H	0.53002600	4.33643000	-1.01113500
C	-1.42819300	0.02628900	-3.07923400
H	-0.68037800	0.13603500	-3.87083600
H	-0.95087000	-0.54731700	-2.27980300
H	-2.27411600	-0.53704200	-3.47785800

H	-0.84465800	5.34711700	-0.53286600
C	-5.02421700	3.53601000	-2.60770200
H	-5.10017300	3.96418700	-3.61241500
H	-5.33016400	4.30440400	-1.89434600
H	-5.73333300	2.70647100	-2.55045600
H	3.74688200	5.60683900	1.62097000
C	-5.75301900	2.17948500	2.80724500
C	-5.03155000	1.67917400	3.89001300
C	-3.75090600	1.16859200	3.69635300
C	-3.17014100	1.14406900	2.42445700
C	-3.89875500	1.65637200	1.34826800
C	-5.18009800	2.17012300	1.53812300
H	-6.75075100	2.58076900	2.95429000
H	-5.46370600	1.69291900	4.88594400
H	-3.18889500	0.78451800	4.54542900
H	-3.45997500	1.66137800	0.35366200
H	-5.73012300	2.56495400	0.68853900
C	-1.79987700	0.51722500	2.23832700
C	-1.09556500	0.88508100	0.97450100
C	0.16255800	1.41692900	1.00153900
O	0.89812800	1.77751300	1.97830900
H	-1.53711200	0.60288800	0.02576200
H	-1.15575000	0.82369700	3.07179800
C	3.37531000	-3.67988700	3.93568700
C	4.05442000	-3.64552400	2.72119700
C	3.49225400	-3.03897400	1.60289600
C	2.21786100	-2.46189800	1.66984500
C	1.50708100	-2.51504100	2.89749500
C	2.11112300	-3.11263200	4.00844500
H	3.82193200	-4.14301500	4.80812900

H	5.04222100	-4.08709800	2.63645200
H	4.03699700	-3.02353100	0.66879800
H	1.55762200	-3.13612700	4.94347600
N	1.63635900	-1.77053500	0.59491100
C	1.72591500	-1.98235100	-0.75967100
O	0.96817300	-1.40755400	-1.52700600
O	2.67851400	-2.84285000	-1.10820800
C	2.72082600	-3.39793300	-2.46417500
C	3.03651400	-2.31788100	-3.49264600
H	3.99581900	-1.84943100	-3.26327000
H	3.09683300	-2.78536600	-4.47987900
H	2.25682700	-1.55438400	-3.50623100
C	3.86488500	-4.39987500	-2.37026000
H	3.64584400	-5.16295700	-1.61861000
H	4.00889400	-4.88867800	-3.33687300
H	4.79179600	-3.88911100	-2.09486600
C	1.40457600	-4.10936100	-2.76080400
H	0.58331200	-3.39807400	-2.85511400
H	1.50116400	-4.66132600	-3.69950600
H	1.17574900	-4.82284000	-1.96392200
C	0.13517600	-2.00374500	3.08190200
H	-0.24137900	-2.02897100	4.11566900
N	-0.58051800	-1.58545200	2.11990300
C	-4.22479600	-1.72005200	1.63613700
C	-2.42997700	-1.93420200	0.03415000
C	-5.14318500	-2.14133200	0.68478100
H	-4.56931700	-1.46014000	2.63281200
C	-3.33515500	-2.35278300	-0.93269500
H	-1.37525800	-1.85993700	-0.21262000
C	-4.67752700	-2.44672600	-0.58830300

