

Electronic Supplementary Information For

**Disclosing the Mechanism and Origin of Stereoselectivity of NHC-Catalyzed  
Transformation Reaction of Enal with Acyl Azolium as Key Intermediate**

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## Part 1: Energy profile for the *Re*-face addition

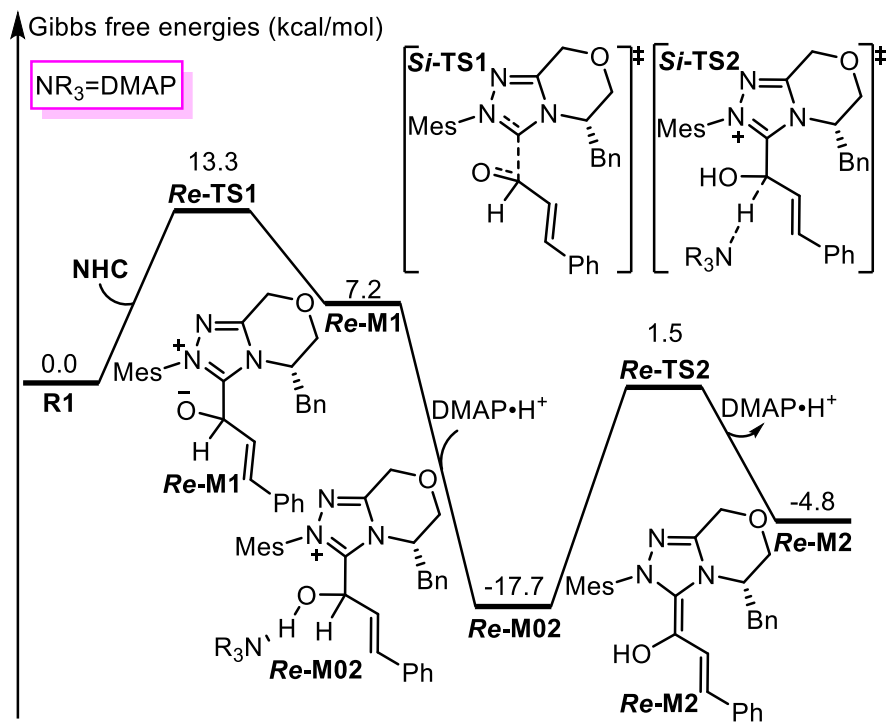
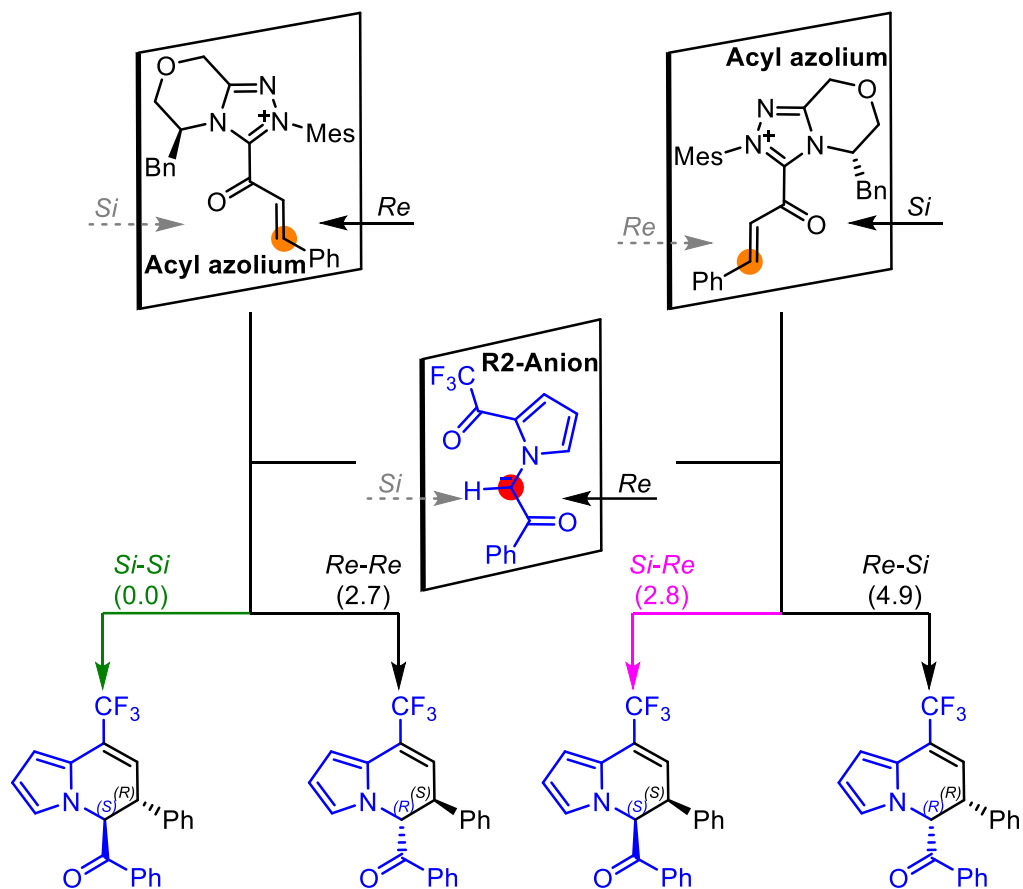


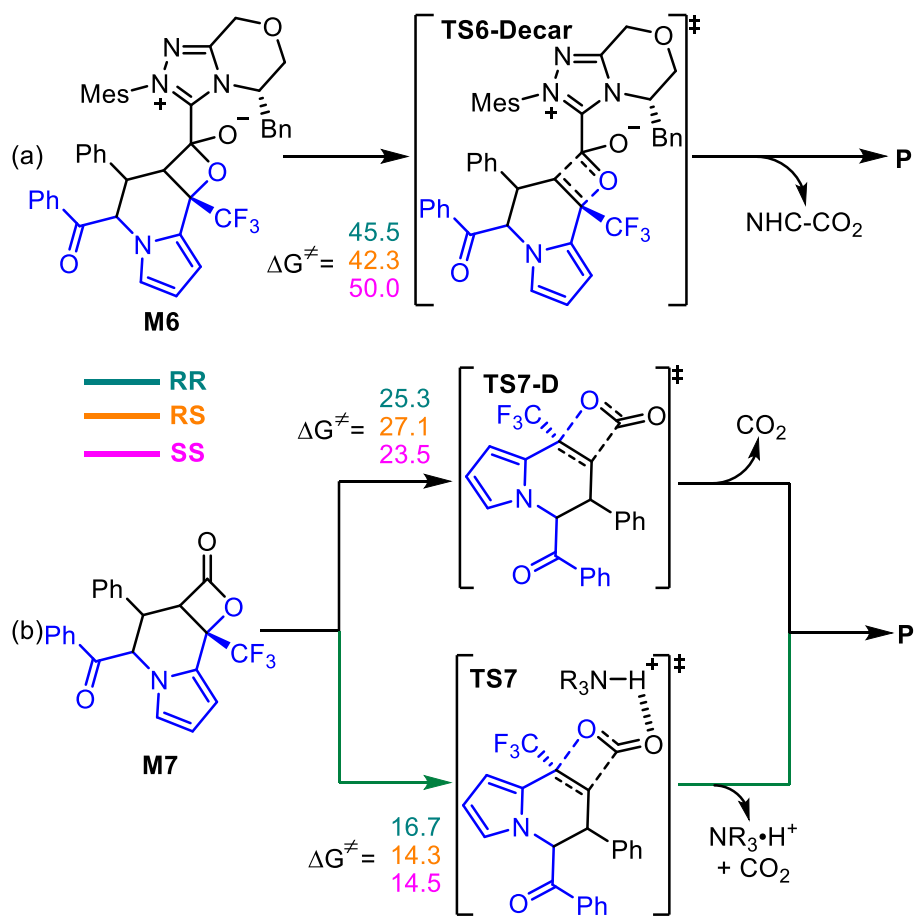
Fig. S1 Energy profile for the formation of *Re*-M2.

## Part 2: Illustration of stereochemistry



Scheme S1 Illustration of the stereoselective addition mode.

### Part 3: Possible pathways for decarboxylation process



**Scheme S2** Possible Pathways for Decarboxylation Process.

## Part 4: Energy profile for the reaction between acyl azolium intermediate Si-M3 and R2-anion

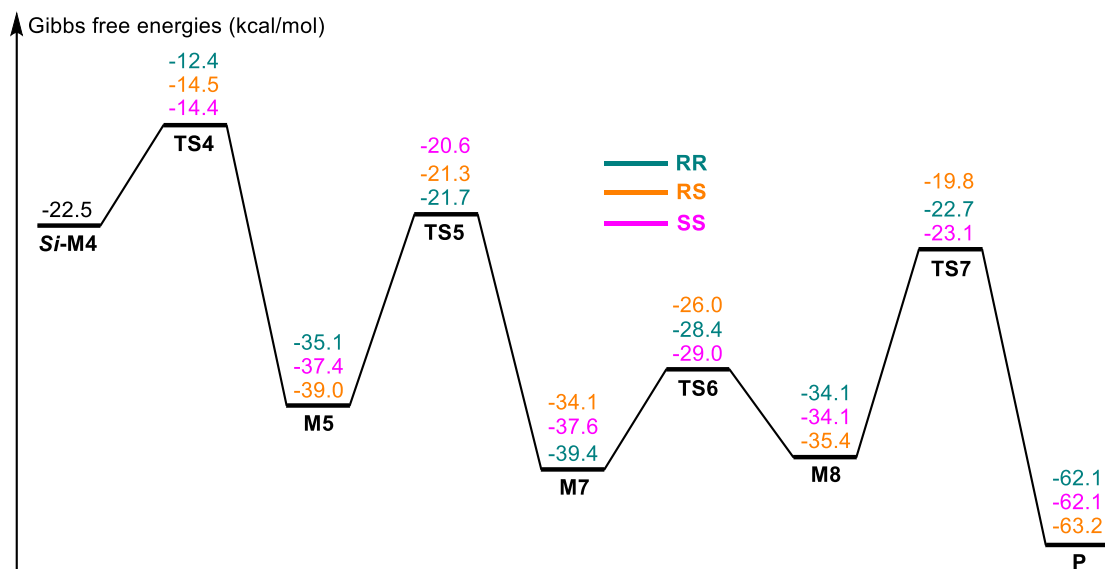


Fig. S2 Energy profile for the reaction between acyl azolium intermediate Si-M3 and R2-anion.

## Part 5: Different configuration of complex Si-M4

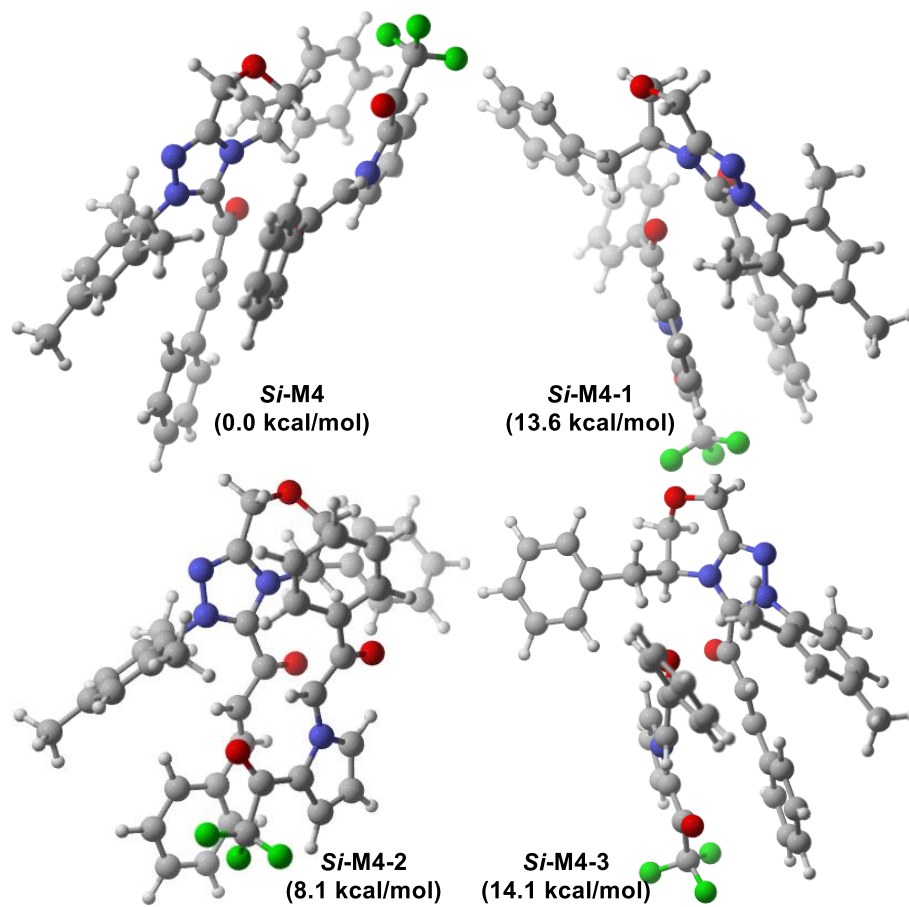
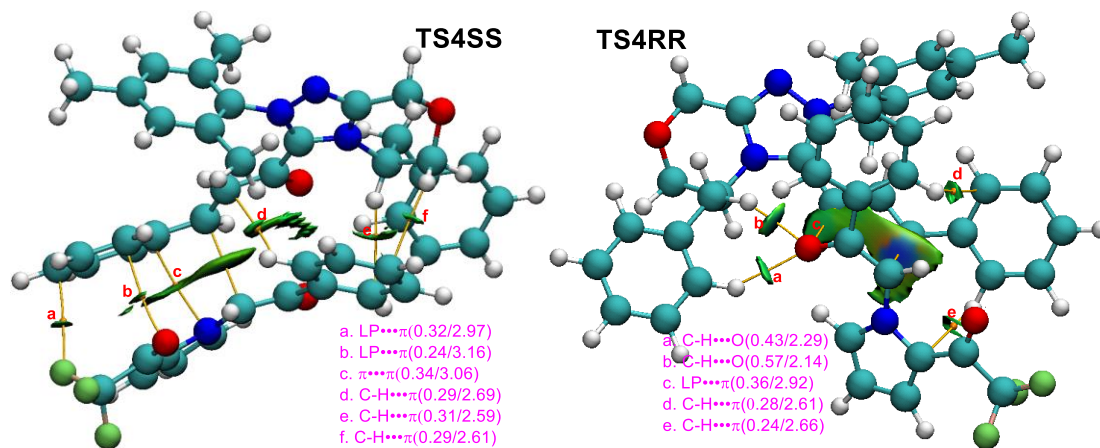


Fig. S3 Different configurations of the complex *Si-M4*.

## Part 6: NCI and AIM analysis for TS4RR and TS4SS



**Fig. S4** NCI and AIM analyses for the enantioselective transition states of **TS4SS** and **TS4RR** (distance in Å and Laplacian of electron density  $\nabla^2\rho$  in  $10^{-1}$  a.u.).

## Part 7: Base effect on the proton transfer process

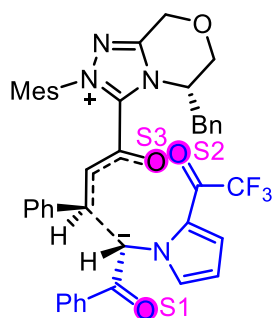
Table S1. Energy barriers for Brønsted acid promoted proton transfer

	H-Bond Abstractor		
	DMAP	DBU	DIPEA
<b>R1+NHC</b>	0.0	0.0	0.0
<b><i>Si</i>-M02</b>	-15.4	-12.0	-15.3
<b><i>Si</i>-TS2</b>	-0.7	3.2	-2.6



## Part 8: Hydrogen bond effect on the C-C bond formation

Table S2. Energy barriers for DMAP•H<sup>+</sup> participated the C-C bond formation step



	S0	S1	S2	S3
RR	4.9	2.9	3.2	3.8
RS	2.7	3.0	3.9	3.3
SR	0.0	0.0	0.0	0.0
SS	2.8	1.6	4.0	1.8

## Part 9: Solvation effect on the C-C bond formation step

**Table S3.** Solvent effects on the C-C bond formation step

	Toluene	Gas phase	THF
RR	4.9	2.1	3.4
RS	2.7	1.7	1.6
SR	0.0	0.0	0.0
SS	2.8	1.5	1.3

## Part 10: Energies and Cartesian coordinates of all the stationary points

### 1. Energies of all the stationary points

	G (a.u.)	G-correct (a.u.)	Imaginary frequency (cm <sup>-1</sup> )
<b>R1</b>	-422.6862870	0.11003	-
<b>R2</b>	-1043.675010	0.172791	-
<b>R2-Anion</b>	-1043.164808	0.160186	-
<b>NHC</b>	-1052.757028	0.353287	-
<b>DQ</b>	-1240.434406	0.560574	-
<b>DQ•H</b>	-1241.147138	0.574546	-
<b>DMAP</b>	-381.9684470	0.129384	-
<b>DMAP•H<sup>+</sup></b>	-382.3898570	0.145535	-
<b>CO<sub>2</sub></b>	-188.5171010	-0.006883	-
<b>Re-TS1</b>	-1475.424292	0.490192	-170.13
<b>Re-M1</b>	-1475.434155	0.489975	-
<b>Re-M02</b>	-1857.873499	0.65837	-
<b>Re-TS2</b>	-1857.831559	0.655358	-772.06
<b>Re-M2</b>	-1475.451377	0.487002	-
<b>Si-TS1</b>	-1475.424367	0.491929	-175.20
<b>Si-M1</b>	-1475.433316	0.493197	-
<b>Si-M02</b>	-1857.870435	0.655231	-
<b>Si-TS2</b>	-1857.834384	0.65347	-941.86
<b>Si-M2</b>	-1475.455900	0.487491	-
<b>Si-TS3</b>	-2715.876541	1.079498	-1227.96
<b>Si-M3</b>	-2715.883194	1.083967	-
<b>Si-M4</b>	-2517.932860	0.669881	-
<b>Si-M4-1</b>	-2517.927713	0.668477	-
<b>Si-M4-2</b>	-2517.936173	0.672081	-
<b>Si-M4-3</b>	-2517.926641	0.670877	-
<b>TS4RR</b>	-2517.918563	0.668321	-192.45
<b>TS4RS</b>	-2517.923285	0.670755	-131.78
<b>TS4SR</b>	-2517.924305	0.668776	-32.49
<b>TS4SS</b>	-2517.921566	0.667895	-113.41
<b>M5RR</b>	-2517.958712	0.674387	-
<b>M5RS</b>	-2517.958352	0.672994	-
<b>M5SR</b>	-2517.954532	0.670438	-
<b>M5SS</b>	-2517.958418	0.672159	-
<b>TS5RR</b>	-2517.936745	0.676588	-194.31
<b>TS5RS</b>	-2517.940179	0.674128	-255.21
<b>TS5SR</b>	-2517.934017	0.673905	-106.19