H	-6.19787200	-2.23141300	0.91174800
H	-3.01443800	-2.60939800	-1.93471300
N	-5.63712500	-2.88374600	-1.60450000
O	-5.21833900	-3.11379700	-2.72716300
O	-6.80737200	-2.99358100	-1.27829400
H	0.75421400	-1.30497900	0.83609500
C	-2.86580300	-1.60426100	1.32362900
C	-1.90391500	-1.05472600	2.35565300
H	-2.27329500	-1.30012100	3.36415100
TS6SS			
C	-4.89234900	-3.28154100	0.50278000
C	-3.68329400	-2.64390100	0.76983300
C	-3.03785000	-2.80662400	1.99429300
C	-3.62673500	-3.62812900	2.95148800
C	-4.84100500	-4.26817300	2.68928700
C	-5.48294500	-4.09623900	1.46622600
C	-5.39779200	-2.95838600	-0.87685600
C	-4.24787600	-2.18897300	-1.56574600
C	-3.21122000	-1.84187200	-0.42820500
H	-2.10653700	-2.28696400	2.19497900
H	-5.28655100	-4.90612200	3.44590000
H	-6.42545300	-4.59526400	1.26199300
H	-5.66042900	-3.84767700	-1.45908400
H	-4.60020900	-1.26352600	-2.01409000
H	-6.29437900	-2.33293900	-0.83032200
H	-3.15018400	-0.76671300	-0.24582300
N	-1.85817600	-2.29206500	-0.81455200
O	-3.68224800	-2.91071200	-2.64913000
C	-0.64271500	-1.89600300	-0.39790300

C	-1.67728600	-3.40643900	-1.58248400
N	0.21418200	-2.78898200	-0.90420500
N	-0.41961800	-3.73321400	-1.65632400
C	-2.87546100	-3.99792100	-2.24843000
H	-3.40290700	-4.67372400	-1.56076000
H	-2.57811700	-4.55491600	-3.13654700
C	1.61231900	-2.98758600	-0.60822400
C	1.95966500	-3.44619200	0.66323600
C	2.54060700	-2.77709400	-1.63352800
C	3.31004200	-3.72096500	0.88988300
C	3.87502400	-3.04937000	-1.34754500
C	4.27553200	-3.53219000	-0.09675300
H	3.61102500	-4.07643200	1.87187600
H	4.62056900	-2.88876300	-2.12220900
C	2.10832000	-2.25517500	-2.97730800
H	1.39373900	-2.93165300	-3.45368200
H	1.62011900	-1.27902800	-2.87802800
C	0.94861300	-3.59018800	1.76872900
H	0.75507200	-2.61381100	2.23105700
H	-0.00418900	-3.99188400	1.41087300
H	1.32820000	-4.25509100	2.54566500
H	2.96928800	-2.13710200	-3.63599200
C	5.72748200	-3.83334600	0.16795100
H	5.89158600	-4.10851700	1.21175500
H	6.35264100	-2.96623300	-0.06410700
H	6.07183500	-4.66046900	-0.45996100
H	-3.14093600	-3.76858700	3.91146000
C	4.57187000	-0.55608800	3.88837900
C	3.58284200	0.27790300	4.40645800
C	2.53512900	0.70465200	3.59425400

C	2.46130200	0.31582300	2.25277700
C	3.45396600	-0.52805400	1.74696100
C	4.49881800	-0.96250800	2.55808000
H	5.38894400	-0.89145900	4.51893000
H	3.62396400	0.59366000	5.44415600
H	1.76576000	1.35668400	4.00080400
H	3.42531100	-0.84644900	0.70775700
H	5.25876200	-1.61992700	2.14447600
C	1.35358300	0.87188200	1.38491600
C	0.86066700	-0.05675300	0.32216500
C	-0.37738600	-0.69889700	0.49491900
O	-1.32710900	-0.36343200	1.21913900
H	1.59114000	-0.54704000	-0.31186400
H	0.49340600	1.08646500	2.02921100
C	-2.65527100	0.38446000	-3.06265000
C	-3.73193700	1.05975900	-2.46726200
C	-3.55986600	1.89073500	-1.37697500
C	-2.27133900	2.13947900	-0.81898700
C	-1.17836600	1.44155200	-1.43798900
C	-1.39657400	0.58630400	-2.53136300
H	-2.80866900	-0.27864500	-3.90675100
H	-4.73439300	0.92715300	-2.86774200
H	-4.41658600	2.38114000	-0.93916500
H	-0.53606100	0.07906400	-2.96729600
N	-1.97819200	2.94092000	0.24232300
C	-2.74725000	3.90733700	0.78356000
O	-2.43136600	4.51548900	1.80361600
O	-3.88876900	4.21397400	0.09572400
C	-4.77533500	5.26584300	0.54475600
C	-4.06417700	6.61676200	0.51867500