<b>TS5SS</b>	-2517.935511	0.678812	-66.34
<b>M6RR</b>	-2517.970163	0.680936	-
<b>M6RS</b>	-2517.959266	0.677351	-
<b>M6SR</b>	-2517.960693	0.678796	-
<b>M6SS</b>	-2517.968485	0.67854	-
<b>TS6RR</b>	-2517.952857	0.678762	-109.22
<b>TS6RS</b>	-2517.946969	0.67376	-148.31
<b>TS6SR</b>	-2517.943407	0.677417	-135.36
<b>TS6SS</b>	-2517.954314	0.673682	-109.49
<b>M7RR</b>	-1465.205070	0.295228	-
<b>M7RS</b>	-1465.201764	0.293107	-
<b>M7SR</b>	-1465.201756	0.293115	-
<b>M7SS</b>	-1465.205062	0.295235	-
<b>TS7RR</b>	-1847.577580	0.458881	-273.36
<b>TS7RS</b>	-1847.570326	0.456912	-250.33
<b>TS7SR</b>	-1847.570713	0.456524	-250.36
<b>TS7SS</b>	-1847.578236	0.458221	-273.50
<b>PRR</b>	-1276.721297	0.280568	-
<b>PRS</b>	-1276.723025	0.279664	-
<b>PSR</b>	-1276.723014	0.279675	-
<b>PSS</b>	-1276.721297	0.280568	-
<b>TS6RR-Decar</b>	-2517.910323	0.677014	-915.80
<b>TS6RS-Decar</b>	-2517.897524	0.674174	-917.30
<b>TS6SR-Decar</b>	-2517.904033	0.675661	-901.63
<b>TS6SS-Decar</b>	-2517.900364	0.675066	-977.18
<b>TS7RR-D</b>	-1465.168817	0.293416	-283.92
<b>TS7RS-D</b>	-1465.154162	0.291334	-429.17
<b>TS7SR-D</b>	-1465.154141	0.291355	-428.28
<b>TS7SS-D</b>	-1465.168795	0.293438	-286.72

## 2. Cartesian coordinates of all the stationary points

### R1

C	-3.40926700	0.38266000	-0.00014200
O	-3.84506800	-0.75055200	0.00018100
H	-4.10252900	1.24611000	0.00011000
C	-1.97287600	0.72176200	-0.00007700
C	-1.05294600	-0.25571400	-0.00006700
H	-1.71240000	1.77589800	-0.00004900
H	-1.43349300	-1.27710100	-0.00009700
C	0.40375300	-0.11049600	-0.00002700
C	1.19223000	-1.26845900	-0.00004200
C	1.04276900	1.13874200	0.00002200

C	2.58049200	-1.18617500	-0.00001000
H	0.70499500	-2.23953300	-0.00008000
C	2.42793600	1.22139700	0.00005500
H	0.45334300	2.05003800	0.00003200
C	3.20134000	0.05958700	0.00003800
H	3.17622900	-2.09289000	-0.00002400
H	2.90955000	2.19369000	0.00009200
H	4.28427700	0.12838800	0.00006200

**R2**

C	0.18395300	2.34443200	-0.91230300
C	-0.76681300	2.20223000	-1.91038900
C	-1.67490900	1.23225400	-1.46936600
C	-1.25434500	0.79769400	-0.21117200
N	-0.10412300	1.50147200	0.10783100
H	1.04709200	2.99350000	-0.85017300
H	-0.78934500	2.74287000	-2.84390100
H	-2.54479800	0.86742900	-1.99494400
C	-1.86339500	-0.19876400	0.63579100
O	-1.43795700	-0.62700500	1.69443500
C	-3.19453600	-0.78436700	0.10635900
F	-3.00347200	-1.40784300	-1.06515800
F	-4.10115300	0.18077500	-0.09266700
F	-3.69492900	-1.65886000	0.96753200
C	0.69523800	1.44878700	1.33119700
H	0.64539500	2.41204600	1.84219500
H	0.29267000	0.67129400	1.97822300
C	2.16337700	1.19631800	0.97444500
O	2.97955400	2.07170500	1.17924200
C	2.53747900	-0.09965300	0.34063900
C	3.81501300	-0.21052700	-0.21875100
C	1.66372100	-1.19051600	0.30682200
C	4.21241500	-1.39877900	-0.81594300
H	4.47745400	0.64750600	-0.17389700
C	2.06865700	-2.38266000	-0.28598500
H	0.67890900	-1.12638400	0.75945000
C	3.33775700	-2.48542000	-0.85020900
H	5.20140800	-1.48249400	-1.25383400
H	1.39333000	-3.23122800	-0.30568000
H	3.64830100	-3.41526300	-1.31583900

**R2-Anion**

C	0.63960700	2.51606800	-0.04687400
C	1.99596600	2.87313500	-0.06601700

C	2.73760000	1.70453700	-0.01472700
C	1.82297500	0.62858200	0.03443600
N	0.53255600	1.16879100	0.01504700
H	-0.26622800	3.09956200	-0.07460000
H	2.37250300	3.88480900	-0.11166000
H	3.81269600	1.60699600	-0.01146400
C	2.12004500	-0.76577000	0.06363400
O	1.36016600	-1.72662300	0.10324700
C	3.63547100	-1.09527200	0.03229900
F	4.28930200	-0.56023100	1.07881000
F	4.22874000	-0.62790400	-1.07988600
F	3.83529100	-2.41155200	0.06860000
C	-0.66350500	0.42255600	0.04467600
H	-0.51629900	-0.62913200	0.19897800
C	-1.90844900	1.01731300	-0.07012700
O	-2.16351100	2.25457200	-0.17486400
C	-3.09261600	0.07033200	-0.03838300
C	-4.34681800	0.61976700	0.24539000
C	-3.01438200	-1.30310700	-0.30128900
C	-5.48557900	-0.17824100	0.29666500
H	-4.39255600	1.69047600	0.41595200
C	-4.15191000	-2.10355200	-0.25289400
H	-2.06081300	-1.74757600	-0.56897200
C	-5.39338100	-1.54674300	0.05079500
H	-6.44981900	0.26782200	0.52504000
H	-4.07028000	-3.16613700	-0.46374900
H	-6.28048400	-2.17240500	0.08486800

**DMAP**

C	-1.94792300	-1.12959500	0.00550300
C	-0.56372600	-1.19682900	-0.00979300
C	0.18364000	-0.00003000	-0.02209600
C	-0.56372200	1.19681100	-0.00968500
C	-1.94789600	1.12962100	0.00561900
N	-2.66360400	0.00000300	0.01279300
H	-2.51903100	-2.05610800	0.01404500
H	-0.08090700	-2.16552500	-0.01111900
H	-0.08085400	2.16548200	-0.01089400
H	-2.51901200	2.05612500	0.01427800
N	1.54973600	-0.00000100	-0.04536900
C	2.26874100	1.25683400	0.01785200
H	2.04680000	1.80779000	0.94057900
H	3.33893100	1.05709300	-0.01292500
H	2.01902900	1.90001600	-0.83355200

C	2.26876100	-1.25681700	0.01805100
H	2.01943100	-1.89997900	-0.83348400
H	3.33895900	-1.05705000	-0.01225100
H	2.04647200	-1.80783300	0.94064900

**DMAP•H<sup>+</sup>**

C	-1.87711000	-1.17932000	0.01119400
C	-0.51430000	-1.21672500	0.00997200
C	0.23533300	-0.00005100	-0.00022500
C	-0.51425600	1.21664000	-0.01059900
C	-1.87707100	1.17934700	-0.01112200
N	-2.54117400	0.00003400	0.00031700
H	-2.48606500	-2.07415400	0.02066200
H	-0.02575200	-2.18010700	0.02080700
H	-0.02562000	2.17997500	-0.02206400
H	-2.48594600	2.07423500	-0.02051000
N	1.56888400	0.00000500	-0.00010600
C	2.30453300	1.26325200	0.01929800
H	2.03991200	1.85004600	0.90328600
H	3.36976500	1.04983900	0.05400500
H	2.09639800	1.84894600	-0.88066600
C	2.30463100	-1.26322200	-0.01894400
H	2.04067900	-1.85003100	-0.90309700
H	3.36986700	-1.04973500	-0.05283900
H	2.09578100	-1.84885100	0.88090200
H	-3.55354900	0.00004000	0.00059000

**NHC**

C	0.57038700	1.74729500	-0.75856400
C	1.51607100	2.60652200	-1.54403100
C	3.16052900	2.02959100	-0.00088800
C	2.23426400	1.46470100	1.07479600
C	-0.09110200	0.45298700	0.97088200
H	1.94841200	2.02303600	-2.37022400
H	3.44983700	1.23614900	-0.70539800
H	2.06845800	2.24335300	1.82763200
N	-0.64303700	1.41327800	-1.06658600
N	-1.01598000	0.62146000	0.00319700
N	0.94168900	1.18640500	0.43900800
H	4.06284300	2.43185200	0.46551300
H	0.98798600	3.46470700	-1.96202900
O	2.53480000	3.09340400	-0.69596600
C	2.80986200	0.22704400	1.77951900
H	3.70023800	0.55476600	2.32757000

H	2.07188100	-0.10219100	2.51524000
C	3.16520900	-0.91411700	0.85525100
C	4.45924400	-1.05143400	0.34517000
C	2.19544400	-1.84927000	0.48275500
C	4.77531500	-2.08966700	-0.52783200
H	5.22754100	-0.33925300	0.63854400
C	2.50731800	-2.88764000	-0.39031300
H	1.19339100	-1.74651200	0.88733900
C	3.79800200	-3.00943300	-0.90063200
H	5.78589500	-2.18255100	-0.91279000
H	1.74089000	-3.60555100	-0.66764000
H	4.04310100	-3.81984600	-1.57950000
C	-2.34326900	0.08654400	0.01417500
C	-3.41441400	0.97033100	0.18994300
C	-2.53312000	-1.28476000	-0.16749200
C	-4.70358900	0.44398200	0.18221500
C	-3.84336000	-1.76687900	-0.16546000
C	-4.93725000	-0.92166100	0.00823800
H	-5.54702000	1.11697000	0.31885100
H	-4.00977300	-2.83177400	-0.31048300
C	-3.17103700	2.44263800	0.38803400
H	-2.40588000	2.60820900	1.15267300
H	-2.80996200	2.90622300	-0.53400000
H	-4.08892200	2.94577600	0.69716000
C	-6.34195100	-1.46763100	0.03406700
H	-6.68614800	-1.60432400	1.06437100
H	-7.03997800	-0.78501200	-0.45691800
H	-6.39916600	-2.43676600	-0.46633200
C	-1.36986400	-2.22407100	-0.34414900
H	-0.58071200	-1.77729900	-0.95513600
H	-0.92892300	-2.47307200	0.62650800
H	-1.69722900	-3.15255300	-0.81666500

**DQ**

C	-2.80847300	1.28105500	0.06787600
C	-1.45904100	1.23397200	0.05902900
C	-0.69378100	0.00006300	-0.00028500
C	-1.45900500	-1.23386200	-0.05985000
C	-2.80843600	-1.28102700	-0.06796900
C	-3.57341300	-0.00003500	0.00065300
H	-0.91526500	2.16404800	0.12828700
H	-0.91519300	-2.16384800	-0.13003400
C	0.69377100	0.00005500	-0.00005900
C	1.45898900	-1.23387000	0.05956000



C	1.45903700	1.23396500	-0.05933500
C	2.80841900	-1.28103800	0.06792500
H	0.91516600	-2.16386300	0.12957200
C	2.80847100	1.28104100	-0.06791000
H	0.91527200	2.16403100	-0.12880500
C	3.57340300	-0.00003300	-0.00034800
C	-3.58544400	-2.59471600	-0.15050900
C	-4.45936000	-2.60904600	-1.41946400
C	-2.64333600	-3.80294600	-0.21744700
C	-4.47076100	-2.75832200	1.10024900
H	-5.19706800	-1.80744900	-1.40366200
H	-3.83784800	-2.50191900	-2.31433100
H	-4.98534500	-3.56707400	-1.48566600
H	-2.00785300	-3.87435100	0.67154200
H	-3.24119500	-4.71682300	-0.27196300
H	-2.00272100	-3.77221700	-1.10497800
H	-4.99399200	-3.71880500	1.04949600
H	-3.85751100	-2.75483900	2.00716400
H	-5.21067300	-1.96174100	1.17089300
C	-3.58550200	2.59476000	0.15010800
C	-4.47236800	2.75712000	-1.09970400
C	-4.45791700	2.61015300	1.42009900
C	-2.64344300	3.80314100	0.21482300
H	-3.86024300	2.75304400	-2.00737600
H	-5.21216700	1.96028900	-1.16877000
H	-4.99579600	3.71750200	-1.04910000
H	-3.83535700	2.50353300	2.31429600
H	-4.98363100	3.56833400	1.48624700
H	-5.19577200	1.80866300	1.40571600
H	-3.24133400	4.71702800	0.26883000
H	-2.00204200	3.77348900	1.10182600
H	-2.00875100	3.87358500	-0.67480700
C	3.58556000	2.59470400	-0.15014000
C	4.45842500	2.60982300	-1.41982800
C	2.64353700	3.80309200	-0.21545800
C	4.47193600	2.75732600	1.09997800
H	5.19638500	1.80844200	-1.40494100
H	3.83619000	2.50282400	-2.31420600
H	4.98401700	3.56806000	-1.48609600
H	2.00857900	3.87377500	0.67396500
H	3.24145400	4.71695700	-0.26951500
H	2.00239500	3.77321000	-1.10264000
H	4.99548900	3.71763800	1.04931400
H	3.85942300	2.75359300	2.00739000

H	5.21162100	1.96044100	1.16960500
C	3.58539500	-2.59475000	0.15046000
C	4.45889400	-2.60927700	1.41971200
C	2.64328100	-3.80299600	0.21689100
C	4.47116500	-2.75812100	-1.10000000
H	5.19678400	-1.80784100	1.40413500
H	3.83711000	-2.50199100	2.31436800
H	4.98462600	-3.56743100	1.48609400
H	2.00796700	-3.87417300	-0.67223700
H	3.24113000	-4.71688700	0.27127700
H	2.00249700	-3.77249600	1.10431000
H	4.99455800	-3.71850800	-1.04912500
H	3.85823900	-2.75468700	-2.00713400
H	5.21095500	-1.96139400	-1.17032300
O	4.79998800	-0.00007300	-0.00088500
O	-4.80000300	-0.00011900	0.00176500

**DQ•H<sup>-</sup>**

C	0.71584900	-0.00080000	0.00734200
C	1.44892300	-1.15209600	0.32636000
C	2.84345600	-1.19357200	0.29979500
C	3.52346400	-0.01201900	-0.04913800
C	2.84035200	1.18609900	-0.32851400
C	1.44534300	1.15260900	-0.31087700
C	-0.75740700	-0.00178800	0.01101300
C	-1.48976700	-1.16107200	-0.29052100
C	-2.87432000	-1.20011900	-0.30995500
C	-3.64052400	-0.00373500	-0.00312200
C	-2.87888400	1.19364200	0.31139000
C	-1.49413000	1.15634700	0.30627800
H	0.89286600	-2.03202500	0.62437500
H	0.88579700	2.04076600	-0.57595300
H	-0.93069700	-2.05448200	-0.55569500
H	-0.93925900	2.05082800	0.57645500
C	3.60287100	-2.47971500	0.67023500
C	2.64285100	-3.62312200	1.02890300
C	4.45931000	-2.96820100	-0.51256100
C	4.49850800	-2.22898500	1.89661000
H	2.01388100	-3.37040400	1.88742400
H	1.99104700	-3.88638900	0.18991500
H	3.22766300	-4.51017800	1.29185200
H	5.27852000	-2.28230800	-0.73107600
H	4.89932800	-3.94312100	-0.27462100
H	3.84533200	-3.08426600	-1.41144200

H	5.02593100	-3.15109900	2.16773500
H	5.23433800	-1.45026300	1.69520100
H	3.88964500	-1.92189400	2.75282000
C	3.59396800	2.49339100	-0.63269900
C	4.46358300	2.88270400	0.57646500
C	4.47672900	2.35577500	-1.88733900
C	2.62700500	3.65693300	-0.89600500
H	3.83463000	3.04201600	1.45790600
H	5.19203900	2.10410700	0.80423300
H	4.99827300	3.81635900	0.36612500
H	3.89794500	1.96194500	-2.72866700
H	4.86682800	3.33813000	-2.17549100
H	5.33824800	1.70855200	-1.71575500
H	3.20647800	4.56926200	-1.06822800
H	2.00729000	3.48022200	-1.78057300
H	1.96626500	3.83522500	-0.04269100
C	-3.64180500	2.47919200	0.65176900
C	-2.70771400	3.65556700	0.96042300
C	-4.52518300	2.88931800	-0.54088800
C	-4.52575400	2.24944200	1.89085100
H	-2.07034000	3.45234600	1.82785200
H	-2.06053900	3.89502000	0.10935300
H	-3.30705200	4.54481300	1.18618800
H	-5.21519800	2.08105000	-0.78305500
H	-5.09329600	3.79747600	-0.30062200
H	-3.90066300	3.09974000	-1.41677900
H	-5.11283700	3.14948800	2.11521000
H	-5.19852300	1.41018400	1.71270900
H	-3.89970300	2.02545100	2.76196600
C	-3.63221800	-2.48568900	-0.66125600
C	-2.69390800	-3.66086300	-0.96131200
C	-4.52876600	-2.89882300	0.52036000
C	-4.50194900	-2.25394000	-1.91021700
H	-2.04553200	-3.45482600	-1.81988300
H	-2.05761600	-3.90276700	-0.10277800
H	-3.29005500	-4.54957300	-1.19751400
H	-5.22291000	-2.09199900	0.75541200
H	-5.09247500	-3.80767400	0.27238900
H	-3.91409800	-3.10906900	1.40316600
H	-5.08999600	-3.15196400	-2.14006100
H	-5.17335500	-1.41192300	-1.73982900
H	-3.86594000	-2.03339700	-2.77515000
O	-4.91500800	-0.00454300	-0.00989800
O	4.92054000	-0.02078600	-0.06802700

H	5.20417700	-0.15960700	-0.97935300
<b>CO<sub>2</sub></b>			
C	0.00000000	0.00052400	0.00000000
O	1.16273800	0.00188000	0.00000000
O	-1.16273800	-0.00227300	0.00000000
<b>Re-TS1</b>			
C	-0.56782200	0.94061900	2.16352500
C	-0.01368700	1.68809000	3.33881600
C	1.85096200	2.18525700	2.05214200
C	1.56719000	1.24488200	0.87787000
C	-0.51841000	-0.01254000	0.16100100
H	-0.37620400	2.72600800	3.33301400
H	1.37310400	3.15877700	1.87748000
H	2.22204500	0.36915800	0.94489500
N	-1.72340800	0.35943100	2.05675200
N	-1.66895700	-0.21987800	0.81125600
N	0.18666800	0.75274300	1.03155400
H	2.92951900	2.33145700	2.13872000
H	-0.33164700	1.20813300	4.26521200
O	1.39478700	1.64731900	3.28063600
C	1.79096200	1.91820400	-0.48735900
H	2.84225400	2.22896400	-0.51143400
H	1.64421100	1.16384900	-1.26742800
C	0.88037500	3.09065000	-0.76695600
C	1.19150300	4.39010500	-0.35464800
C	-0.31147100	2.87219700	-1.46468500
C	0.31509300	5.44423600	-0.60167200
H	2.13472900	4.58227600	0.15244000
C	-1.19022300	3.92491100	-1.70936000
H	-0.50870100	1.87253800	-1.84748100
C	-0.88373800	5.21162700	-1.27184700
H	0.57245000	6.44770400	-0.27755200
H	-2.11028400	3.74069600	-2.25666900
H	-1.56651500	6.03257200	-1.46639600
C	-2.78376800	-0.99767400	0.35068900
C	-3.46663900	-0.59229300	-0.80050700
C	-3.13424900	-2.14354700	1.07334500
C	-4.54569700	-1.37359800	-1.21446200
C	-4.22301500	-2.88492600	0.61973000
C	-4.94280800	-2.51328500	-0.51662500
H	-5.08945800	-1.07862400	-2.10838700
H	-4.50864400	-3.78218100	1.16333900

C	-3.04651200	0.62065500	-1.58705600
H	-2.81509200	1.46232200	-0.92720200
H	-2.14764200	0.41314800	-2.18135100
H	-3.84581200	0.92247100	-2.26680100
C	-6.13552600	-3.31623600	-0.96704600
H	-7.04777200	-2.95887100	-0.47843700
H	-6.28351900	-3.23301100	-2.04592200
H	-6.01846000	-4.37263900	-0.71478200
C	-2.35310800	-2.57744300	2.28582100
H	-1.27593000	-2.53596200	2.09500100
H	-2.55374600	-1.92399600	3.13855200
H	-2.61570100	-3.60060000	2.55958600
C	0.03640200	-0.91441900	-1.52742900
O	0.19776900	-0.12216000	-2.48407600
H	-0.87625100	-1.54637200	-1.48630100
C	1.22060700	-1.60749300	-0.90044800
C	2.44800600	-1.45534100	-1.40741200
H	1.01958300	-2.25320800	-0.04529300
H	2.52736400	-0.83575300	-2.30026700
C	3.69247200	-2.04929200	-0.89545500
C	4.83177500	-2.05465400	-1.71025200
C	3.79201200	-2.60141600	0.39008400
C	6.02712800	-2.61176500	-1.26721400
H	4.77009800	-1.62112100	-2.70465400
C	4.98527200	-3.15727200	0.83456000
H	2.93014700	-2.58267900	1.05100000
C	6.10782000	-3.16737400	0.00687200
H	6.89659800	-2.61020100	-1.91684100
H	5.04362200	-3.57807400	1.83342300
H	7.03966700	-3.59931600	0.35697500

**Re-M1**

C	-0.99470900	1.43506900	1.61272100
C	-0.69838400	2.58888200	2.51350500
C	1.57555900	2.43698800	2.05017500
C	1.40155200	1.43041000	0.87582100
C	-0.45122500	-0.22069000	0.28616000
H	-0.72611500	3.53588800	1.95463000
H	1.58442200	3.45676200	1.64818600
H	2.08193200	0.58527000	0.99476100
N	-2.09948500	0.77100900	1.45473900
N	-1.74336400	-0.25189800	0.61649600
N	0.04116500	0.86492400	0.92142200
H	2.53108500	2.24602800	2.53996300

H	-1.42083300	2.62328400	3.32888700
O	0.58473800	2.34893500	3.05505400
C	1.67377500	2.09715200	-0.49043100
H	2.68089200	2.52645100	-0.43780300
H	1.64955500	1.30505600	-1.24598700
C	0.64906500	3.15145600	-0.83540900
C	0.84541100	4.50679300	-0.55177200
C	-0.55596900	2.75398100	-1.42972200
C	-0.15373300	5.44220000	-0.81557000
H	1.79329300	4.83781300	-0.13326000
C	-1.55488800	3.68829000	-1.68959400
H	-0.66424800	1.70556100	-1.70780700
C	-1.36185200	5.03237600	-1.37360500
H	0.01537700	6.49054200	-0.59058400
H	-2.48320400	3.36890200	-2.15438500
H	-2.14135800	5.75935000	-1.57815500
C	-2.71910200	-1.23899700	0.23903500
C	-3.33096800	-1.13275300	-1.01165200
C	-3.01114700	-2.25192600	1.15466500
C	-4.27985100	-2.10164000	-1.33573800
C	-3.96834300	-3.19352600	0.78360500
C	-4.61221900	-3.13088300	-0.45375000
H	-4.76948500	-2.04954800	-2.30478800
H	-4.21221400	-3.99654600	1.47449000
C	-2.95356400	-0.03147100	-1.96371200
H	-3.05781700	0.94527800	-1.47760200
H	-1.90381600	-0.13587300	-2.27252800
H	-3.59760300	-0.04985000	-2.84445400
C	-5.66638500	-4.14297900	-0.82080700
H	-6.65807500	-3.79246300	-0.51707200
H	-5.69184600	-4.31268500	-1.89940300
H	-5.48678800	-5.09903200	-0.32422200
C	-2.30030000	-2.32057700	2.47981100
H	-1.21703800	-2.40422600	2.33902700
H	-2.48399700	-1.41874000	3.07080400
H	-2.63656800	-3.18585100	3.05252100
C	0.22613400	-1.06919000	-0.80911900
O	0.29253700	-0.31381900	-1.90514500
H	-0.44563600	-1.96315500	-0.87664400
C	1.54600900	-1.60903100	-0.26177700
C	2.67466700	-1.45005400	-0.95580400
H	1.50842200	-2.16094600	0.67949900
H	2.57362200	-0.89822400	-1.89019200
C	4.01968500	-1.93381300	-0.60451900

C	5.09221900	-1.61654400	-1.44773000
C	4.28422100	-2.69825900	0.54167100
C	6.38540800	-2.04221900	-1.15948900
H	4.90104000	-1.02817200	-2.34105700
C	5.57412100	-3.12412700	0.83179700
H	3.47175700	-2.96708500	1.21002100
C	6.63204800	-2.79794900	-0.01702800
H	7.19999200	-1.78464300	-1.82904800
H	5.75688800	-3.71670000	1.72284500
H	7.63852600	-3.13344100	0.21104200

**Re-M02**

C	-1.95542500	-2.22544600	1.73664500
C	-3.13890000	-3.02736400	2.18303200
C	-4.55287900	-1.60827800	1.02291400
C	-3.46769000	-0.66302800	0.45875100
C	-0.94724600	-0.50114900	0.86743100
H	-3.35146600	-3.83462900	1.46869400
H	-4.72627100	-2.43270300	0.32152400
H	-3.62867900	0.35394400	0.82270400
N	-0.70035100	-2.37797100	2.05011100
N	-0.08753100	-1.30060500	1.49256300
N	-2.15190700	-1.08718600	0.99701500
H	-5.47738600	-1.04070800	1.13590300
H	-2.93940100	-3.45660600	3.16507800
O	-4.22514600	-2.13573700	2.29133900
C	-3.46383200	-0.66029600	-1.08311200
H	-4.45839800	-0.31867700	-1.39095900
H	-2.74184200	0.08636400	-1.42623500
C	-3.14739200	-2.00548500	-1.69475600
C	-4.15856900	-2.88975400	-2.08259800
C	-1.81459700	-2.39317300	-1.86497500
C	-3.84598800	-4.14495800	-2.59881600
H	-5.19974000	-2.58932600	-1.99058100
C	-1.49940200	-3.64890600	-2.37700400
H	-1.02959300	-1.67977900	-1.62901100
C	-2.51516600	-4.53121900	-2.73811800
H	-4.64246000	-4.81827900	-2.89782500
H	-0.45963200	-3.93265300	-2.50960100
H	-2.27158300	-5.50865600	-3.14086200
C	1.33331300	-1.09880200	1.63149200
C	2.17353500	-1.63374600	0.65376400
C	1.78987600	-0.37266800	2.73382600
C	3.54012100	-1.41461000	0.80603400

C	3.16442000	-0.16727400	2.82973000
C	4.04877600	-0.67878400	1.87740900
H	4.22120000	-1.80949300	0.05679800
H	3.55323000	0.40336400	3.66885200
C	1.61224800	-2.37458000	-0.52795600
H	0.90298300	-3.14810700	-0.21737800
H	1.08049900	-1.67547600	-1.18312800
H	2.41192800	-2.84324500	-1.10366800
C	5.53120300	-0.45179800	2.00691200
H	5.99926700	-1.26948100	2.56404500
H	6.00607100	-0.40347200	1.02234700
H	5.74094200	0.47618900	2.54496600
C	0.82808500	0.16904000	3.75792100
H	0.18377600	0.94648000	3.33093900
H	0.17950100	-0.62223900	4.14417900
H	1.36876500	0.60971400	4.59591400
C	-0.55322100	0.79216500	0.17693400
O	-0.33548400	0.54251700	-1.17543500
H	0.64713500	0.74132200	-1.34545700
C	-1.56567200	1.87885300	0.44505300
C	-2.10447400	2.60751100	-0.53502100
H	-1.80489000	2.05397300	1.49325400
H	-1.80388600	2.36761600	-1.55370800
C	-3.08396600	3.69519500	-0.38486900
C	-3.68279800	4.21656200	-1.53786700
C	-3.44895100	4.22743900	0.85987700
C	-4.62932400	5.23283700	-1.45406400
H	-3.40197700	3.81609400	-2.50802600
C	-4.39309000	5.24222800	0.94440000
H	-2.98386200	3.85880400	1.76913100
C	-4.98827500	5.74746200	-0.21187600
H	-5.08356100	5.62360200	-2.35845700
H	-4.66270500	5.64671400	1.91445000
H	-5.72338800	6.54228800	-0.14247900
C	3.01198000	0.22024200	-2.17542000
C	4.39223200	0.21839000	-2.19074800
C	5.09882700	1.03491800	-1.27565000
C	4.30894000	1.82580700	-0.40872800
C	2.93305000	1.74386400	-0.48067300
N	2.26617300	0.95714900	-1.33843800
H	2.46570400	-0.40382000	-2.87844700
H	4.90820200	-0.40249800	-2.91066300
H	4.75791400	2.49016800	0.31765800
H	2.32779500	2.35214600	0.18701800



N	6.45617100	1.05464600	-1.22761000
C	7.13264000	2.01871900	-0.37483800
H	6.88681500	1.85202500	0.67955600
H	8.20849200	1.90397100	-0.49240300
H	6.86223800	3.04791400	-0.63766300
C	7.22328000	0.25858800	-2.17208500
H	7.05510200	0.57939800	-3.20701300
H	8.28285700	0.36295400	-1.94604300
H	6.96193600	-0.80122600	-2.08808200
H	0.39148300	1.06853600	0.67423300

**Re-TS2**

C	-1.28497700	-3.25309200	1.22155600
C	-2.34047500	-3.99785300	1.98596400
C	-3.88054900	-2.43650800	1.23881100
C	-2.89952900	-1.41771400	0.63172500
C	-0.38532300	-1.52940800	0.19061700
H	-2.75558800	-4.80676000	1.36869500
H	-4.15299200	-3.18128700	0.47444700
H	-2.91991300	-0.49127600	1.21069100
N	-0.06831100	-3.62432200	0.95908000
N	0.47696600	-2.55193200	0.31483300
N	-1.54045600	-1.99286500	0.74148900
H	-4.78627600	-1.91718000	1.55152500
H	-1.90540600	-4.43069100	2.88788200
O	-3.34008100	-3.08492700	2.37063200
C	-3.25653300	-1.14344300	-0.83792000
H	-2.50184000	-0.49231500	-1.28714900
H	-3.23866800	-2.09770400	-1.37702800
C	-4.62361400	-0.50443800	-0.93350400
C	-4.79318300	0.82796700	-0.54339800
C	-5.73348400	-1.22657700	-1.37537500
C	-6.04735000	1.42687100	-0.59832200
H	-3.93356900	1.40230400	-0.20765700
C	-6.99102400	-0.62856300	-1.42973900
H	-5.61262400	-2.26063000	-1.68862800
C	-7.15047800	0.69866100	-1.04096500
H	-6.15782700	2.46496500	-0.30096700
H	-7.84462300	-1.19984800	-1.77975000
H	-8.12906000	1.16502700	-1.08645500
C	1.87340300	-2.55531500	-0.01509600
C	2.26745700	-2.96665200	-1.28922800
C	2.77698800	-2.20316800	0.99416300
C	3.64056200	-3.00321900	-1.54843900

C	4.13332000	-2.26368100	0.68809600
C	4.58140200	-2.66169100	-0.57555900
H	3.97888900	-3.31848000	-2.53185900
H	4.85848400	-1.98919400	1.45022400
C	1.24969400	-3.36121700	-2.32435000
H	0.62970800	-4.18559300	-1.95929700
H	0.59184600	-2.51694300	-2.55008100
H	1.74114800	-3.68311200	-3.24333700
C	6.05789200	-2.71664600	-0.86832900
H	6.53261300	-3.52433700	-0.30361100
H	6.24897100	-2.88887100	-1.92888800
H	6.54779300	-1.78363700	-0.57424900
C	2.28262900	-1.76450200	2.34587800
H	1.63587000	-0.88320000	2.25797900
H	1.69640200	-2.55564500	2.82255000
H	3.11792700	-1.51122100	2.99965900
C	-0.08671000	-0.21251900	-0.34085800
O	0.12203200	-0.28074800	-1.74466000
H	1.29941200	0.32644300	0.07092600
C	-0.90546400	0.90121000	0.13180800
C	-1.28080600	1.95501800	-0.61876500
H	-1.11036400	0.90406800	1.20476900
H	-1.11016100	1.90849100	-1.69294400
C	-1.98263000	3.14373600	-0.11746000
C	-2.74572500	3.91485600	-1.00732100
C	-1.95391100	3.52863200	1.23174700
C	-3.47164100	5.01486700	-0.56332600
H	-2.78012300	3.63124800	-2.05587500
C	-2.68133000	4.62654700	1.67641200
H	-1.34498300	2.97123500	1.93800600
C	-3.44624900	5.37417500	0.78248300
H	-4.05956900	5.59188600	-1.26991100
H	-2.64460000	4.90649800	2.72449400
H	-4.01018500	6.23284900	1.13098400
C	2.41012400	2.08456500	0.75790900
C	3.55942500	2.83166700	0.78067700
C	4.69023900	2.40827200	0.02590700
C	4.54119500	1.21242200	-0.72954200
C	3.35382800	0.52683900	-0.68821800
N	2.30814900	0.94814000	0.04485900
H	1.52482400	2.37817500	1.31314900
H	3.58360100	3.73351500	1.37605400
H	5.34340900	0.82411100	-1.34209600
H	3.20557200	-0.39341800	-1.24616600

N	5.84053200	3.10441100	0.02676500
C	6.98391100	2.62469600	-0.73879000
H	6.75610800	2.58935000	-1.80877700
H	7.81975200	3.30412900	-0.58816100
H	7.28712700	1.62643200	-0.40630400
C	5.95242400	4.33356800	0.80254600
H	5.81881000	4.13897600	1.87140200
H	6.94276300	4.75677800	0.65069200
H	5.21075200	5.07022400	0.47922800
H	0.77178100	0.39582500	-1.98191100

**Re-M2**

C	-1.41967500	1.55938400	1.69927100
C	-1.49488300	2.72774800	2.63733700
C	0.66966800	3.26358700	2.05857400
C	0.99905500	2.00133300	1.24117800
C	-0.42919600	0.00510800	0.45409600
H	-1.90363200	3.60686100	2.11858000
H	0.22010600	4.02320900	1.40477100
H	1.79234900	1.45690300	1.76202800
N	-2.39420100	0.82186600	1.30212100
N	-1.80399000	-0.12242600	0.46980800
N	-0.19456400	1.15140700	1.20864700
H	1.59569600	3.66403800	2.47548100
H	-2.14240900	2.48332100	3.48060700
O	-0.20315600	2.99643300	3.13516200
C	1.50235900	2.39326000	-0.16846900
H	2.35987500	3.05867200	-0.01373800
H	1.87987200	1.50324000	-0.67712300
C	0.46718300	3.07919900	-1.03086500
C	0.40976200	4.47431100	-1.11231800
C	-0.45592400	2.33070700	-1.77006500
C	-0.55591800	5.10896100	-1.88942500
H	1.13853700	5.07044600	-0.56767100
C	-1.42258600	2.96251000	-2.54784400
H	-0.40126300	1.24528200	-1.75176800
C	-1.47989100	4.35303400	-2.60565700
H	-0.58086300	6.19280900	-1.93981100
H	-2.12566500	2.36427200	-3.11947800
H	-2.23238800	4.84406800	-3.21404300
C	-2.53422900	-1.32595400	0.21330100
C	-2.57258300	-2.31339100	1.20149000
C	-3.19650300	-1.46799200	-1.00865900
C	-3.30463700	-3.47222300	0.93943000

C	-3.91977600	-2.63806300	-1.22711400
C	-3.98704900	-3.64790500	-0.26438500
H	-3.34518100	-4.25243500	1.69595000
H	-4.43996400	-2.76765100	-2.17342500
C	-1.83791000	-2.12060600	2.50215800
H	-0.76090800	-2.01543000	2.33210500
H	-2.17826500	-1.21156300	3.00752200
H	-1.99915900	-2.97002200	3.16816800
C	-4.80331500	-4.89017800	-0.51447800
H	-4.74416000	-5.19762800	-1.56142800
H	-4.46251900	-5.72024400	0.10826200
H	-5.85866800	-4.71276500	-0.28335300
C	-3.07679000	-0.40019700	-2.05959900
H	-3.25066900	0.59170700	-1.63324200
H	-2.06112600	-0.41016500	-2.47089300
H	-3.78609000	-0.56911800	-2.87223700
C	0.45630500	-0.81308500	-0.21035800
O	-0.08604900	-1.62034400	-1.20660100
H	-0.11434000	-2.53444400	-0.89040900
C	1.86457600	-0.88479800	0.03043400
C	2.72570800	-1.65043200	-0.67953800
H	2.23781400	-0.31826600	0.87947000
H	2.32836800	-2.22060900	-1.51575100
C	4.15934300	-1.79190000	-0.43165500
C	4.90174200	-2.68426700	-1.22298600
C	4.85364800	-1.07543900	0.55994100
C	6.26780000	-2.85955500	-1.03385500
H	4.38803500	-3.24710900	-1.99802400
C	6.21778100	-1.25108600	0.75032200
H	4.32284100	-0.36632700	1.18874200
C	6.93685600	-2.14465900	-0.04365700
H	6.81155600	-3.55793000	-1.66276800
H	6.72673800	-0.68386200	1.52393000
H	8.00289200	-2.27835800	0.10739500

#### Si-TS1

C	-2.47695500	1.51996200	0.38500700
C	-3.86424000	2.05542300	0.51980600
C	-4.35524200	1.49808400	-1.69670000
C	-3.08799400	0.60171900	-1.85484900
C	-0.80092400	0.62695600	-0.77174200
H	-4.55831400	1.26959600	0.85363600
H	-5.20410400	0.86610700	-1.40930800
H	-2.58964800	0.82575400	-2.80093200

N	-1.45443200	1.62418700	1.17763500
N	-0.43904600	1.05181500	0.44427900
N	-2.12603500	0.92563600	-0.79919400
H	-4.58344100	1.97177500	-2.65233400
H	-3.88601000	2.88593200	1.22531100
O	-4.22264600	2.54713800	-0.75910800
C	-3.45152300	-0.90253400	-1.82602300
H	-4.17778500	-1.07502300	-2.62837100
H	-2.55043000	-1.48503800	-2.04239800
C	-4.01338000	-1.33662200	-0.49339000
C	-5.38990600	-1.41431000	-0.26029600
C	-3.13581600	-1.62630000	0.55852000
C	-5.88251600	-1.73147700	1.00412500
H	-6.08422000	-1.23253000	-1.07748000
C	-3.62635200	-1.93698900	1.82352900
H	-2.06642500	-1.62799800	0.35845500
C	-5.00075000	-1.98009000	2.05284700
H	-6.95406900	-1.78692700	1.16754300
H	-2.93313200	-2.15749300	2.62985200
H	-5.38248500	-2.22295900	3.03927700
C	0.88828900	0.98573700	0.98497100
C	1.24484300	-0.12882200	1.74438200
C	1.78406600	2.00582800	0.66526700
C	2.56519000	-0.21187800	2.17972800
C	3.09467600	1.87961200	1.12326600
C	3.50426400	0.77154600	1.86426000
H	2.87591800	-1.08075500	2.75548000
H	3.81828800	2.65207900	0.87340600
C	0.25523400	-1.23294000	1.99473900
H	-0.70215300	-0.83353600	2.34464300
H	0.07234800	-1.77435800	1.05735400
H	0.63676800	-1.93261000	2.74081400
C	4.94645900	0.59718600	2.25671500
H	5.03799400	0.17705800	3.26167000
H	5.43566700	-0.09104600	1.55808700
H	5.48645000	1.54621600	2.22596300
C	1.34701800	3.17760700	-0.17281300
H	1.08973700	2.85587900	-1.18791200
H	0.45746600	3.65380100	0.24984200
H	2.14167700	3.92254100	-0.24000000
C	0.01197100	-0.92892700	-1.80010500
O	-0.40255400	-1.95781800	-1.22561600
H	-0.47483500	-0.59597400	-2.74139800
C	1.45361600	-0.51818800	-1.74414700