H	-3.63083500	6.78819500	-0.47135700
H	-4.78601800	7.41392400	0.72062100
H	-3.27245400	6.65014600	1.26607200
C	-5.88764400	5.23895100	-0.50019600
H	-6.39299400	4.26849800	-0.49353600
H	-6.62575900	6.01730300	-0.28862000
H	-5.47338200	5.40865100	-1.49781700
C	-5.34513200	4.94536400	1.92458900
H	-4.56525800	4.98257400	2.68395300
H	-6.12706400	5.66947600	2.17317800
H	-5.79186800	3.94629700	1.91810400
C	0.20172000	1.55279500	-0.97303200
H	0.95290800	1.17985500	-1.66530400
N	0.55808900	2.54219400	-0.12317400
C	4.20852600	2.35472500	0.82923000
C	3.16846300	2.61980600	-1.32673900
C	5.46450200	2.46312800	0.25192700
H	4.13463100	2.24503500	1.90574000
C	4.41823200	2.72969100	-1.92566200
H	2.28461500	2.74503000	-1.94005000
C	5.54599800	2.63332100	-1.12462300
H	6.36698900	2.42671800	0.84876200
H	4.52279000	2.89799500	-2.99003600
N	6.86733600	2.74031100	-1.74829500
O	6.91813300	2.89529900	-2.95688900
O	7.84775400	2.66591500	-1.02705800
H	-0.31893400	2.91652100	0.33327000
C	3.04244100	2.39819900	0.04842200
C	1.68986300	2.28987400	0.73291200
H	1.67804000	3.03370700	1.53657900

M7SS

C	-5.30294600	-1.04200600	1.65407700
C	-3.97446800	-0.63203700	1.55892400
C	-3.28224300	-0.16480800	2.67424500
C	-3.94466700	-0.11922400	3.89777200
C	-5.27700000	-0.52828300	3.99805700
C	-5.96487300	-0.98801700	2.87846600
C	-5.84115200	-1.48755600	0.32084400
C	-4.61979600	-1.51728900	-0.62603700
C	-3.46087500	-0.77510700	0.13930600
H	-2.25398100	0.17139800	2.58770800
H	-5.78021800	-0.48584500	4.95862900
H	-7.00013800	-1.30548400	2.95819400
H	-6.31466600	-2.47403600	0.35546300
H	-4.81388600	-0.99276100	-1.56135200
H	-6.59258800	-0.78465000	-0.05340100
H	-3.21982000	0.18267300	-0.33600800
N	-2.24001500	-1.60105300	0.12758100
O	-4.28027000	-2.83698500	-1.02499100
C	-0.94933800	-1.26230200	0.23774300
C	-2.29630600	-2.96401400	0.18526700
N	-0.27943600	-2.40617100	0.39767900
N	-1.11232100	-3.48265900	0.36047800
C	-3.63034200	-3.60205900	-0.03211100
H	-4.19832900	-3.63497500	0.90823900
H	-3.50497600	-4.61696700	-0.40853600
C	1.11535300	-2.53523200	0.74006000
C	1.54655400	-1.92755100	1.93016200
C	1.98649200	-3.18842900	-0.13771000

C	2.91535700	-1.92137100	2.18328700
C	3.34921800	-3.13304900	0.16120700
C	3.83461700	-2.48745800	1.29674200
H	3.27395400	-1.44120700	3.09100200
H	4.04824300	-3.60713000	-0.52406300
C	1.53449100	-3.94301800	-1.36050600
H	1.80805900	-4.99676000	-1.25665700
H	0.45810400	-3.89364100	-1.51459900
C	0.61008200	-1.24585600	2.89573200
H	0.52821300	-0.17354100	2.67659300
H	-0.39259900	-1.68134900	2.88823500
H	1.00563400	-1.33094400	3.90934400
H	2.03965400	-3.56121800	-2.25292800
C	5.31017200	-2.42024800	1.58547800
H	5.57263800	-1.45982100	2.03883500
H	5.90257200	-2.54623700	0.67653800
H	5.60049100	-3.20671700	2.28939000
H	-3.42337200	0.24120000	4.77829500
C	2.70613900	3.27174400	3.39709400
C	1.83112200	4.02584700	2.61894700
C	1.40716800	3.54792500	1.38109500
C	1.85682400	2.31720600	0.89345900
C	2.73663800	1.56848200	1.68594100
C	3.15511700	2.03871000	2.92756600
H	3.03378800	3.63946500	4.36419500
H	1.46948300	4.98361400	2.97961600
H	0.70355400	4.12118300	0.78222600
H	3.11613800	0.61360600	1.32899000
H	3.83765900	1.44244000	3.52615900
C	1.35404000	1.84134500	-0.44694500

C	0.90169100	0.38511400	-0.47327700
C	-0.41725600	0.16218200	0.19760400
O	-1.11527800	1.01253900	0.69673300
H	1.64247500	-0.23684700	0.04113600
H	0.49548300	2.45402300	-0.73260400
C	-1.92530400	-2.10816300	-3.45904700
C	-2.96174400	-1.17523100	-3.48723500
C	-2.75509200	0.13827600	-3.08799200
C	-1.49631800	0.58031200	-2.60940400
C	-0.44931700	-0.38602200	-2.57375900
C	-0.67409100	-1.68893700	-3.02094000
H	-2.08541900	-3.13003300	-3.78561300
H	-3.94610100	-1.47534900	-3.83817400
H	-3.56756700	0.85365900	-3.13755300
H	0.15812500	-2.38587000	-3.02470400
N	-1.15856000	1.86035600	-2.24796700
C	-1.96228500	2.71987200	-1.62368800
O	-1.63289400	3.86725400	-1.30675500
O	-3.21480100	2.23105700	-1.28370800
C	-4.17621700	3.06044800	-0.59601300
C	-4.51398800	4.30628100	-1.41412100
H	-4.82730800	4.01342000	-2.42139000
H	-5.34289100	4.83955600	-0.93878600
H	-3.65173500	4.96646400	-1.48683200
C	-5.41118900	2.16494200	-0.50343400
H	-5.21115300	1.30123000	0.13862800
H	-6.24789900	2.71763500	-0.06709500
H	-5.70352700	1.81280100	-1.49791000
C	-3.67860700	3.40179100	0.80591800
H	-2.79661500	4.03890500	0.75270000

H	-4.46773700	3.91464100	1.36495300
H	-3.42053900	2.47853100	1.33590700
C	0.90951100	-0.04462700	-1.99257200
H	1.50849300	-0.96232600	-2.05229900
N	1.61473200	1.04575300	-2.69548500
C	4.58393400	2.18084400	-0.66680900
C	4.11257500	0.07231900	-1.73560900
C	5.83178000	1.72122700	-0.27426900
H	4.27989400	3.18885900	-0.40062900
C	5.35746500	-0.41091800	-1.34984700
H	3.46605700	-0.54817800	-2.34473000
C	6.18901300	0.41932100	-0.61074500
H	6.51691900	2.34424300	0.28669700
H	5.68650100	-1.40706000	-1.61997500
N	7.49199900	-0.09077400	-0.18104500
O	7.78991700	-1.23546900	-0.48557100
O	8.21300000	0.65022600	0.46484300
H	0.87047000	1.63900900	-3.06105400
C	3.69871900	1.35904000	-1.37804300
C	2.30748100	1.86586300	-1.69296000
H	2.39144400	2.89159600	-2.06539600