C	2.36866400	-1.30572600	-1.17307000
H	1.70610800	0.42553400	-2.22500200
H	2.00640200	-2.23783100	-0.74036200
C	3.81571100	-1.05937000	-1.08025200
C	4.64892600	-2.08233500	-0.61065800
C	4.40667300	0.15824900	-1.44965400
C	6.02936200	-1.91138400	-0.53820700
H	4.20355000	-3.02740200	-0.31146600
C	5.78222700	0.33406300	-1.37241700
H	3.77947900	0.97937800	-1.78403100
C	6.60250800	-0.70302400	-0.92444200
H	6.65550400	-2.72264800	-0.18036400
H	6.21990300	1.28436500	-1.66225700
H	7.67740200	-0.56425000	-0.86934600

**Si-M1**

C	2.43552000	-1.50592800	0.53066700
C	3.79216000	-2.11528200	0.66856400
C	4.27737100	-1.67323200	-1.56556300
C	3.02591600	-0.77693500	-1.79740400
C	0.79445000	-0.59061500	-0.59955700
H	4.53224500	-1.35483000	0.95820500
H	5.12222700	-1.03789400	-1.27645000
H	2.49546400	-1.10446500	-2.69422000
N	1.43415600	-1.50081100	1.35771000
N	0.42357600	-0.91728900	0.64055000
N	2.08984100	-0.96325500	-0.67794400
H	4.52537000	-2.18325100	-2.49712300
H	3.77410200	-2.91121500	1.41286500
O	4.10330400	-2.68082300	-0.58965500
C	3.40877000	0.71362300	-1.95102000
H	4.11510400	0.77484700	-2.78670800
H	2.49988000	1.27184600	-2.20112900
C	4.01207800	1.28704300	-0.68975900
C	5.39409000	1.34273300	-0.48289500
C	3.15839700	1.74655800	0.32109100
C	5.91543900	1.80746300	0.72316200
H	6.07074700	1.03135700	-1.27566700
C	3.67975800	2.20650300	1.52745000
H	2.08827500	1.76272100	0.11527100
C	5.05789000	2.22835500	1.73647800
H	6.99055300	1.84526200	0.86761400
H	3.00739700	2.56221600	2.30278200
H	5.46249100	2.58824900	2.67710800

C	-0.88701400	-0.75216700	1.20771900
C	-1.22208500	0.48264100	1.76043800
C	-1.78900100	-1.80978300	1.08019300
C	-2.54671500	0.65914200	2.15613100
C	-3.09968100	-1.58391800	1.49133800
C	-3.50003700	-0.34745900	2.00105300
H	-2.84824700	1.62120800	2.56324700
H	-3.83273400	-2.37933400	1.38048100
C	-0.21766800	1.59812300	1.82299200
H	0.73005700	1.25167400	2.24916100
H	-0.01997400	1.94750300	0.79998500
H	-0.59397300	2.42280700	2.43094200
C	-4.94860200	-0.07893500	2.30453300
H	-5.48350200	-0.99881800	2.55163700
H	-5.05989800	0.62386700	3.13367700
H	-5.42723100	0.36163200	1.42180200
C	-1.36054800	-3.12232600	0.48007800
H	-1.05656100	-2.99751000	-0.56552200
H	-0.50542800	-3.54166700	1.01793700
H	-2.17804300	-3.84430900	0.51021800
C	0.06862600	0.30886200	-1.62981100
O	0.42935300	1.55799500	-1.34052200
H	0.44706100	-0.08370600	-2.61288900
C	-1.42325600	-0.00897100	-1.62770000
C	-2.31903800	0.93894200	-1.35325200
H	-1.71471200	-1.03063600	-1.87688100
H	-1.91037500	1.92583800	-1.13825200
C	-3.78198900	0.78985100	-1.29245100
C	-4.57109000	1.92540400	-1.06965400
C	-4.43236500	-0.44610200	-1.43119900
C	-5.96008000	1.83991600	-1.00853800
H	-4.08162600	2.88835000	-0.95074300
C	-5.81717000	-0.53560100	-1.36808700
H	-3.84483900	-1.34801900	-1.57707500
C	-6.59047200	0.60838300	-1.16233000
H	-6.54867500	2.73671500	-0.84173500
H	-6.29903900	-1.50225500	-1.47915200
H	-7.67230300	0.53618600	-1.11617000

**Si-M02**

C	-3.36735900	0.79183400	1.70720800
C	-4.48620200	1.72868100	2.03140400
C	-3.14873100	3.56971900	1.58585000
C	-1.98010700	2.74690400	0.96858000

C	-1.31246900	0.27408300	1.20277000
H	-5.07046600	1.96224500	1.12962400
H	-3.82926600	3.88614900	0.78684900
H	-1.02706900	3.03411400	1.40578000
N	-3.30471700	-0.49695800	1.86211600
N	-2.01954100	-0.80464400	1.53366700
N	-2.16149400	1.31291000	1.30454000
H	-2.73402000	4.45716600	2.06459900
H	-5.13564200	1.28135100	2.78358700
O	-3.88610300	2.88375600	2.57453500
C	-1.91055500	2.92821400	-0.56219900
H	-1.83895500	4.00533300	-0.74821800
H	-0.97662400	2.47475500	-0.90239800
C	-3.09441400	2.33885400	-1.29154100
C	-4.19886000	3.11880800	-1.64867500
C	-3.11617900	0.97307000	-1.59828700
C	-5.30996400	2.54422300	-2.26247200
H	-4.18550500	4.18953800	-1.46025500
C	-4.22394800	0.39551800	-2.21167600
H	-2.24078100	0.36409700	-1.37865900
C	-5.32911500	1.17937400	-2.53650600
H	-6.15622800	3.16653600	-2.53379700
H	-4.21833600	-0.66346700	-2.45076000
H	-6.19253400	0.73181600	-3.01705900
C	-1.54824400	-2.16339700	1.60693400
C	-1.80197800	-3.01155200	0.52440800
C	-0.87656900	-2.56558700	2.76394900
C	-1.30474400	-4.31002100	0.60969700
C	-0.40023700	-3.87510800	2.79584500
C	-0.59841800	-4.75485400	1.73041600
H	-1.48097700	-4.99426500	-0.21633800
H	0.12952900	-4.21850100	3.68016400
C	-2.55437000	-2.53486000	-0.68965100
H	-3.41331500	-1.91863300	-0.41021900
H	-1.90954900	-1.93243900	-1.34283000
H	-2.91395700	-3.38526300	-1.27092300
C	-0.10038100	-6.17361000	1.80682500
H	0.79296500	-6.24581600	2.43035300
H	-0.86554000	-6.82148500	2.24578300
H	0.13456800	-6.56402700	0.81475300
C	-0.69766200	-1.63207200	3.93306100
H	0.03980200	-0.84908400	3.72586500
H	-1.64051800	-1.14053700	4.18834500
H	-0.35232700	-2.18378800	4.80801200



C	0.15425700	0.26369400	0.81443900
O	0.57087600	1.57799700	0.69514000
C	0.35243700	-0.57101600	-0.43876100
C	0.66160800	-0.02861000	-1.61913100
H	0.27800200	-1.64710800	-0.30746000
H	0.76790100	1.05500300	-1.67289800
C	0.91033900	-0.76172600	-2.87116800
C	1.36719800	-0.04682300	-3.98450400
C	0.71226200	-2.14516500	-2.99570800
C	1.62585300	-0.69119300	-5.19042400
H	1.52017600	1.02572800	-3.89915700
C	0.96849400	-2.78787000	-4.19943900
H	0.35390500	-2.72590600	-2.14951900
C	1.42706300	-2.06393900	-5.30074600
H	1.98042100	-0.12081200	-6.04240600
H	0.81048400	-3.85812000	-4.28236600
H	1.62511100	-2.56989900	-6.23968900
H	1.59162300	1.54655700	0.57800200
C	3.85472200	1.93627300	1.54643800
C	5.22999200	1.92387300	1.64673000
C	5.99433000	1.30492400	0.62789000
C	5.26281300	0.72926400	-0.43933400
C	3.88510700	0.79948000	-0.43492500
N	3.16740800	1.39105100	0.53185300
H	3.25995100	2.41144100	2.32253200
H	5.69992900	2.38941200	2.50256000
H	5.76005900	0.23395700	-1.26244000
H	3.31850200	0.35665800	-1.25065100
N	7.34801200	1.26597900	0.67275100
C	8.09076200	0.62502900	-0.39934000
H	7.90818700	1.11731800	-1.36091500
H	9.15508000	0.68648100	-0.18044200
H	7.82029000	-0.43236500	-0.49208000
C	8.05295400	1.88589400	1.78199100
H	7.78233400	1.41946900	2.73568500
H	9.12443100	1.76485200	1.63497000
H	7.83324300	2.95747600	1.84345000
H	0.67116800	-0.26018600	1.63898600

**Si-TS2**

C	-2.09775100	-2.96820700	-1.14224900
C	-3.22668000	-3.95071200	-1.25521800
C	-4.57916600	-2.44571700	-0.12382400
C	-3.49746500	-1.43437700	0.28980300

C	-1.03164200	-1.22338200	-0.33615500
H	-3.76060800	-3.80911100	-2.20535300
H	-4.98192400	-2.17358500	-1.11250200
H	-3.34873200	-1.44727600	1.37073500
N	-0.92459400	-3.02276200	-1.69244800
N	-0.27190200	-1.92653300	-1.19382800
N	-2.22512800	-1.86781400	-0.32709400
H	-5.39367900	-2.41065100	0.60037400
H	-2.83284800	-4.96748600	-1.22008900
O	-4.08651800	-3.76970100	-0.15531800
C	-3.87589600	-0.01947900	-0.16880900
H	-3.03451600	0.65773200	-0.00507500
H	-4.08673300	-0.04324900	-1.24391500
C	-5.07707700	0.47328400	0.60314900
C	-4.90474600	0.93065800	1.91300200
C	-6.36007800	0.45063800	0.05525200
C	-5.99736300	1.35484000	2.66207600
H	-3.89992500	0.96089200	2.32885300
C	-7.45558300	0.87614300	0.80382500
H	-6.50280600	0.10671500	-0.96637400
C	-7.27633100	1.32667600	2.10856200
H	-5.85207900	1.71464300	3.67569200
H	-8.44822300	0.85825400	0.36556700
H	-8.12933000	1.65910200	2.69099800
C	1.13330300	-1.74369000	-1.42006400
C	1.57512600	-0.91204200	-2.45047600
C	2.00615900	-2.42477000	-0.56332200
C	2.95279800	-0.70227900	-2.55263200
C	3.36930100	-2.19882500	-0.71740500
C	3.85675400	-1.32376900	-1.69157000
H	3.32445600	-0.03827600	-3.32959400
H	4.06631600	-2.69665100	-0.04748400
C	0.63018400	-0.30535600	-3.45531000
H	0.95748800	0.69569000	-3.74654300
H	0.61038000	-0.92181200	-4.35921400
H	-0.39381600	-0.24089900	-3.08223400
C	5.33574700	-1.06549700	-1.80650600
H	5.79493800	-1.74537400	-2.53095100
H	5.53246800	-0.04364300	-2.14137700
H	5.83264800	-1.22098500	-0.84419700
C	1.46946000	-3.35242400	0.49291300
H	0.72871600	-2.84870600	1.12589700
H	0.97035600	-4.21205800	0.03554900
H	2.27523900	-3.71861800	1.13145800

C	-0.60236900	-0.08445800	0.47380000
O	-1.46642100	0.10863600	1.58202800
H	0.81722600	-0.18276000	0.99663500
C	-0.35474400	1.15219500	-0.29108800
C	-0.55133900	2.39297300	0.18167400
H	0.08972700	1.01039500	-1.27461300
H	-1.02828400	2.50464800	1.15277100
C	-0.17721800	3.63089100	-0.51752900
C	-0.69486100	4.85284700	-0.06682000
C	0.69981200	3.65141100	-1.61342200
C	-0.36830300	6.04869700	-0.69697800
H	-1.36796900	4.85700000	0.78618200
C	1.02541300	4.84533700	-2.24544800
H	1.14161300	2.72486000	-1.97374300
C	0.49190500	6.05086400	-1.79190400
H	-0.78593700	6.98133000	-0.33115000
H	1.70379700	4.83766000	-3.09290400
H	0.74938100	6.98221000	-2.28511900
C	2.51605600	-0.81820600	2.32008900
C	3.86305600	-0.82449300	2.58544800
C	4.72647800	0.03333500	1.84990200
C	4.10974800	0.88772200	0.89845400
C	2.75313000	0.81644700	0.69813300
N	1.96182800	-0.02324800	1.38919100
H	1.83663400	-1.47100300	2.85986800
H	4.24149100	-1.48531800	3.35282400
H	4.68517500	1.59064900	0.31192900
H	2.25714500	1.44389800	-0.03520100
N	6.05974900	0.03436100	2.04418200
C	6.89970300	0.97796900	1.31792100
H	6.63196500	2.01278800	1.55566000
H	7.93798300	0.81588900	1.59903700
H	6.81061700	0.82938300	0.23681300
C	6.65220100	-0.83677500	3.05065400
H	6.41747900	-1.88577900	2.84520000
H	7.73355900	-0.71971300	3.02662900
H	6.29796100	-0.58415200	4.05588300
H	-0.99986200	-0.15695000	2.38181400

**Si-M2**

C	-2.59171400	-1.24920000	0.86582100
C	-4.02075200	-1.57175100	1.16806600
C	-4.39093700	0.58355900	1.91950100
C	-2.97898400	1.11789300	1.55926200

C	-0.76002000	0.01650900	0.88193700
H	-4.65415100	-1.36312200	0.29219400
H	-5.07140500	0.74440100	1.07300900
H	-2.53709200	1.61769200	2.42021600
N	-1.69779600	-2.01438500	0.34723000
N	-0.55174000	-1.22705200	0.31226500
N	-2.10844600	-0.01092100	1.22237000
H	-4.77102300	1.13760500	2.77916600
H	-4.11786100	-2.62367500	1.43832300
O	-4.41489300	-0.78433400	2.27125500
C	-3.05695400	2.13946900	0.40005700
H	-3.74738400	2.93060300	0.71508300
H	-2.07061200	2.59669800	0.28881700
C	-3.51587100	1.53670600	-0.90610300
C	-4.84527600	1.63985900	-1.32797600
C	-2.61536600	0.83283500	-1.71470200
C	-5.27268700	1.03692400	-2.50887600
H	-5.55251000	2.20798400	-0.72811900
C	-3.03870800	0.22749600	-2.89425100
H	-1.56972100	0.77553800	-1.42103900
C	-4.37085500	0.32199700	-3.29196100
H	-6.30880100	1.13078000	-2.81806500
H	-2.32394900	-0.31015600	-3.50986100
H	-4.70043600	-0.14861400	-4.21248400
C	0.69957100	-1.85896400	0.05501700
C	1.49240900	-2.27074200	1.13337100
C	1.10655300	-2.01978400	-1.27151900
C	2.73972800	-2.82261000	0.85146700
C	2.35894200	-2.58675200	-1.50914700
C	3.19198300	-2.98018300	-0.46143100
H	3.37417900	-3.14047100	1.67573200
H	2.69444600	-2.71359700	-2.53549200
C	1.01306100	-2.08547500	2.54707300
H	1.06159200	-1.02861900	2.83153200
H	-0.02753600	-2.40630800	2.65174500
H	1.62875500	-2.65803400	3.24279700
C	4.56377400	-3.54340600	-0.73018800
H	5.33541900	-2.79938600	-0.50647500
H	4.76126400	-4.41664500	-0.10310300
H	4.67450900	-3.83765600	-1.77574700
C	0.22820000	-1.54292100	-2.39681500
H	-0.80480200	-1.87139800	-2.25415600
H	0.22291200	-0.44696700	-2.43698600
H	0.59164400	-1.91393500	-3.35694500

C	0.12464900	1.05981900	1.04874100
O	-0.33207300	2.17091200	1.76261200
H	0.19370600	2.22820300	2.57222300
C	1.46424000	1.09345800	0.54539400
C	2.33045300	2.11917400	0.71426700
H	1.79518200	0.22782700	-0.01799600
H	1.99194900	3.02301900	1.21600300
C	3.70887600	2.12782800	0.22403700
C	4.42719600	3.33446700	0.20410300
C	4.36885200	0.97007700	-0.22869400
C	5.73478700	3.39245500	-0.26495700
H	3.93966300	4.23985100	0.55660200
C	5.67272600	1.03042500	-0.70315000
H	3.86272500	0.00822800	-0.19215100
C	6.36627900	2.24056600	-0.72745400
H	6.26169900	4.34190100	-0.27112600
H	6.15772600	0.12197000	-1.04862800
H	7.38657800	2.28179500	-1.09440100

**Si-TS3**

C	5.04655500	0.91302300	0.98564200
C	6.28507700	0.52793900	1.72399200
C	5.68341200	-1.72546200	1.67554800
C	4.63086300	-1.50286700	0.54130800
C	3.09558500	0.51703100	0.05279200
H	7.10998800	0.30665100	1.03151100
H	6.62592300	-2.05612000	1.22153500
H	3.73363900	-2.07998000	0.75988600
N	4.51794800	2.08807200	0.83717200
N	3.31674100	1.84266100	0.23284000
N	4.23158700	-0.08168500	0.51634200
H	5.32091400	-2.50926300	2.34157100
H	6.57709400	1.33225400	2.39889900
O	5.93196600	-0.60237400	2.49471300
C	5.17302300	-1.94931600	-0.83565800
H	5.47617100	-2.99668100	-0.72967900
H	4.33830200	-1.91297600	-1.53906100
C	6.32632200	-1.10832200	-1.32064400
C	7.65504500	-1.50823100	-1.14813800
C	6.07640700	0.13397100	-1.91429600
C	8.70576300	-0.67259000	-1.52158900
H	7.86962900	-2.48554900	-0.72293400
C	7.12152000	0.97505400	-2.28315500
H	5.04618600	0.43471400	-2.09244900