M8SS

C	5.40459100	-1.76319800	-1.76114900
C	4.05156500	-1.44860200	-1.65751800
C	3.16728900	-1.65920300	-2.71065100
C	3.67141400	-2.21400200	-3.88590000
C	5.02605400	-2.53663200	-3.99869900
C	5.90383500	-2.31007400	-2.93966200
C	6.13638100	-1.42146000	-0.48713300

C	5.02044900	-1.20618400	0.55644100
C	3.73968500	-0.88038700	-0.28740100
H	2.12606900	-1.36738200	-2.60016900
H	5.39989500	-2.96845200	-4.92183500
H	6.95605700	-2.56305700	-3.02994200
H	6.82300400	-2.20230000	-0.14772100
H	5.24876100	-0.39136600	1.24467700
H	6.71864500	-0.50178200	-0.61030400
H	3.53185500	0.18860100	-0.33786300
N	2.57923300	-1.55357000	0.30738000
O	4.85558400	-2.34303000	1.39887000
C	1.27692000	-1.21661100	0.36341500
C	2.69248700	-2.85551300	0.70766800
N	0.65691700	-2.33535700	0.75506400
N	1.53359500	-3.36668600	0.99160300
C	4.07841100	-3.39624100	0.85740200
H	4.46901200	-3.74790400	-0.10596700
H	4.08677100	-4.22057600	1.57046200
C	-0.75288600	-2.61393300	0.83911200
C	-1.45200600	-2.80916300	-0.36026700
C	-1.34319300	-2.72049400	2.09668100
C	-2.81739600	-3.06150900	-0.26379400
C	-2.71654900	-2.97774500	2.13744900
C	-3.46532200	-3.14798100	0.97391800
H	-3.38958500	-3.20498200	-1.17760100
H	-3.20505700	-3.05603800	3.10547900
C	-0.53073900	-2.59484800	3.35709600
H	-0.02002500	-3.53877600	3.57255300
H	0.23477100	-1.81953700	3.27064900
C	-0.75048700	-2.71782900	-1.68943000

H	-0.37171800	-1.70358500	-1.87490100
H	0.10888900	-3.39718300	-1.71882100
H	-1.43220500	-2.98944200	-2.49742800
H	-1.17331900	-2.35177600	4.20561100
C	-4.93659700	-3.46496100	1.03477400
H	-5.50784200	-2.85311000	0.33076000
H	-5.33861700	-3.29791200	2.03675400
H	-5.11104400	-4.51377800	0.77452500
H	3.00576900	-2.39322200	-4.72419200
C	-2.51229800	1.35496100	-4.60408300
C	-1.80764700	2.47580400	-4.17335500
C	-1.37222400	2.56169100	-2.85278500
C	-1.63588800	1.53974600	-1.93808000
C	-2.34905800	0.42059600	-2.38274900
C	-2.77850800	0.32597500	-3.70252500
H	-2.84909300	1.28166300	-5.63322600
H	-1.58919600	3.28203900	-4.86683600
H	-0.81021900	3.43324100	-2.52522200
H	-2.59339000	-0.38232300	-1.68973000
H	-3.32901300	-0.55270000	-4.02547000
C	-1.21625400	1.71428700	-0.49954000
C	-0.70755500	0.46197400	0.22757800
C	0.75419600	0.15746500	-0.19991000
O	0.96566700	0.15225900	-1.46917800
H	-1.32365300	-0.38380900	-0.07885300
H	-0.42216400	2.47275500	-0.46782200
C	1.25995300	1.02699100	4.79672700
C	2.49364800	1.32479700	4.21213500
C	2.61441600	1.38309900	2.83181500
C	1.49452900	1.17486200	2.01594600

C	0.26064700	0.87309200	2.59185500
C	0.15648800	0.80159600	3.98516400
H	1.16525500	0.96969000	5.87582200
H	3.36504200	1.49686500	4.83572500
H	3.57189500	1.60037000	2.36598600
H	-0.81132200	0.57035000	4.42413500
N	1.62526100	1.18492500	0.60883800
C	2.18584100	2.27174600	-0.03293000
O	2.75471400	2.23220000	-1.10433500
O	2.02359800	3.39067800	0.70684300
C	2.68307100	4.63308700	0.33259700
C	2.09039400	5.16061700	-0.97008800
H	1.00402100	5.25238500	-0.87315000
H	2.50091500	6.15227000	-1.18104800
H	2.32073200	4.49454900	-1.80152400
C	2.33623800	5.55615500	1.49542100
H	2.72391700	5.14585500	2.43199400
H	2.77582700	6.54351600	1.33360100
H	1.25197900	5.66490200	1.58454000
C	4.19406600	4.43616600	0.24651800
H	4.46594000	3.80691700	-0.60022800
H	4.67591100	5.41121600	0.13302200
H	4.56281400	3.97956400	1.17039800
C	-0.96866600	0.73921100	1.73365700
H	-1.57197700	-0.08074900	2.14257300
N	-1.76533600	1.99386800	1.81629400
C	-4.47030700	1.95079100	-0.79446700
C	-4.13598600	0.60904000	1.17950600
C	-5.68658400	1.32861100	-1.03088300
H	-4.12560300	2.72047900	-1.47876300

C	-5.34950700	-0.03164900	0.95916700
H	-3.55937700	0.36467500	2.06335500
C	-6.09579900	0.33023200	-0.15371700
H	-6.30640700	1.59594500	-1.87724200
H	-5.72177800	-0.78784900	1.63895100
N	-7.36391800	-0.35580500	-0.40363300
O	-7.65764300	-1.29742800	0.31666000
O	-8.06137500	0.04220000	-1.32087100
H	-1.12106800	2.75043600	2.03588100
C	-3.66869300	1.58598400	0.29621200
C	-2.31695800	2.24640200	0.48291800
H	-2.44745800	3.32409100	0.33894800

TS7SS

C	-5.48941800	-1.73832300	1.40556200
C	-4.18865900	-1.24435500	1.36490500
C	-3.53452800	-0.80032500	2.50977800
C	-4.21463000	-0.88470500	3.72270500
C	-5.51689200	-1.39053800	3.77713600
C	-6.16694800	-1.81452600	2.61998300
C	-5.97212800	-2.11049200	0.02616000
C	-4.70541400	-2.09682600	-0.85947900
C	-3.64323600	-1.27017800	-0.04581000
H	-2.53469000	-0.37676800	2.43570700
H	-6.02897300	-1.45095300	4.73254000
H	-7.18008800	-2.20291600	2.66599900
H	-6.45048300	-3.09339300	-0.02289600
H	-4.88492900	-1.62693700	-1.82768700
H	-6.69836800	-1.37750700	-0.34101400
H	-3.54074200	-0.26537300	-0.45161400