C	8.44122700	0.57642200	-2.07788600
H	9.73074900	-0.99941200	-1.37974700
H	6.90747400	1.93747100	-2.73744900
H	9.25862800	1.22955600	-2.36481300
C	2.47976800	2.95248300	-0.12810400
C	1.85512500	3.66921300	0.89494400
C	2.30445700	3.25208100	-1.48477200
C	0.98237300	4.69322600	0.52000700
C	1.41832200	4.27550800	-1.80440500
C	0.73867000	4.99696400	-0.81853100
H	0.47274200	5.25580600	1.29780000
H	1.25037500	4.51522900	-2.85137300
C	2.10760400	3.35204500	2.34429700
H	2.04342500	2.27766800	2.53917000
H	3.11164600	3.67074400	2.63859000
H	1.38116600	3.86161100	2.97871900
C	-0.24500800	6.06764100	-1.21068500
H	-1.06969200	5.63429500	-1.78482100
H	-0.66246800	6.56577800	-0.33379600
H	0.23040400	6.82377700	-1.84166100
C	3.03675900	2.49165400	-2.55601500
H	4.10931900	2.46016900	-2.33966500
H	2.67327600	1.46070100	-2.63104400
H	2.89699200	2.97025400	-3.52603000
C	1.94078800	-0.16643500	-0.50181000
O	2.16318500	-1.39711300	-0.92054500
H	1.86375500	-2.21094400	-0.13909400
C	0.72050900	0.51588300	-0.60758400
C	-0.40034900	0.05273300	-1.27053300
H	0.66594600	1.48834600	-0.13488700
H	-0.35271000	-0.93091400	-1.72996200
C	-1.59739200	0.81420100	-1.46896500
C	-2.68571400	0.21936700	-2.14321100
C	-1.75901800	2.15093100	-1.02121500
C	-3.86165800	0.91797200	-2.38316000
H	-2.58299900	-0.80648200	-2.48955200
C	-2.93696000	2.83358800	-1.24623400
H	-0.94571400	2.65906800	-0.51010800
C	-4.00708300	2.21837900	-1.91686600
H	-4.68202000	0.43063800	-2.89902100
H	-3.03710900	3.85614200	-0.89240500
H	-4.93485300	2.75730500	-2.07999200
C	-0.67809200	-3.23612600	-0.13509800
C	-1.92219000	-2.65307500	-0.24029300

C	-2.36189400	-1.60921600	0.61707800
C	-1.51175800	-1.28273100	1.70654200
C	-0.26830800	-1.84978200	1.88334400
C	0.22384800	-2.71444400	0.85067200
H	-2.58169300	-2.96940600	-1.03849200
H	-1.89281600	-0.60293200	2.45781300
C	-3.61935200	-0.95210200	0.41827600
C	-3.89516800	0.30537600	1.03370700
C	-4.67386000	-1.55432500	-0.34326500
C	-5.09486300	0.94919800	0.92729500
H	-3.08826500	0.77837100	1.57999600
C	-5.90205300	-0.98618600	-0.50046700
H	-4.48977900	-2.53222700	-0.77105500
C	-6.17823700	0.32061000	0.13921600
C	0.56495000	-1.58470300	3.14521200
C	1.80021300	-0.72711500	2.83210000
C	-0.25077500	-0.84564500	4.21431400
C	1.01669700	-2.92896500	3.74409000
H	2.47550300	-1.26112400	2.16458000
H	1.49413500	0.20610600	2.34752400
H	2.34047400	-0.48325100	3.75428200
H	-1.16776900	-1.38628700	4.46795200
H	0.35110200	-0.75457700	5.12347600
H	-0.52210300	0.16636000	3.89579000
H	1.60735600	-2.75315900	4.64977400
H	0.14850300	-3.53726400	4.01646300
H	1.62545800	-3.48789600	3.03140700
C	-0.25080700	-4.39621300	-1.04740400
C	0.89207700	-4.01020100	-2.00505000
C	0.20381000	-5.57343200	-0.16487800
C	-1.42353700	-4.88387100	-1.90953700
H	0.65543000	-3.09595300	-2.55802200
H	1.82857900	-3.85050000	-1.47198000
H	1.04167000	-4.81930600	-2.72885400
H	-0.61645700	-5.91420200	0.47493400
H	0.51473000	-6.41259400	-0.79687200
H	1.04493900	-5.28136100	0.46613700
H	-1.11005000	-5.76804100	-2.47208800
H	-2.28914400	-5.16202700	-1.29991400
H	-1.73847300	-4.12642800	-2.63563600
C	-7.02553800	-1.67469000	-1.27845200
C	-7.48507200	-0.78536900	-2.44932000
C	-6.57295700	-3.01631000	-1.86705700
C	-8.21681500	-1.95227700	-0.34153800

H	-7.79076200	0.19904600	-2.09612500
H	-6.67987600	-0.66991600	-3.18316500
H	-8.33215200	-1.25744000	-2.95961900
H	-6.28646900	-3.72859800	-1.08638400
H	-7.39943300	-3.45675200	-2.43290900
H	-5.72693100	-2.89364100	-2.55227900
H	-9.00502900	-2.47688200	-0.89307100
H	-7.90402200	-2.58969700	0.49206000
H	-8.62295800	-1.02350700	0.05793700
C	-5.39736900	2.23662400	1.69986900
C	-6.47218500	1.91906800	2.75953300
C	-4.15513300	2.76471800	2.42781700
C	-5.91213900	3.36580700	0.78817000
H	-7.39787900	1.59328900	2.28369200
H	-6.12333300	1.12957800	3.43310400
H	-6.67796600	2.81350000	3.35825400
H	-3.34124100	2.97486200	1.72471500
H	-4.40949400	3.69675500	2.94212600
H	-3.79058500	2.05809300	3.18083300
H	-6.21135700	4.21968600	1.40667400
H	-5.12223400	3.70390700	0.11257400
H	-6.76967300	3.03810200	0.20217400
O	-7.29429400	0.85706400	0.04097100
O	1.50877100	-2.97484300	0.74859800

**Si-M3**

C	5.11490600	0.89866400	0.99008600
C	6.31889100	0.50156800	1.78007300
C	5.66990100	-1.74110900	1.74468700
C	4.65903300	-1.51925200	0.57257800
C	3.19098500	0.52424300	0.03349300
H	7.16360000	0.25209400	1.12284400
H	6.62082700	-2.09223900	1.32567500
H	3.73631700	-2.06479500	0.76774800
N	4.60236900	2.08058300	0.80011600
N	3.41275600	1.83536600	0.19082500
N	4.29103000	-0.08707000	0.52092600
H	5.27261300	-2.50782100	2.41065800
H	6.60087300	1.31023100	2.45411300
O	5.90454500	-0.60698500	2.55140200
C	5.23889900	-1.99157300	-0.77951000
H	5.55331900	-3.03088400	-0.63467300
H	4.42581000	-1.98777200	-1.50798400
C	6.39075900	-1.14476000	-1.25901700



C	7.72193500	-1.50351500	-1.02748300
C	6.12903000	0.06284300	-1.91542700
C	8.76260200	-0.65705300	-1.40528400
H	7.94768300	-2.45678400	-0.55600800
C	7.16384500	0.91399200	-2.28967700
H	5.09784700	0.32479300	-2.14533700
C	8.48511700	0.55886400	-2.02472000
H	9.79046200	-0.95045100	-1.21834100
H	6.94192000	1.84788500	-2.79660200
H	9.29554400	1.21872900	-2.31583300
C	2.56232800	2.93748100	-0.18512600
C	1.93882400	3.65810400	0.83580400
C	2.36836900	3.19983100	-1.54526200
C	1.04546300	4.65848100	0.44912100
C	1.46546900	4.20578000	-1.87321100
C	0.78412300	4.93304500	-0.89321400
H	0.53226900	5.22514200	1.22130700
H	1.28185600	4.42331600	-2.92218600
C	2.20628300	3.37197200	2.28951800
H	2.17790500	2.29996600	2.50707400
H	3.19721300	3.73400000	2.57818100
H	1.46186800	3.86544300	2.91539300
C	-0.23138000	5.96947900	-1.29241700
H	-1.10769200	5.48574000	-1.73594100
H	-0.56318600	6.55465800	-0.43303000
H	0.17855300	6.65329700	-2.04015200
C	3.09092500	2.42339300	-2.61318300
H	4.16201800	2.36398700	-2.39613400
H	2.69977300	1.40331400	-2.70194900
H	2.96711800	2.90818100	-3.58218600
C	2.00280400	-0.18476300	-0.57827500
O	2.24910400	-1.30233500	-1.05725500
H	1.85783800	-2.85685200	0.08180300
C	0.76222200	0.51512700	-0.56926100
C	-0.31721500	0.08726500	-1.29655500
H	0.70129500	1.42982300	0.00565100
H	-0.22510600	-0.86097300	-1.82379600
C	-1.54602800	0.81314500	-1.46198100
C	-2.61365900	0.20172200	-2.14543100
C	-1.73044700	2.12444700	-0.96724700
C	-3.81996700	0.86149300	-2.32945300
H	-2.48369200	-0.81024100	-2.52092300
C	-2.93409700	2.77635800	-1.14852300
H	-0.91809300	2.63705900	-0.45864400

C	-3.99356700	2.13968900	-1.81279400
H	-4.64331100	0.35869000	-2.82365000
H	-3.06555200	3.78104400	-0.75747700
H	-4.94939200	2.64125300	-1.92493900
C	-0.66817000	-3.14839500	-0.15423800
C	-1.92359400	-2.55146200	-0.26667300
C	-2.40994100	-1.60482300	0.64945300
C	-1.58795000	-1.31088400	1.74845900
C	-0.30760100	-1.83868300	1.89956900
C	0.16310700	-2.70565000	0.89328300
H	-2.56123100	-2.81915100	-1.09943600
H	-1.98638100	-0.66135800	2.51693000
C	-3.71278900	-0.95874200	0.46618900
C	-3.99210300	0.28811700	1.05779500
C	-4.74742700	-1.55826000	-0.28803300
C	-5.20605600	0.93272000	0.93318000
H	-3.19404300	0.77498500	1.60936300
C	-5.97847600	-0.97076600	-0.48113100
H	-4.56403300	-2.54308200	-0.70725400
C	-6.26993200	0.32278600	0.13748500
C	0.53667300	-1.51363500	3.14293800
C	1.78552700	-0.71166500	2.74612100
C	-0.24125200	-0.66948300	4.16092000
C	0.95682700	-2.81578900	3.84737000
H	2.40834800	-1.29383100	2.06718400
H	1.48422600	0.21709400	2.24734500
H	2.37999500	-0.45370500	3.63047900
H	-1.14679400	-1.18068500	4.50026600
H	0.39246900	-0.49083700	5.03517800
H	-0.52775100	0.30459300	3.75130700
H	1.53719100	-2.58153600	4.74694400
H	0.07157600	-3.38215800	4.15222800
H	1.56325000	-3.44592100	3.19565200
C	-0.25783200	-4.29799100	-1.09901800
C	0.98759000	-3.99166000	-1.95409600
C	0.00725000	-5.55383700	-0.24821200
C	-1.38660300	-4.63703400	-2.08371500
H	0.91430400	-3.01638900	-2.44227300
H	1.91662200	-4.01541300	-1.37876800
H	1.08526600	-4.75839800	-2.73006900
H	-0.89664500	-5.84172200	0.29699100
H	0.29798100	-6.38898900	-0.89540100
H	0.80655100	-5.37644300	0.47360200
H	-1.08790300	-5.50112500	-2.68427900

H	-2.31528400	-4.89357700	-1.56630500
H	-1.58978900	-3.80852800	-2.77136800
C	-7.08136700	-1.66169300	-1.28990300
C	-7.51788000	-0.76625400	-2.46435400
C	-6.61998300	-3.00016200	-1.87782900
C	-8.29518400	-1.94069300	-0.38470500
H	-7.81632800	0.21653800	-2.09906200
H	-6.69970900	-0.65201500	-3.18550000
H	-8.36144800	-1.22634700	-2.99333600
H	-6.35172200	-3.71896500	-1.09619200
H	-7.43336300	-3.43616300	-2.46747700
H	-5.75532700	-2.87454400	-2.53989500
H	-9.09049500	-2.43093500	-0.95957800
H	-8.00892200	-2.60628700	0.43687500
H	-8.67501300	-1.00799600	0.03230400
C	-5.50828500	2.22647700	1.69891900
C	-6.61767800	1.93059400	2.72700000
C	-4.28473200	2.74688500	2.46266300
C	-5.98527100	3.35723500	0.76924000
H	-7.51857200	1.59094000	2.21434000
H	-6.29028100	1.15124300	3.42340900
H	-6.85095900	2.83291400	3.30567000
H	-3.44855800	2.95456300	1.78442300
H	-4.54683400	3.67961300	2.97386200
H	-3.94226700	2.03475400	3.22132100
H	-6.32363600	4.21084400	1.36931600
H	-5.16577900	3.70597700	0.13301200
H	-6.80754300	3.01069100	0.14383700
O	-7.39701500	0.87686900	0.00810700
O	1.48185700	-3.13429000	0.93408500

#### Si-M4

C	1.69628100	-0.49783800	-1.09591600
C	2.74109100	0.58597400	-1.36043800
H	1.60903300	-0.73939600	-0.03297400
H	2.59175700	1.43586300	-0.68124200
N	0.40419500	0.10866000	-1.49053300
O	2.65175300	1.00792500	-2.71848900
C	0.29308100	1.12768500	-2.39540100
C	1.51859500	1.80969900	-2.93347600
H	1.41196400	1.97777100	-4.00626300
H	1.61859400	2.78237800	-2.42975500
N	-0.95533600	1.42104900	-2.62944400
C	-0.84155700	-0.21486300	-1.11436000

N	-1.65339500	0.56913800	-1.82978300
C	-3.08975400	0.52039500	-1.89569100
C	-3.70516900	-0.66529400	-2.31389500
C	-3.80317900	1.66529500	-1.52435700
C	-5.09777600	-0.70527600	-2.27186700
C	-5.19397400	1.56872400	-1.50926400
C	-5.85543600	0.38867700	-1.85360500
H	-5.60207100	-1.61888900	-2.57631300
H	-5.77240000	2.43911000	-1.21061100
H	3.74040600	0.17648900	-1.21316200
C	1.95246300	-1.76038500	-1.93755600
H	1.03301600	-2.34918600	-1.96349200
H	2.19998600	-1.44815600	-2.95770000
C	3.06458100	-2.58520600	-1.33635400
C	2.75846400	-3.59373000	-0.41937500
C	4.40376000	-2.33846900	-1.64878200
C	3.77141500	-4.34642900	0.16699200
H	1.71744200	-3.77632600	-0.16475400
C	5.42013900	-3.07551200	-1.04631300
H	4.65317100	-1.56857500	-2.37552200
C	5.10513700	-4.08394800	-0.13879200
H	3.51985300	-5.13300900	0.87199500
H	6.45626400	-2.86522200	-1.29208700
H	5.89554400	-4.66595300	0.32447300
C	-7.35262400	0.28028200	-1.74496400
H	-7.76911500	-0.30074000	-2.57105800
H	-7.62108000	-0.23113100	-0.81392000
H	-7.82469300	1.26463700	-1.73845200
C	-2.93204100	-1.86774300	-2.79251500
H	-1.98897900	-1.58912400	-3.27040100
H	-2.70509200	-2.55204600	-1.96843400
H	-3.52742800	-2.41991100	-3.52155500
C	-3.10860000	2.95103100	-1.17252300
H	-3.78532000	3.61203800	-0.62989300
H	-2.22700700	2.78079300	-0.54906300
H	-2.77481700	3.46203000	-2.08046900
C	-3.22055500	-2.14468500	1.00018100
C	-2.49810300	-1.10308400	0.57003900
H	-2.80407700	-3.14286900	0.86962900
C	-4.54372500	-2.04721700	1.62565700
C	-5.04460500	-3.13202500	2.35507300
C	-5.33781700	-0.89820800	1.48932800
C	-6.29505100	-3.06331300	2.96098000
H	-4.44021900	-4.02939000	2.45396800

C	-6.58755300	-0.83226900	2.09205100
H	-4.98393000	-0.06462500	0.88794200
C	-7.06857300	-1.91274300	2.83271700
H	-6.66619100	-3.90858200	3.53100400
H	-7.19221600	0.06243300	1.98019500
H	-8.04592600	-1.85898200	3.30095600
C	-1.24153600	-1.32254300	-0.16146300
O	-0.60247100	-2.35514900	-0.19470100
H	-2.81528400	-0.07375200	0.69820100
C	4.03718800	0.35038300	1.56656100
C	4.56868700	-0.92721600	1.80482400
H	5.59126200	-1.22367000	1.62576900
C	3.54017700	-1.71789900	2.31040300
H	3.59879700	-2.75688700	2.59568700
C	2.39499000	-0.92608200	2.36453000
H	1.38201400	-1.15531900	2.65373900
N	2.68790500	0.32034300	1.91840100
C	4.69422000	1.50014800	1.01922000
C	1.75707000	1.38253900	1.77855400
H	2.16929700	2.36960600	1.90282400
C	0.42042600	1.14715900	1.57056200
O	-0.14223000	-0.00673900	1.47270400
C	-0.46898500	2.35846900	1.53481300
C	-0.07054300	3.58723700	0.99694000
C	-1.74532500	2.25014700	2.10154100
C	-0.91661700	4.69272300	1.05839200
H	0.91008700	3.67411000	0.53531500
C	-2.58445700	3.35749000	2.17566500
H	-2.04269500	1.28885000	2.51036500
C	-2.17000000	4.58451900	1.65840800
H	-0.59560300	5.64116000	0.63876700
H	-3.56151500	3.26599800	2.64098200
H	-2.82351000	5.44962000	1.71363000
O	4.23896400	2.62059500	0.84698000
C	6.14048800	1.24329900	0.52783300
F	6.15280900	0.31054300	-0.44369800
F	6.67624700	2.35290700	0.03320700
F	6.93658700	0.80122600	1.51194500

**Si-M4-1**

C	3.84799400	0.87318300	0.09469300
C	5.15357700	1.60575900	0.40320300
H	3.54922100	0.18605700	0.88855200
H	5.09112000	2.13237300	1.36558100

N	2.83014700	1.94677300	0.04244000
O	5.43827000	2.51220800	-0.65531900
C	3.12508400	3.18803100	-0.44906600
C	4.54660400	3.59886000	-0.72954700
H	4.62866500	4.03118700	-1.72852700
H	4.80749100	4.37329600	0.00623300
N	2.06959200	3.95481800	-0.46310500
C	1.52909200	1.95091300	0.37225700
N	1.08502100	3.16761500	0.05024700
C	-0.26085600	3.65557600	0.20249100
C	-1.03641900	3.76579800	-0.95485500
C	-0.74742100	3.90599000	1.48655200
C	-2.37973300	4.09407500	-0.78929000
C	-2.09811700	4.23404900	1.59472800
C	-2.92969100	4.31079900	0.47691200
H	-3.01337200	4.16955800	-1.66896400
H	-2.51228300	4.42207100	2.58217900
H	5.97918800	0.89435500	0.43358600
C	3.90947000	0.15622600	-1.26488800
H	2.90062800	-0.18746700	-1.49913300
H	4.24455600	0.87526400	-2.01919500
C	4.85109500	-1.02032700	-1.19649700
C	4.38382400	-2.23825800	-0.69651600
C	6.18883400	-0.91032300	-1.58308300
C	5.24094500	-3.32773900	-0.57695500
H	3.34073200	-2.31660400	-0.40480300
C	7.04700100	-2.00206200	-1.46974700
H	6.55533400	0.03648600	-1.97487300
C	6.57489100	-3.21152100	-0.96387200
H	4.86095600	-4.26557700	-0.18284000
H	8.08370000	-1.90881900	-1.77811600
H	7.24486500	-4.06105900	-0.87602900
C	-4.39984800	4.59157500	0.64165000
H	-4.92327000	3.68274900	0.95738900
H	-4.57316300	5.35248200	1.40629200
H	-4.84798300	4.93035600	-0.29438100
C	-0.43728300	3.53442700	-2.31562900
H	0.31091800	4.29838200	-2.54504100
H	0.05801000	2.55920000	-2.37017100
H	-1.21199600	3.56698200	-3.08283100
C	0.11998800	3.79538400	2.71294300
H	1.16285500	4.04142500	2.49707300
H	-0.23904900	4.47764900	3.48538300
H	0.09137800	2.78043200	3.12273000