N	-2.33212900	-1.91706700	-0.10476000
O	-4.27015200	-3.41071000	-1.18276600
C	-1.07756000	-1.39833200	-0.08706700
C	-2.25719100	-3.28355800	-0.02407100
N	-0.31802700	-2.50067500	0.01948400
N	-1.02605900	-3.68164500	0.04573100
C	-3.52770000	-4.05518300	-0.16185500
H	-4.07881300	-4.08690300	0.78764500
H	-3.32061900	-5.07417300	-0.48840100
C	1.11024200	-2.57886100	0.14403000
C	1.67500800	-2.37368300	1.40806700
C	1.86879200	-2.87887900	-0.98848100
C	3.06226400	-2.45528400	1.50954800
C	3.25569700	-2.94267800	-0.83602400
C	3.86628700	-2.74036800	0.40219100
H	3.52768600	-2.29462800	2.47972800
H	3.86974800	-3.16811100	-1.70491500
C	1.20671300	-3.14435800	-2.31499600
H	0.77355700	-4.14957600	-2.33253400
H	0.39247700	-2.43846600	-2.50650600
C	0.81199100	-2.03056500	2.59246500
H	0.36012000	-1.03848300	2.46590200
H	-0.00314800	-2.75288300	2.70484400
H	1.40546100	-2.03105800	3.50881600
H	1.93096300	-3.06947500	-3.12885100
C	5.35782000	-2.86960900	0.56820200
H	5.74743500	-2.09729200	1.23887100
H	5.88020800	-2.79668800	-0.38832900
H	5.60795000	-3.83912100	1.01138000
H	-3.73192500	-0.54898700	4.63501900

C	2.86983200	2.78595900	4.02803600
C	2.25364600	3.79413400	3.29143100
C	1.73750500	3.51781400	2.02720100
C	1.83289800	2.23891700	1.47196500
C	2.45024900	1.23456100	2.22447400
C	2.96206300	1.50379300	3.48957200
H	3.27038800	2.99507300	5.01483900
H	2.16781000	4.79525400	3.70223800
H	1.25256500	4.30800400	1.45855000
H	2.55590000	0.23326800	1.81704000
H	3.43920600	0.70832300	4.05443500
C	1.34258300	2.01560400	0.06274700
C	0.76729000	0.62581700	-0.26221000
C	-0.65019400	0.51711100	0.30497800
O	-0.81343600	0.67458800	1.52199200
H	1.36934500	-0.13845700	0.22974800
H	0.55619200	2.75672500	-0.13939700
C	-1.51348100	-0.02035300	-4.66226000
C	-2.70562600	0.43042500	-4.09515400
C	-2.73938800	0.84641400	-2.77142300
C	-1.56979200	0.84560000	-1.99741200
C	-0.37058500	0.40145400	-2.56197400
C	-0.35885700	-0.03127700	-3.89040000
H	-1.48793200	-0.35836700	-5.69234700
H	-3.61880600	0.44365900	-4.68108800
H	-3.67370700	1.18498300	-2.33291400
H	0.58272400	-0.37296900	-4.31391000
N	-1.60733300	1.16846600	-0.62356700
C	-2.56156700	2.05741200	-0.11869600
O	-3.18372900	1.89537500	0.90434000

O	-2.67302700	3.11359300	-0.93914000
C	-3.70453100	4.12355000	-0.71425100
C	-3.44378800	4.84670200	0.60302100
H	-2.41176300	5.20825400	0.63004900
H	-4.11278500	5.70862400	0.67750400
H	-3.61374600	4.18858400	1.45464400
C	-3.50921600	5.06698000	-1.89461600
H	-3.62984200	4.52564200	-2.83690700
H	-4.24803900	5.87102700	-1.85262500
H	-2.50912800	5.50752500	-1.86914400
C	-5.09040500	3.48768100	-0.76322700
H	-5.23470600	2.78248500	0.05539200
H	-5.84575000	4.27445400	-0.68528700
H	-5.23685100	2.97378500	-1.71833400
C	0.92053800	0.48954100	-1.79606700
H	1.50873400	-0.41121500	-2.00991100
N	1.69609300	1.66883600	-2.26861400
C	4.58628700	1.99424200	0.13161500
C	4.12925200	0.47866800	-1.68545300
C	5.80493600	1.37229600	0.35979800
H	4.30453200	2.84283000	0.74652700
C	5.35297600	-0.14809300	-1.48475300
H	3.49343200	0.15897500	-2.50238200
C	6.16259800	0.30163800	-0.45242400
H	6.47453800	1.70705100	1.14199400
H	5.67948400	-0.96663600	-2.11475000
N	7.44112200	-0.36910000	-0.21555000
O	7.81153100	-1.20385700	-1.02563200
O	8.06882300	-0.06693300	0.78565800
H	1.03258400	2.36317500	-2.60435200