C	-1.25363100	-0.12636500	1.87916800
C	-0.58537500	0.74175900	1.09822000
H	-0.69373100	-0.64997300	2.65363200
C	-2.68831100	-0.40606200	1.78625500
C	-3.21685600	-1.51649600	2.45597800
C	-3.55644900	0.41937600	1.05617200
C	-4.57285000	-1.81248000	2.38112300
H	-2.54755700	-2.16187700	3.01831200
C	-4.91128000	0.12367100	0.98338900
H	-3.16992200	1.29773800	0.54396000
C	-5.42298100	-0.99694100	1.63874000
H	-4.96333600	-2.68952000	2.88640300
H	-5.57024700	0.75987900	0.40152900
H	-6.47989400	-1.23300300	1.56566800
C	0.83486500	0.96221000	1.30158500
O	1.50474700	0.64988700	2.27739000
H	-1.05377700	1.21261900	0.24058000
C	-2.77901000	-1.32097700	-1.64833400
C	-3.07483000	-0.33525300	-2.59555900
H	-4.04122200	-0.17793700	-3.04965500
C	-1.90369700	0.38734500	-2.82703700
H	-1.77054300	1.20745000	-3.51645000
C	-0.90998200	-0.16595900	-2.02413400
H	0.13738700	0.06431900	-1.90881500
N	-1.43154700	-1.20118300	-1.31161000
C	-3.67878800	-2.29273000	-1.08082700
C	-0.72385600	-2.05272400	-0.43563500
H	-1.27670400	-2.92281700	-0.12540000
C	0.56078800	-1.81341600	-0.01137800
O	1.26189300	-0.75637900	-0.25433800
C	1.17137600	-2.87507800	0.86018100
C	0.96912000	-4.23818300	0.61627200
C	2.02204400	-2.49899200	1.90590500
C	1.58841500	-5.20129700	1.40902800
H	0.34440600	-4.54296300	-0.21771800
C	2.63827700	-3.46092100	2.69956900
H	2.18155100	-1.44101300	2.09183500
C	2.42521300	-4.81669900	2.45383400
H	1.42595900	-6.25455600	1.20107200
H	3.28849000	-3.15291000	3.51299100
H	2.91158900	-5.56757300	3.06882700
C	-5.12618200	-2.25567500	-1.63867500
O	-3.43259400	-3.16355500	-0.26612300
F	-5.68789800	-1.03624300	-1.59049100

F	-5.90899500	-3.08633200	-0.95853300
F	-5.13336100	-2.63556400	-2.92669900

**Si-M4-2**

C	3.48631200	0.28133600	-0.40128600
C	4.66912500	0.87894900	0.35747000
H	3.15744000	-0.64963100	0.06870600
H	4.48241300	0.88235200	1.43878400
N	2.37403600	1.26044200	-0.27420000
O	4.93047700	2.20178700	-0.09794800
C	2.58228100	2.57862400	0.02047300
C	3.94881300	3.08975300	0.37228500
H	4.10923300	4.06430800	-0.09129300
H	4.00151300	3.19665600	1.46629600
N	1.46848300	3.25403100	-0.00213200
C	1.04924800	1.10423700	-0.46584000
N	0.51950700	2.32728000	-0.31386500
C	-0.79857900	2.79569100	-0.67158600
C	-1.10313000	2.87887900	-2.03497800
C	-1.69176400	3.14692900	0.33920900
C	-2.38055300	3.31303400	-2.37443500
C	-2.95878100	3.57923700	-0.05714400
C	-3.32140000	3.65994600	-1.40096200
H	-2.65025700	3.37818500	-3.42558400
H	-3.68049400	3.84650500	0.71000000
H	5.55724700	0.28089700	0.14413800
C	3.81940700	0.06668000	-1.88430200
H	2.88495800	-0.06380900	-2.43595800
H	4.32985800	0.95811500	-2.26492100
C	4.68509400	-1.16004200	-2.05054000
C	4.20591000	-2.40581600	-1.62788000
C	5.96237100	-1.07453300	-2.60521200
C	4.99465500	-3.54246000	-1.76892800
H	3.21695600	-2.47348400	-1.17829000
C	6.75041000	-2.21503800	-2.74935200
H	6.34098300	-0.10817500	-2.92890900
C	6.26726100	-3.45134000	-2.33191300
H	4.61585900	-4.50320300	-1.43490500
H	7.74155600	-2.13430800	-3.18472100
H	6.88024600	-4.34069900	-2.43937200
C	-4.70627100	4.08711500	-1.81012900
H	-4.66712900	4.93730500	-2.49684600
H	-5.21755300	3.27033800	-2.32922200
H	-5.30695400	4.37132100	-0.94437800



C	-0.10639400	2.48094300	-3.09151400
H	0.89793000	2.84868000	-2.85919600
H	-0.05556900	1.39001600	-3.18849000
H	-0.40061300	2.88459900	-4.06133700
C	-1.33165100	3.00998400	1.79255500
H	-1.36509300	1.95416700	2.08477600
H	-0.33296500	3.40687200	1.99461300
H	-2.05008700	3.54601600	2.41446500
C	-1.78963900	-1.04823500	-1.62487800
C	-1.10065800	-0.15482200	-0.89719100
H	-1.23149800	-1.80652700	-2.17201500
C	-3.25074000	-1.07908700	-1.72584600
C	-3.87892300	-2.22174400	-2.23593700
C	-4.04324600	0.01549800	-1.34338200
C	-5.26315600	-2.27424200	-2.36119900
H	-3.26950500	-3.07370300	-2.52509000
C	-5.42475900	-0.03778100	-1.47313600
H	-3.57480600	0.91881500	-0.96173100
C	-6.03904800	-1.18081500	-1.98493500
H	-5.73596100	-3.16778000	-2.75598100
H	-6.02584100	0.81506700	-1.17304600
H	-7.11875300	-1.21852100	-2.08820500
C	0.36209700	-0.18020200	-0.87789000
O	1.06547100	-1.07201900	-1.33668200
H	-1.60780800	0.56007100	-0.26118300
C	-2.16092100	-2.25123500	1.26589900
C	-2.56503200	-3.47946700	0.71586100
H	-3.58425300	-3.82831900	0.65400200
C	-1.42866700	-4.11047300	0.22395500
H	-1.37498300	-5.06782800	-0.27277000
C	-0.33779300	-3.27997000	0.48921900
H	0.71555300	-3.40366300	0.30586000
N	-0.76989600	-2.16825700	1.13686800
C	-2.99561200	-1.17219500	1.69088600
O	-2.67521100	-0.01487800	1.94029100
C	-4.49296600	-1.52977700	1.86951700
F	-5.19700300	-0.44803900	2.19210000
F	-4.64147500	-2.43231200	2.85168600
F	-5.03938900	-2.05468100	0.76314300
C	0.02880900	-1.13113900	1.65568900
H	-0.51322900	-0.41674500	2.25322900
C	1.42036400	-1.26195800	1.74771300
O	2.11666100	-2.15124100	1.19077600
C	2.14519500	-0.24162200	2.59229000

C	1.70628100	1.07136700	2.78687700
C	3.33788300	-0.64756000	3.20034600
C	2.44553100	1.96262700	3.56099300
H	0.78607600	1.40584500	2.31638600
C	4.06601400	0.23253400	3.99599700
H	3.67708200	-1.66341200	3.02621100
C	3.62772400	1.54457900	4.17191800
H	2.09459900	2.98307000	3.68905600
H	4.98311900	-0.10135800	4.47153700
H	4.20083000	2.23525600	4.78230800

**Si-M4-3**

C	-3.85520400	-0.53775000	-1.15601800
C	-5.16764400	-0.37127700	-1.92085200
H	-3.17159000	-1.22384600	-1.65883400
H	-4.97907600	-0.07302000	-2.96149500
N	-3.23250000	0.80417700	-1.18822300
O	-5.98099000	0.58797000	-1.25901200
C	-3.98529800	1.94157700	-1.10486700
C	-5.47396300	1.90044900	-1.32462900
H	-5.98480100	2.49528500	-0.56567000
H	-5.67029300	2.34804200	-2.30984100
N	-3.23211800	2.99912800	-0.97397100
C	-1.94449500	1.17669800	-1.11971300
N	-1.96481100	2.50387400	-0.99023000
C	-0.82331400	3.34281600	-0.73386900
C	-0.52607200	3.59036400	0.60803800
C	-0.01286900	3.73457500	-1.79833200
C	0.67571900	4.24262200	0.87793600
C	1.17397500	4.38818200	-1.47427900
C	1.54134300	4.62990500	-0.14820100
H	0.94998300	4.42447400	1.91414700
H	1.84033600	4.69453000	-2.27663400
H	-5.72085000	-1.31107600	-1.91260900
C	-4.08607100	-0.93193000	0.31510500
H	-3.15649800	-0.73747400	0.85669400
H	-4.88072000	-0.29135000	0.71204600
C	-4.46057600	-2.38580200	0.44309400
C	-3.45582800	-3.33711500	0.64210400
C	-5.78922600	-2.80802700	0.35352800
C	-3.77368200	-4.68929400	0.73185700
H	-2.42905500	-2.99349800	0.74801400
C	-6.10900900	-4.16055600	0.44457700
H	-6.57672100	-2.06778000	0.22668000

C	-5.10034800	-5.10342900	0.62850500
H	-2.98639400	-5.41948300	0.89005600
H	-7.14511600	-4.47760600	0.37896300
H	-5.34836200	-6.15755400	0.70146600
C	2.87813700	5.24851000	0.16277600
H	3.66522700	4.49054700	0.07832500
H	3.11684000	6.04993100	-0.54045800
H	2.90537800	5.65393900	1.17602900
C	-1.44965300	3.11282300	1.69303300
H	-2.39106900	3.67106500	1.67416700
H	-1.68079300	2.04995900	1.55904700
H	-0.98813300	3.22521500	2.67564700
C	-0.37297700	3.40264200	-3.22132100
H	-0.15173900	2.35157100	-3.44158100
H	-1.43533600	3.57207800	-3.41558500
H	0.20710800	4.01452500	-3.91364700
C	1.67432100	0.25405600	-1.62080500
C	0.56245400	0.70775200	-1.02369200
H	1.56190000	-0.41361000	-2.47553800
C	3.04022300	0.53973000	-1.17892500
C	4.10715000	-0.08624400	-1.83372900
C	3.31769600	1.38367300	-0.09206500
C	5.41787000	0.10915700	-1.40800500
H	3.89750500	-0.75996300	-2.66002400
C	4.62440400	1.57621200	0.33315500
H	2.50722900	1.88813500	0.42698700
C	5.67876600	0.93720600	-0.32126800
H	6.22976100	-0.40526800	-1.91113500
H	4.82418900	2.21608300	1.18725800
H	6.69783600	1.07859700	0.02353700
C	-0.75649800	0.31397000	-1.51399000
O	-0.99709900	-0.53341300	-2.35498600
H	0.59714800	1.33206300	-0.13945500
C	2.55963900	-2.68701600	-0.20980500
C	2.34168100	-3.50926600	-1.32474800
H	3.10977400	-4.03499500	-1.87110700
C	0.97084100	-3.51069900	-1.58146900
H	0.45306300	-4.03392200	-2.37141000
C	0.37138200	-2.70031400	-0.62104500
H	-0.65457400	-2.40296500	-0.47950200
N	1.32071900	-2.20699000	0.20839800
C	3.81788900	-2.31536400	0.38257000
O	4.02336000	-1.56405200	1.31972900
C	5.05989800	-3.01342100	-0.23622600

F	6.18230900	-2.51896400	0.27663300
F	5.13675200	-2.88252700	-1.57389600
F	5.02724200	-4.33014300	0.02192900
C	1.09753500	-1.34474900	1.31040600
H	1.91709600	-1.29627600	2.00649200
C	-0.05764600	-0.64213900	1.51072300
O	-1.11940900	-0.62240600	0.76211500
C	-0.07951900	0.21419300	2.74581500
C	1.02020100	0.98902400	3.12985500
C	-1.25025000	0.28263600	3.50916800
C	0.95352600	1.80699800	4.25666400
H	1.92909900	0.94626300	2.53458300
C	-1.31493800	1.08856300	4.64037100
H	-2.10738100	-0.30805900	3.19783300
C	-0.21278700	1.85790800	5.01700400
H	1.81433100	2.40551300	4.54042200
H	-2.22507600	1.11978600	5.23199500
H	-0.26356900	2.49165000	5.89696400

#### TS4RR

C	-3.79525200	-1.14900200	-1.07190600
C	-5.21772400	-1.28999000	-1.60571300
H	-3.06272000	-1.57535700	-1.75808000
H	-5.28579700	-0.91554700	-2.63690100
N	-3.54282100	0.31169300	-1.01647000
O	-6.12073700	-0.58882500	-0.76189900
C	-4.54518200	1.21860000	-0.81318500
C	-5.98969000	0.80633700	-0.88843600
H	-6.55214800	1.27642400	-0.08035300
H	-6.39688500	1.15499700	-1.84876900
N	-4.06785900	2.41965700	-0.64104700
C	-2.37922600	0.98360300	-0.95414400
N	-2.71909400	2.25625000	-0.73076700
C	-1.84041000	3.38763200	-0.58254900
C	-1.50405100	3.77756200	0.71464300
C	-1.31245400	3.97411100	-1.73222900
C	-0.58150200	4.81473100	0.84276500
C	-0.39361200	5.00482800	-1.54921900
C	-0.00948800	5.42749200	-0.27479900
H	-0.28840000	5.13534300	1.83926800
H	0.04524100	5.47791400	-2.42378800
H	-5.51176800	-2.33973300	-1.58763900
C	-3.62063500	-1.70856000	0.34931100
H	-2.61295700	-1.44436100	0.68722900

H	-4.36002300	-1.22185600	0.99546800
C	-3.79104400	-3.20657100	0.38999800
C	-2.68486500	-4.03888400	0.19613700
C	-5.04767400	-3.78029000	0.60612300
C	-2.83979400	-5.42276800	0.21088000
H	-1.70473000	-3.58631100	0.06576800
C	-5.20129200	-5.16405100	0.62060900
H	-5.90719800	-3.13303700	0.77083700
C	-4.09609400	-5.98783100	0.42028400
H	-1.97436200	-6.06227300	0.06734400
H	-6.18102400	-5.59844300	0.79362000
H	-4.21283800	-7.06684100	0.43564700
C	1.04332100	6.49226500	-0.11372700
H	2.04045800	6.05162900	-0.21940600
H	0.94331100	7.26630100	-0.87807200
H	0.98558500	6.96424700	0.86909400
C	-2.05114700	3.04050800	1.90600000
H	-3.14429500	3.00876000	1.88773100
H	-1.68354600	2.00539600	1.92128700
H	-1.72899100	3.51367000	2.83412200
C	-1.68403300	3.47248200	-3.10137600
H	-1.22778900	2.49402500	-3.29033700
H	-2.76755500	3.36397100	-3.20524200
H	-1.33044200	4.16048300	-3.87035400
C	1.37346200	0.53771200	-0.87561400
C	0.10116700	1.02701900	-0.67647700
H	1.46475300	-0.29814700	-1.56763800
C	2.60976400	1.27760700	-0.59661900
C	3.82412500	0.76655100	-1.07921000
C	2.62504200	2.48929300	0.11233700
C	5.02518400	1.41451400	-0.81883400
H	3.81906100	-0.15509700	-1.65577200
C	3.82730100	3.13888600	0.36740600
H	1.69474500	2.92380300	0.47043800
C	5.03075500	2.60137300	-0.08888900
H	5.95489500	0.98889700	-1.18287200
H	3.82718800	4.06860900	0.92822900
H	5.96706500	3.10882200	0.11923200
C	-1.01556500	0.37952100	-1.26981300
O	-1.04263100	-0.55179500	-2.07901700
H	-0.06899700	1.86448000	-0.01511400
C	3.58872700	-2.51476400	-0.44845800
C	3.61830000	-3.35781700	-1.56669400
H	4.50888600	-3.78512600	-2.00195100

C	2.30010300	-3.54628400	-1.98342300
H	1.95893200	-4.14512100	-2.81448900
C	1.48261200	-2.80881700	-1.13197300
H	0.41847700	-2.63087000	-1.13897800
N	2.25420700	-2.19660500	-0.19423600
C	4.70494100	-2.00443600	0.30574400
O	4.69572800	-1.38448400	1.35448100
C	6.08637100	-2.23265600	-0.35816800
F	7.05470200	-1.68641400	0.36721500
F	6.12188500	-1.67097500	-1.58082300
F	6.36723900	-3.53583000	-0.50935000
C	1.82289800	-1.25232800	0.76109500
H	2.62356800	-0.86563500	1.36882700
C	0.49314000	-1.17737500	1.20618200
O	-0.49131800	-1.73641200	0.66837400
C	0.21613300	-0.26478900	2.36926900
C	1.03319500	0.81361600	2.72656900
C	-0.94947700	-0.50419100	3.10575500
C	0.69186900	1.62781800	3.80437400
H	1.93454200	1.02508200	2.15896800
C	-1.27985500	0.29705600	4.19371000
H	-1.57368200	-1.34461100	2.81872900
C	-0.45904800	1.36750400	4.54589500
H	1.33120100	2.46515700	4.06789400
H	-2.17547100	0.08523800	4.76975700
H	-0.71586200	1.99597700	5.39321800

**TS4RS**

C	4.00694800	0.82268500	0.15347700
C	5.35377800	1.50405900	0.38804900
H	3.74028900	0.14818900	0.96918800
H	5.38076000	1.99015000	1.37329300
N	3.01951800	1.92647300	0.16901600
O	5.58712200	2.45185500	-0.64572700
C	3.32911500	3.18822500	-0.25695500
C	4.75211500	3.58053800	-0.55019100
H	4.80698700	4.12177700	-1.49626900
H	5.08546300	4.25049500	0.25580200
N	2.28094300	3.96410100	-0.23645900
C	1.71059000	1.91913900	0.47501100
N	1.28311800	3.15862200	0.22026500
C	-0.06012700	3.65002700	0.37872100
C	-0.83194600	3.79609400	-0.77461600
C	-0.54912400	3.85067000	1.67083900

C	-2.17570300	4.12341600	-0.60041700
C	-1.89742400	4.17826500	1.78890400
C	-2.72617300	4.29758000	0.67096800
H	-2.80850600	4.22718900	-1.47784400
H	-2.31559100	4.32812900	2.78096500
H	6.15455600	0.76668900	0.32910700
C	3.94714500	0.10794400	-1.20761500
H	2.91694100	-0.21244100	-1.37679000
H	4.24081100	0.82478500	-1.98161100
C	4.85969700	-1.09402000	-1.22173600
C	4.38842700	-2.31977800	-0.74324400
C	6.17860900	-0.99845200	-1.67260600
C	5.22925100	-3.42827000	-0.70392100
H	3.35175200	-2.38872800	-0.42297700
C	7.01831200	-2.10959000	-1.63917500
H	6.54492200	-0.04731500	-2.05428600
C	6.54547000	-3.32563000	-1.15046600
H	4.85065700	-4.37394400	-0.32782900
H	8.03963000	-2.02628400	-1.99744000
H	7.19916200	-4.19176300	-1.12443000
C	-4.19567000	4.57622800	0.84482200
H	-4.71282200	3.66969800	1.17672300
H	-4.36458700	5.34587000	1.60194700
H	-4.65299600	4.90299600	-0.09101900
C	-0.23497800	3.58318900	-2.13924700
H	0.53991600	4.32647400	-2.34688200
H	0.22487600	2.59179500	-2.21605100
H	-1.00555200	3.65966100	-2.90739800
C	0.33014700	3.68271800	2.88149900
H	1.30783000	4.14939800	2.73085000
H	-0.13744800	4.14121900	3.75396400
H	0.49449200	2.62354900	3.10769500
C	-1.08499400	-0.39115900	1.55473400
C	-0.39635500	0.65338600	0.98696600
H	-0.52718700	-1.03666100	2.23171900
C	-2.54753800	-0.49781100	1.61755900
C	-3.12189000	-1.54013600	2.35973100
C	-3.39412900	0.41633600	0.97586600
C	-4.49984000	-1.67719700	2.44828100
H	-2.46791900	-2.25784400	2.84926600
C	-4.77626000	0.27514900	1.06137100
H	-2.97533000	1.23927100	0.40117100
C	-5.33314800	-0.77304500	1.79112700
H	-4.92676000	-2.49740200	3.01606800

H	-5.42043100	0.97878800	0.54417100
H	-6.41127000	-0.88481800	1.84686300
C	0.99480600	0.80708900	1.23557500
O	1.70055500	0.25637900	2.08527700
H	-0.87480700	1.31520400	0.27616600
C	-2.85263000	-1.08641300	-1.75579800
C	-2.97962400	-0.10668200	-2.74445700
H	-3.89378700	0.13712000	-3.26441600
C	-1.72161900	0.47024000	-2.92814300
H	-1.45643900	1.24496200	-3.63209800
C	-0.84255700	-0.15825900	-2.05151200
H	0.21496100	-0.04041900	-1.88319300
N	-1.51718600	-1.11144300	-1.34733600
C	-3.88300100	-1.94285100	-1.22702300
C	-0.98537500	-1.96377400	-0.36449700
H	-1.68692400	-2.69019000	0.00823300
C	0.38763200	-2.05742400	-0.09576800
O	1.25942000	-1.23860900	-0.49532900
C	0.79575700	-3.16361700	0.83841900
C	0.17760600	-4.41812100	0.82041800
C	1.85229100	-2.93910400	1.72695000
C	0.60475300	-5.42680900	1.67983600
H	-0.62311000	-4.61427600	0.11360600
C	2.27757900	-3.94715100	2.58593800
H	2.30896500	-1.95395600	1.74088700
C	1.65510200	-5.19441600	2.56454000
H	0.12263500	-6.39905300	1.64998200
H	3.09192400	-3.75860500	3.27896100
H	1.98812700	-5.98192200	3.23349300
C	-5.30086700	-1.68768300	-1.79957100
O	-3.77160100	-2.85455400	-0.42709800
F	-5.67660100	-0.40152900	-1.70503900
F	-6.20306100	-2.42143600	-1.15793100
F	-5.34676800	-2.01327100	-3.10156500

**TS4SR**

C	3.71369800	-0.16236500	-0.17410900
C	4.86792100	0.06708800	0.79696900
H	3.09414100	-1.00354500	0.13673900
H	4.50063400	0.09903800	1.83298100
N	2.87423100	1.05648200	-0.09437500
O	5.54026300	1.27621400	0.47426400
C	3.37559600	2.27164900	0.27457500
C	4.77204200	2.40498100	0.81053000



H	5.25399800	3.28721200	0.38683200
H	4.70413200	2.52798900	1.90159300
N	2.46945500	3.20486400	0.18132800
C	1.57580700	1.24082800	-0.39536700
N	1.35578700	2.54966700	-0.23835800
C	0.18286100	3.30321500	-0.60808200
C	-0.09623000	3.43820900	-1.97255100
C	-0.62905000	3.81721900	0.40261300
C	-1.27079400	4.10001800	-2.31500200
C	-1.79114000	4.47859300	0.00090600
C	-2.13485700	4.61304300	-1.34365400
H	-1.52178400	4.21211900	-3.36658200
H	-2.45020600	4.88246800	0.76494400
H	5.59273600	-0.74222000	0.69490200
C	4.19223000	-0.36865600	-1.61750700
H	3.32754700	-0.26278600	-2.27770200
H	4.92493400	0.40676000	-1.86376300
C	4.78895900	-1.74699600	-1.76482300
C	3.94701100	-2.86483800	-1.74916100
C	6.16744200	-1.93292400	-1.87106500
C	4.48112800	-4.14613600	-1.84281800
H	2.87220000	-2.71642900	-1.66158600
C	6.70237400	-3.21662600	-1.96755500
H	6.82429600	-1.06639500	-1.88051500
C	5.86003300	-4.32436800	-1.95311400
H	3.82050900	-5.00743100	-1.83459100
H	7.77611700	-3.34939600	-2.05418400
H	6.27498900	-5.32423600	-2.02907000
C	-3.42769300	5.26828200	-1.75075000
H	-3.28103600	5.93412400	-2.60466800
H	-4.15645500	4.50706700	-2.04866000
H	-3.85773900	5.84527500	-0.92993400
C	0.80600000	2.85499400	-3.02829700
H	1.86255900	3.00874000	-2.78954100
H	0.63473500	1.77778300	-3.13711900
H	0.60528600	3.31898100	-3.99487300
C	-0.32803700	3.58868000	1.85737300
H	-0.81999600	4.34659000	2.46959700
H	-0.71197700	2.61106700	2.16965000
H	0.74278100	3.61678200	2.06723000
C	-1.69066700	-0.52396600	-1.13288500
C	-0.76489300	0.39324100	-0.72653900
H	-1.34038600	-1.49924500	-1.47339600
C	-3.10530200	-0.22849400	-1.33879800

C	-3.89460800	-1.17489600	-2.00834400
C	-3.69989200	0.97321500	-0.91732600
C	-5.24219500	-0.93224900	-2.24931500
H	-3.44449000	-2.12238100	-2.29386300
C	-5.04631600	1.20961700	-1.15469800
H	-3.11371200	1.72176200	-0.39021000
C	-5.82119900	0.25887300	-1.82294900
H	-5.84389600	-1.68565900	-2.74688800
H	-5.49795200	2.13593800	-0.81249300
H	-6.87567600	0.44569000	-2.00028600
C	0.63663600	0.12360800	-0.82778500
O	1.19016300	-0.88284800	-1.26497600
H	-1.07924500	1.35344600	-0.34491000
C	0.33385000	-1.32174100	1.96886200
C	1.63496100	-1.85985900	1.90561800
H	2.50029200	-1.46135000	2.41505700
C	1.57689000	-2.99115200	1.10189000
H	2.39698900	-3.64162500	0.83221900
C	0.24856200	-3.15493800	0.69556900
H	-0.23007700	-3.90208300	0.08419700
N	-0.50616700	-2.16522500	1.22881700
C	-0.09355600	-0.12739600	2.62524200
C	-1.89891200	-2.02758300	1.14704900
H	-2.30732100	-1.32352900	1.84752600
C	-2.69432400	-2.88052400	0.37529500
O	-2.26817300	-3.72617100	-0.45571600
C	-4.18791900	-2.73158200	0.53514000
C	-4.81049200	-1.62818400	1.13086500
C	-4.98820700	-3.73736300	-0.01388500
C	-6.19720300	-1.53556600	1.16892700
H	-4.21882800	-0.80745600	1.52415200
C	-6.37555200	-3.65179400	0.03411000
H	-4.48831800	-4.57318400	-0.49141200
C	-6.98628000	-2.54648400	0.62288800
H	-6.66396000	-0.66210400	1.61457000
H	-6.98251000	-4.44435600	-0.39386300
H	-8.06901900	-2.47057200	0.65362000
O	-1.20460700	0.38807400	2.64667200
C	1.02757600	0.63036000	3.38721400
F	1.94224700	1.13630300	2.51987700
F	0.53043600	1.65244100	4.07304500
F	1.69774300	-0.14982300	4.24140400

TS4SS

C	3.95254800	-0.23201800	0.16858900
C	5.07919400	-0.21403900	1.19884400
H	3.14899700	-0.90428500	0.47750700
H	4.68056500	-0.11154600	2.21591700
N	3.38106700	1.13824300	0.17833500
O	5.97788300	0.84926800	0.90845300
C	4.04041200	2.22480300	0.67772700
C	5.42471200	2.09513900	1.24899100
H	6.06843600	2.87766000	0.84395400
H	5.36360500	2.21992900	2.33975500
N	3.29367300	3.29476100	0.63552000
C	2.15234000	1.55762200	-0.18410700
N	2.12352200	2.86257700	0.09505700
C	1.03734000	3.78300800	-0.11339300
C	0.78909000	4.24260100	-1.40600700
C	0.25850800	4.12427100	0.99546400
C	-0.30831900	5.08601800	-1.57536000
C	-0.82654800	4.96653700	0.77126200
C	-1.12788600	5.44850400	-0.50611500
H	-0.53170000	5.46038900	-2.57074400
H	-1.45796700	5.24489600	1.61083700
H	5.63988400	-1.14812000	1.12528800
C	4.47419900	-0.62273100	-1.22193100
H	3.76249200	-0.27823200	-1.97297000
H	5.43587500	-0.12625700	-1.38824200
C	4.61912500	-2.12594700	-1.30075300
C	3.47558700	-2.93501800	-1.29115100
C	5.87785500	-2.72739200	-1.34753200
C	3.59959200	-4.32004900	-1.33216900
H	2.48183500	-2.49238900	-1.24520700
C	6.00006600	-4.11564700	-1.39199900
H	6.76861900	-2.10327500	-1.35373200
C	4.86013200	-4.91457000	-1.38377200
H	2.69918900	-4.92692800	-1.32215300
H	6.98515200	-4.56992000	-1.43202300
H	4.95335700	-5.99552100	-1.41740700
C	-2.33941300	6.31535400	-0.72557400
H	-2.23173500	6.92711200	-1.62326100
H	-3.23144800	5.69312400	-0.85037800
H	-2.51281900	6.97539000	0.12715300
C	1.64069400	3.81034100	-2.56900500
H	2.70542700	3.84836500	-2.32283500
H	1.39804100	2.78296800	-2.86329700
H	1.46343400	4.45376800	-3.43154000

C	0.56404300	3.55578200	2.35501300
H	0.55769900	2.45980100	2.32305700
H	1.55295200	3.86873500	2.70190800
H	-0.18002400	3.87821500	3.08387900
C	-1.17445300	0.14512500	-1.26391500
C	-0.26675400	1.02161100	-0.72100200
H	-0.77267000	-0.69212800	-1.83229000
C	-2.60640700	0.39521200	-1.38498300
C	-3.31689600	-0.24972600	-2.40577900
C	-3.29419200	1.25652400	-0.51629000
C	-4.68080500	-0.03298500	-2.56496000
H	-2.79194100	-0.93311100	-3.06640800
C	-4.65716700	1.46466800	-0.67049000
H	-2.76554600	1.72312600	0.31017300
C	-5.35247700	0.82330300	-1.69807300
H	-5.22090700	-0.54890800	-3.35191000
H	-5.18704600	2.10956900	0.02329400
H	-6.42142900	0.97664100	-1.80416100
C	1.10938300	0.65843600	-0.80413500
O	1.55131000	-0.36785400	-1.32423700
H	-0.57672800	1.93404300	-0.22830300
C	-3.98117100	-2.20903400	0.11456300
C	-4.78615300	-2.96329100	-0.75257000
H	-5.86511000	-2.99273800	-0.73055800
C	-3.94145900	-3.63364700	-1.63301500
H	-4.22756100	-4.30104400	-2.43223800
C	-2.63103700	-3.29151600	-1.29924300
H	-1.68044200	-3.60436200	-1.69961500
N	-2.64876900	-2.44086200	-0.23923400
C	-4.40404900	-1.35502200	1.18682900
O	-3.72301800	-0.67820300	1.94283700
C	-5.93637000	-1.32419300	1.42636700
F	-6.23796300	-0.47877000	2.40772300
F	-6.39505000	-2.53751000	1.77005200
F	-6.61965300	-0.93869800	0.33610100
C	-1.53444900	-1.89431500	0.41645800
H	-1.79296100	-1.29067800	1.26810500
C	-0.23235100	-2.41054000	0.24706200
O	0.13293600	-3.24868500	-0.61083800
C	0.76171900	-1.94569500	1.28117900
C	0.66703700	-0.72933800	1.97257100
C	1.81358300	-2.81613200	1.59439400
C	1.59508700	-0.40385300	2.96215700
H	-0.14658200	-0.04477100	1.74890900

C	2.72649100	-2.50147000	2.59532700
H	1.88483200	-3.74511100	1.03894300
C	2.61626800	-1.29472000	3.28887300
H	1.50170000	0.53407500	3.50326300
H	3.52120200	-3.19971900	2.84066900
H	3.31609000	-1.05502400	4.08422300

**M5RR**

C	3.60669700	0.56810400	0.69257000
C	4.82082500	0.16748900	1.46427500
C	4.07581300	-2.01243000	1.55347500
C	2.85023900	-1.82509900	0.61880300
C	1.60970300	0.29012300	-0.14858400
H	5.62966500	-0.15232800	0.79158100
H	4.94457000	-2.30915900	0.95034200
H	1.93289700	-2.14472400	1.11397400
N	3.19870500	1.76981700	0.41790700
N	1.95921300	1.58413700	-0.12051400
N	2.67765600	-0.37717400	0.34487900
H	3.84547000	-2.81606000	2.25418600
H	5.16022500	1.00792100	2.06963800
O	4.42445000	-0.88068500	2.31974200
C	3.05525400	-2.67191800	-0.65692700
H	3.49441200	-3.62180000	-0.32941400
H	2.07187200	-2.86659500	-1.07936300
C	3.93370500	-2.01143000	-1.68923100
C	5.31611300	-2.21125900	-1.74071600
C	3.34250400	-1.15803400	-2.62867800
C	6.09522300	-1.55998700	-2.69587500
H	5.78753700	-2.90310300	-1.04696200
C	4.11786600	-0.51470900	-3.58899200
H	2.26101800	-1.03318000	-2.59981700
C	5.49817300	-0.70779900	-3.62029600
H	7.16675600	-1.73034100	-2.72505000
H	3.64316600	0.13130600	-4.32177100
H	6.10231000	-0.20723200	-4.36993100
C	1.22109900	2.73642000	-0.57267100
C	0.64476900	3.57107200	0.39015800
C	1.10365100	2.96011800	-1.94382100
C	-0.07708900	4.67035700	-0.06884400
C	0.36554000	4.07092400	-2.35130800
C	-0.23014900	4.93340600	-1.43242200
H	-0.54345900	5.33042500	0.65856600
H	0.25092100	4.26052000	-3.41531400

C	0.73389100	3.24668700	1.85618900
H	0.19747100	2.31583400	2.07407500
H	1.76975100	3.10771500	2.17591400
H	0.28565900	4.04454600	2.45036000
C	-1.00934900	6.13699500	-1.89422800
H	-1.35277700	6.01441500	-2.92328200
H	-1.88117900	6.30781500	-1.25790800
H	-0.38918500	7.03807300	-1.85224600
C	1.71095900	2.01269200	-2.93921800
H	2.72983400	1.73533700	-2.65480300
H	1.11759700	1.09214700	-2.99442500
H	1.73582800	2.46206100	-3.93348200
C	0.31002900	-0.33075200	-0.57456200
O	0.36002500	-1.53585600	-0.98411800
C	-0.79037600	0.46135900	-0.39865300
C	-2.13868500	-0.13097700	-0.64343600
H	-0.70220200	1.43799700	0.04886700
H	-2.06126300	-0.79817000	-1.51040600
C	-3.25038400	0.86622500	-0.91279100
C	-3.16763200	2.21190000	-0.54106600
C	-4.41750900	0.42878500	-1.55059500
C	-4.22346800	3.08702800	-0.78677600
H	-2.27681600	2.59552300	-0.05399100
C	-5.47581900	1.29862400	-1.79323100
H	-4.49434800	-0.60859600	-1.86899100
C	-5.38324200	2.63427900	-1.40847500
H	-4.13500000	4.12772600	-0.48953900
H	-6.36979700	0.93383800	-2.28881500
H	-6.20569300	3.31650000	-1.59822200
C	-3.43056400	0.53763900	2.18065000
C	-2.99897600	1.25820300	3.28479600
C	-1.71967000	0.79056000	3.60701300
C	-1.39744800	-0.21671000	2.69372300
N	-2.47746300	-0.36003800	1.82799600
H	-4.34916600	0.60260700	1.62003900
H	-3.56368100	2.02118600	3.79832600
H	-1.09946100	1.11239300	4.42943200
C	-0.23385600	-1.06636200	2.66445500
O	-0.09182600	-2.10261500	2.03676700
C	0.99442500	-0.59789400	3.48631100
F	0.69513900	-0.27147800	4.74791400
F	1.55309900	0.48301100	2.90883500
F	1.91436700	-1.55783100	3.52252200
C	-2.45013100	-1.09681300	0.56976500

H	-1.59898700	-1.77575500	0.61582800
C	-3.70865200	-1.92300100	0.35823500
O	-4.73823700	-1.69808400	0.96418700
C	-3.63763300	-3.01688700	-0.66442300
C	-4.83301200	-3.67541000	-0.97653200
C	-2.44612200	-3.39619200	-1.29721800
C	-4.84434500	-4.70381400	-1.90855200
H	-5.74048700	-3.36236700	-0.47095300
C	-2.46612900	-4.43043900	-2.23036300
H	-1.50188100	-2.89505800	-1.08660100
C	-3.65737700	-5.08304600	-2.53608800
H	-5.77350400	-5.21070600	-2.14748800
H	-1.54376200	-4.72402500	-2.72035900
H	-3.66300300	-5.88742200	-3.26501800

**M5RS**

C	0.81563900	-1.12377600	-1.40364100
O	1.06256700	-0.90156800	-2.62862800
C	-0.29264800	-0.89894900	-0.63911800
C	-1.55020700	-0.34482500	-1.22234000
H	-0.28621100	-1.17112600	0.41031600
H	-1.48987400	-0.42102300	-2.31399000
C	-2.78839300	-1.09257000	-0.75601500
C	-3.01414900	-1.32364800	0.60471300
C	-3.75180300	-1.51099500	-1.67538900
C	-4.17737600	-1.95377100	1.03471600
H	-2.27858800	-1.00346400	1.33895900
C	-4.91571800	-2.14747000	-1.24920200
H	-3.59037300	-1.32405900	-2.73385100
C	-5.13352100	-2.36769700	0.10801200
H	-4.33900300	-2.12075400	2.09565400
H	-5.65406600	-2.46612200	-1.97839000
H	-6.04278700	-2.85656000	0.44361200
C	-0.25079200	1.97860000	-2.71139500
C	0.71006500	2.96146800	-2.91060000
C	0.94749600	3.55949700	-1.66991300
C	0.12463000	2.93014300	-0.73075300
N	-0.60519300	1.95646500	-1.40692800
H	-0.70112800	1.29820400	-3.41534800
H	1.18375000	3.19499000	-3.85174200
H	1.65180000	4.34794000	-1.45175400
C	0.07648700	3.15180000	0.69002700
O	-0.58950900	2.55387800	1.52200000
C	0.95767900	4.31685700	1.20931600