C	3.71928800	1.54018300	-0.87339100
C	2.37763400	2.21870200	-1.09491400
H	2.56113800	3.28837500	-1.24296000
PSS			
C	-1.66461500	3.57344900	1.71781600
C	-1.18438600	2.72050900	2.70961900
C	-0.74498900	1.44414200	2.37325600
C	-0.78763100	0.99442200	1.04949900
C	-1.26074600	1.86086200	0.06106000
C	-1.69530000	3.14173800	0.39454200
H	-2.00567500	4.57114500	1.97457100
H	-1.14768600	3.05032400	3.74301300
H	-0.36959000	0.77859600	3.14740000
H	-1.28659100	1.54598700	-0.97728900
H	-2.05913700	3.80403700	-0.38446200
C	-0.38638000	-0.43032500	0.76529400
C	0.07855900	-0.77618000	-0.66036000
C	1.34436700	-0.05354300	-1.02726700
O	1.35122500	0.93847600	-1.72758200
H	-0.67678700	-0.47315900	-1.38974400
H	0.42660400	-0.70063800	1.45216300
C	2.83821600	-4.52693600	0.96713300
C	3.91123400	-3.64744300	1.07759500
C	3.80177600	-2.34436600	0.61171200
C	2.61074200	-1.90311900	0.02480800
C	1.50518900	-2.76191800	-0.04576400
C	1.64934700	-4.07326600	0.41106300
H	2.92465700	-5.55118800	1.31208000
H	4.84499000	-3.97351900	1.52313500

H	4.65026800	-1.67656700	0.69085100
H	0.81022100	-4.75853300	0.31784300
N	2.51563000	-0.57133500	-0.47523300
C	3.70860900	0.19632900	-0.69291400
O	4.68306100	-0.25197200	-1.24100100
O	3.55459200	1.39748600	-0.17539700
C	4.49601200	2.47774600	-0.49836800
C	4.56338900	2.65260900	-2.01106800
H	3.55165600	2.73680100	-2.41626600
H	5.11188900	3.57021800	-2.23893700
H	5.07227700	1.81468700	-2.48909000
C	3.84305300	3.68586700	0.15874600
H	3.74991300	3.53026100	1.23655900
H	4.45264400	4.57541100	-0.01681900
H	2.84696000	3.84888400	-0.26044500
C	5.85373000	2.17814500	0.12409800
H	6.31963100	1.31141500	-0.34528700
H	6.50563800	3.04576300	-0.01009600
H	5.74363200	1.99339200	1.19636900
C	0.17088000	-2.30477200	-0.60750600
H	0.04490400	-2.73336100	-1.60913900
N	-0.98416700	-2.68636400	0.23654800
C	-3.64471000	-0.22675100	1.23560100
C	-3.29241200	-1.43404000	-0.82299700
C	-4.86121300	0.24622100	0.76730700
H	-3.30581400	0.06543300	2.22524400
C	-4.50726500	-0.96860600	-1.31377800
H	-2.68839900	-2.11174100	-1.41663400
C	-5.26780500	-0.13363000	-0.50710300
H	-5.48906800	0.89328900	1.36648300

H	-4.86729200	-1.24655800	-2.29631100
N	-6.55182300	0.35869800	-1.01306200
O	-6.89390300	0.01982800	-2.13356800
O	-7.21326000	1.08251300	-0.28780300
H	-0.73481700	-3.42453600	0.88367100
C	-2.84416900	-1.06215400	0.44596500
C	-1.49080200	-1.51628700	0.96435000
H	-1.59228400	-1.73572200	2.03215400