F	2.23151100	4.22720900	0.80633100
F	0.47939600	5.48760500	0.76012200
F	0.94983500	4.34618800	2.53731200
C	-1.70596900	1.16337400	-0.86542800
H	-1.66268500	1.25565800	0.21520800
C	-3.04969300	1.65337400	-1.42122000
O	-3.18838800	1.78238400	-2.62178100
C	-4.18904700	1.84115700	-0.47645500
C	-5.48432300	1.68238800	-0.98059000
C	-3.99956600	2.16804700	0.86990400
C	-6.58136800	1.83346000	-0.14370000
H	-5.60462600	1.42856500	-2.02876000
C	-5.10377800	2.33796900	1.70061700
H	-3.00040900	2.31651400	1.27024200
C	-6.39066200	2.16318500	1.19845500
H	-7.58477200	1.69553500	-0.53282400
H	-4.95755100	2.60519400	2.74188000
H	-7.24799900	2.28496200	1.85294000
C	3.97045500	-2.43778500	-0.12848900
C	5.46725300	-2.45976600	-0.20710500
C	5.37753900	-0.51974300	-1.47715800
C	3.86033800	-0.45516300	-1.68742400
C	1.95582200	-1.78097000	-0.66101000
H	5.90073000	-1.93733700	0.65750500
H	5.64989900	0.00945900	-0.55387100
H	3.58708200	-0.70305800	-2.71481200
N	3.18011600	-3.25071600	0.51069900
N	1.92780800	-2.82543500	0.17035800
N	3.26145800	-1.51539000	-0.85033300
H	5.86997000	-0.03332300	-2.32093900
H	5.81896200	-3.49199500	-0.21201500
O	5.85760900	-1.85056500	-1.41598600
C	3.28887500	0.93624200	-1.35363500
H	3.82370600	1.64592900	-1.99627800
H	2.24419000	0.95135600	-1.67608000
C	3.41296700	1.35559500	0.09375300
C	4.53616000	2.04656600	0.55834700
C	2.38139300	1.08136800	0.99900700
C	4.63963600	2.43215400	1.89318900
H	5.33108800	2.30581500	-0.13760600
C	2.47683900	1.47311900	2.33272200
H	1.47357800	0.60035100	0.63859700
C	3.61111600	2.14323300	2.78555000
H	5.51756000	2.97391400	2.23050700



H	1.64734100	1.28117300	3.00685400
H	3.68281100	2.45742000	3.82170400
C	0.75477000	-3.49660000	0.66190700
C	0.00505800	-4.26555500	-0.23257200
C	0.38354900	-3.27456100	1.98681800
C	-1.17771300	-4.81842400	0.24863400
C	-0.80954400	-3.85449300	2.42015200
C	-1.60391200	-4.61665700	1.56437200
H	-1.79177000	-5.41078500	-0.42517100
H	-1.13040500	-3.69152700	3.44586200
C	0.44705400	-4.45724700	-1.65893000
H	0.35209700	-3.52906900	-2.23340600
H	1.49483000	-4.76962900	-1.70691000
H	-0.16119000	-5.22196100	-2.14419500
C	-2.90945000	-5.20506900	2.03077000
H	-3.09357200	-4.97923600	3.08318000
H	-3.73859100	-4.79851500	1.44336400
H	-2.91584400	-6.29187200	1.90722000
C	1.22404400	-2.41188800	2.89044700
H	2.18710900	-2.88541800	3.10195600
H	1.43876300	-1.44262000	2.42493600
H	0.71055900	-2.23187600	3.83605900

**M5SR**

C	3.67790400	0.34598300	1.00440400
C	4.92343800	-0.32799400	1.47438100
C	4.33970100	-2.29511300	0.34161000
C	3.31322000	-1.55325900	-0.57292700
C	1.75392300	0.39943400	-0.03807500
H	5.75207600	-0.17233500	0.76918000
H	5.28762500	-2.39127100	-0.20359400
H	2.39738600	-2.13111300	-0.69859100
N	3.09515900	1.41653000	1.45508200
N	1.90324100	1.44564700	0.78632500
N	2.90219300	-0.29968500	0.08256900
H	3.96049400	-3.29407400	0.56180500
H	5.20139200	0.04918000	2.45833400
O	4.58898200	-1.69569700	1.59737400
C	3.89317700	-1.27459100	-1.97746600
H	4.24437200	-2.23468800	-2.37165900
H	3.05466600	-0.93657500	-2.58909800
C	5.00935000	-0.26236100	-1.97187300
C	6.35532000	-0.64075700	-1.95721100
C	4.70142100	1.10298500	-1.92923600

C	7.36532300	0.31528000	-1.86376800
H	6.61585000	-1.69411700	-2.02609300
C	5.70545500	2.06090600	-1.82960400
H	3.65832500	1.40811000	-1.98344600
C	7.04215200	1.66765300	-1.78696500
H	8.40451800	0.00259100	-1.85359700
H	5.44628600	3.11458100	-1.79399300
H	7.82747200	2.41239400	-1.71020100
C	0.97894400	2.51931600	1.03083900
C	0.20996600	2.47682900	2.19468000
C	0.86474800	3.52603600	0.07041100
C	-0.72583000	3.49580300	2.37396500
C	-0.08678700	4.51672200	0.29412600
C	-0.89826900	4.50902700	1.43061500
H	-1.34590800	3.48477000	3.26688500
H	-0.20556100	5.30755600	-0.44207900
C	0.31957700	1.33074700	3.16384500
H	-0.19860600	0.44893300	2.76963800
H	1.35925600	1.05366300	3.35272300
H	-0.14923500	1.58897700	4.11497400
C	-1.96612400	5.55583100	1.61002200
H	-2.85946300	5.28181500	1.03898800
H	-2.25463100	5.65448600	2.65857200
H	-1.63019900	6.53077800	1.24904800
C	1.71136300	3.50807000	-1.17245600
H	2.76747000	3.35776100	-0.92628000
H	1.39643400	2.69361700	-1.83525700
H	1.61365700	4.44698800	-1.71915700
C	0.61551900	-0.00384000	-0.94616900
O	0.94852100	-0.73667200	-1.92574700
C	-0.62438400	0.42506800	-0.55388800
C	-1.84605400	-0.00536400	-1.29889200
H	-0.75479100	1.02201900	0.33688600
H	-1.57546400	-0.24888100	-2.33361800
C	-2.94909400	1.03619600	-1.28580600
C	-3.36897100	1.61033800	-0.08075500
C	-3.62250600	1.37559000	-2.46030100
C	-4.43830800	2.50008000	-0.05271100
H	-2.86576800	1.34631500	0.84753900
C	-4.68981800	2.27114300	-2.43656600
H	-3.31300700	0.92161500	-3.39795600
C	-5.10254200	2.83366500	-1.23211700
H	-4.75887600	2.92774100	0.89252200
H	-5.20161600	2.52468200	-3.35974900

H	-5.93873600	3.52522400	-1.21042700
C	-1.08125800	-3.09989700	-1.82558600
C	-0.01248300	-3.93073100	-1.52039000
C	0.31895100	-3.69705600	-0.18328200
C	-0.57026500	-2.73652400	0.30980900
N	-1.43855200	-2.40552300	-0.72162400
H	-1.61014800	-2.94810600	-2.75284500
H	0.46585400	-4.61533500	-2.20390800
H	1.09234600	-4.18419400	0.39305700
C	-0.62572600	-2.17937600	1.63439400
O	-1.50148400	-1.48823900	2.13238800
C	0.61265600	-2.47259200	2.51862200
F	1.73195000	-1.99352900	1.94397700
F	0.79295400	-3.78606600	2.71231300
F	0.48808300	-1.89439800	3.70719500
C	-2.42028300	-1.32490400	-0.67201800
H	-2.60535200	-1.12137900	0.37603200
C	-3.72358100	-1.68659700	-1.38097100
O	-3.71571800	-2.07118100	-2.53574200
C	-5.00835100	-1.43515300	-0.66135400
C	-6.14741800	-1.19706100	-1.43760700
C	-5.10594400	-1.43436500	0.73399700
C	-7.36903400	-0.94748500	-0.82719400
H	-6.04701700	-1.20016000	-2.51802300
C	-6.33642000	-1.20358700	1.34193800
H	-4.23548700	-1.63031300	1.35346700
C	-7.46423300	-0.95316900	0.56438700
H	-8.24753900	-0.74832400	-1.43196000
H	-6.41272100	-1.21573200	2.42401400
H	-8.41947300	-0.76128700	1.04271900

#### M5SS

C	-0.81174800	-0.14758400	-1.13034400
O	-0.05696400	0.05820900	-2.14093800
C	-1.06579400	0.65809100	-0.06029500
C	-0.36366800	1.98754500	0.01044900
H	-1.72009400	0.34334500	0.74528000
H	-0.44438000	2.43158900	-0.99264600
C	-1.04418100	2.96687000	0.95605800
C	-2.44308200	3.04105600	0.90820800
C	-0.36432300	3.81729400	1.83183400
C	-3.14136500	3.93969900	1.70609400
H	-2.98511800	2.37965700	0.23556300
C	-1.06563900	4.71776700	2.63408300

H	0.71632100	3.76733600	1.91469100
C	-2.45336600	4.78565600	2.57455500
H	-4.22541800	3.97793700	1.64932700
H	-0.51731700	5.36470000	3.31159300
H	-2.99477800	5.48725200	3.20100300
C	0.88865400	0.89050200	2.50424500
C	1.60088300	0.08087600	3.37922600
C	2.74803300	-0.34470600	2.70252500
C	2.71315300	0.22359400	1.42896100
N	1.55514300	0.97944200	1.33079600
H	-0.05458900	1.39479100	2.64476400
H	1.30406900	-0.17086000	4.38606900
H	3.52286800	-0.99761600	3.07546500
C	3.66682300	0.09466600	0.35476600
O	3.65178700	0.66913600	-0.71915000
C	4.79525800	-0.93508700	0.59576900
F	5.49130100	-0.66649600	1.70859900
F	4.27831200	-2.16807300	0.73191800
F	5.64108500	-0.95473200	-0.42664100
C	1.16291700	1.72443000	0.13603600
H	1.36925100	1.07010400	-0.71584700
C	2.06605700	2.94662900	-0.04648900
O	2.75637600	3.36017900	0.86414000
C	2.06946200	3.60920800	-1.38670400
C	2.63240200	4.88727200	-1.46831800
C	1.56272900	2.99399000	-2.53828400
C	2.68034600	5.55489500	-2.68455800
H	3.02797900	5.33619400	-0.56328100
C	1.62165900	3.66684100	-3.75632900
H	1.12677500	1.99662100	-2.50149800
C	2.17431700	4.94279200	-3.83120400
H	3.11223200	6.54865200	-2.74237900
H	1.23505500	3.18869800	-4.65027600
H	2.21352100	5.46132900	-4.78415300
C	-1.85809100	-3.60374500	-1.52882900
C	-1.55013700	-4.97212700	-2.05635300
C	0.65624200	-4.32398700	-2.35820300
C	0.50410700	-2.83872600	-1.99681400
C	-1.46887300	-1.49398400	-1.12606400
H	-1.27973000	-5.64743700	-1.23225000
H	0.87918800	-4.90746500	-1.45526200
H	0.63504100	-2.19562500	-2.86834400
N	-2.99162800	-3.13794400	-1.09023000
N	-2.72997700	-1.82082600	-0.84029600

N	-0.89389800	-2.63205100	-1.55853800
H	1.48578300	-4.42885900	-3.05930700
H	-2.42392400	-5.37055600	-2.57285500
O	-0.49690700	-4.85476800	-2.98470400
C	1.51547700	-2.41159900	-0.91256500
H	2.50977700	-2.66064500	-1.30154200
H	1.47099700	-1.32137800	-0.83389800
C	1.30354100	-3.06008900	0.43553400
C	1.93377400	-4.26360000	0.77102200
C	0.47116700	-2.45811800	1.38311000
C	1.70894400	-4.86951200	2.00372100
H	2.62702900	-4.71856300	0.06724500
C	0.24604400	-3.06048600	2.61896800
H	0.03803300	-1.48238600	1.16760100
C	0.85454500	-4.27329000	2.92901900
H	2.21081600	-5.80071400	2.24625600
H	-0.38815800	-2.56448400	3.34797500
H	0.68265300	-4.74130900	3.89288800
C	-3.76382500	-0.93324800	-0.38303200
C	-4.28791300	-0.00550400	-1.28486000
C	-4.15077700	-1.01339300	0.95545100
C	-5.24639300	0.88044700	-0.79409100
C	-5.10889700	-0.10318600	1.39655700
C	-5.66375200	0.84849400	0.53826700
H	-5.67118800	1.61888100	-1.46921400
H	-5.42116700	-0.13159500	2.43730100
C	-3.81714000	0.04728900	-2.71392000
H	-2.78375900	0.40566000	-2.77925000
H	-3.85218500	-0.94446500	-3.17522600
H	-4.44814100	0.71901900	-3.29751200
C	-6.71022700	1.81020700	1.03843800
H	-6.52732400	2.08289300	2.08051100
H	-6.72674100	2.72294400	0.43871100
H	-7.70617700	1.35900000	0.98479100
C	-3.53104600	-2.03067700	1.87570500
H	-3.84782800	-3.04317700	1.60860200
H	-2.43747300	-2.01021600	1.80862200
H	-3.81778400	-1.83871000	2.91060300

**TS5RR**

C	3.76348200	-1.31849700	0.56979900
C	5.09912000	-1.78525300	0.08778500
C	4.70411000	-0.86755500	-2.00833300
C	3.38238300	-0.14625100	-1.63896000

C	1.78878800	-0.47256700	0.30776500
H	5.86925500	-1.02024300	0.26124700
H	5.54614700	-0.18157100	-1.85043200
H	2.54895400	-0.45207300	-2.28095400
N	3.11346700	-1.65158100	1.65121500
N	1.88153900	-1.10420600	1.47224600
N	2.99063200	-0.56618400	-0.27317000
H	4.66383000	-1.13757900	-3.06412400
H	5.37467100	-2.70664300	0.60042900
O	4.94623500	-2.05902400	-1.28808200
C	3.56219200	1.38382000	-1.74374500
H	4.05429900	1.56851300	-2.70529100
H	2.57113400	1.83639500	-1.78598500
C	4.36892900	1.96867400	-0.60884300
C	5.75099400	2.15726900	-0.70051200
C	3.72727000	2.30574300	0.58975900
C	6.47990200	2.63814200	0.38626100
H	6.26174400	1.94561300	-1.63670000
C	4.45227100	2.78559700	1.67625000
H	2.64570400	2.20749800	0.64672900
C	5.83387400	2.94452500	1.58033000
H	7.55182700	2.78087300	0.29465900
H	3.93719200	3.04766800	2.59579100
H	6.40044900	3.31993000	2.42612100
C	0.80338000	-1.25142400	2.41535000
C	0.21028900	-2.51397400	2.53340800
C	0.32328900	-0.10986000	3.05949400
C	-0.93385900	-2.60221700	3.31966300
C	-0.82819500	-0.25751700	3.83412300
C	-1.47353100	-1.48566500	3.96534600
H	-1.43241400	-3.56361700	3.41214400
H	-1.23326300	0.61546300	4.33943700
C	0.76288600	-3.70915400	1.80378900
H	0.07863400	-4.55396100	1.89084700
H	0.90642500	-3.49653700	0.74040300
H	1.73346300	-4.00240300	2.21331100
C	-2.71532500	-1.62204400	4.80490000
H	-2.47363800	-2.05204300	5.78234100
H	-3.18935200	-0.65188400	4.96677800
H	-3.44038800	-2.27719600	4.31653900
C	0.99404700	1.23362600	2.92210300
H	2.07956600	1.13303700	2.83007500
H	0.63120400	1.77482200	2.04072400
H	0.78065300	1.84789600	3.79854000

C	0.55665800	0.22597700	-0.20774700
O	0.70227700	1.39862000	-0.53957200
C	-0.64551700	-0.53849900	-0.37269900
C	-1.88965800	0.34129900	-0.20136200
H	-0.68233200	-1.45905700	0.20665500
H	-1.59524400	1.21669400	0.38947900
C	-3.00782100	-0.35498600	0.54344400
C	-3.36894800	-1.67657100	0.26437000
C	-3.70302500	0.33862100	1.53824000
C	-4.39870600	-2.28917900	0.97395200
H	-2.84121400	-2.22930200	-0.50976200
C	-4.73545900	-0.27129900	2.24495400
H	-3.43005800	1.36889700	1.75835100
C	-5.08463900	-1.59037700	1.96488500
H	-4.66982700	-3.31501700	0.74518200
H	-5.26479000	0.28200100	3.01470900
H	-5.88846400	-2.07013500	2.51480700
C	-3.98707800	-0.59450900	-2.91737700
C	-3.83796100	-1.83341200	-3.49418700
C	-2.48695200	-2.22926700	-3.32405400
C	-1.84776000	-1.20770300	-2.65378700
N	-2.76394700	-0.20836600	-2.42130900
H	-4.85056400	0.03623200	-2.81618600
H	-4.61979000	-2.38886200	-3.99132700
H	-2.02735500	-3.14683300	-3.65925200
C	-0.41580900	-1.05148800	-2.20982600
O	0.34599900	-0.22523100	-2.81004200
C	0.18990900	-2.46214200	-2.02281400
F	0.37161500	-3.05485200	-3.20978500
F	-0.55260600	-3.29742800	-1.27288200
F	1.40961200	-2.41700900	-1.43369400
C	-2.36370700	0.90651100	-1.58329400
H	-1.48433200	1.36074400	-2.05240000
C	-3.42353900	1.97130000	-1.34713300
O	-4.60900700	1.76196300	-1.50790300
C	-2.96524000	3.30142700	-0.81848000
C	-3.96115800	4.19758100	-0.41218700
C	-1.61986800	3.67359900	-0.71993200
C	-3.62065200	5.44825700	0.08489500
H	-4.99760300	3.88974900	-0.49813800
C	-1.28320500	4.92945900	-0.22059000
H	-0.82680500	2.99382400	-1.01320900
C	-2.27853900	5.81641700	0.18032300
H	-4.39809400	6.13771800	0.39719500

H	-0.23845800	5.21347700	-0.14839200
H	-2.01035400	6.79463900	0.56685400

**TS5RS**

C	-0.51760800	-0.32456200	-1.12253500
O	-0.46793900	-1.18154300	-1.99451800
C	0.52051600	-0.01407400	-0.16704000
C	1.90163400	-0.44038200	-0.64101100
H	0.46534500	0.98319700	0.25655000
H	1.78775900	-0.83950400	-1.65562500
C	2.86320800	0.73196800	-0.67654700
C	3.05015200	1.53996100	0.45123400
C	3.59870600	1.00867700	-1.83057500
C	3.96066300	2.59143000	0.42567500
H	2.47866900	1.34486300	1.35526100
C	4.50276500	2.06920100	-1.86204100
H	3.46668300	0.38012100	-2.70802600
C	4.68858800	2.86142700	-0.73256900
H	4.09995600	3.20381400	1.31160600
H	5.06631800	2.27012100	-2.76756600
H	5.39816700	3.68261500	-0.75237400
C	1.65296400	-4.00882000	0.26296400
C	0.49424100	-4.61794800	0.68182600
C	-0.38383100	-3.59605700	1.11956600
C	0.27220800	-2.39494400	0.96734100
N	1.52172200	-2.65179800	0.42785800
H	2.54795300	-4.43325200	-0.16074800
H	0.30555900	-5.68132600	0.66533000
H	-1.38123000	-3.69409600	1.52295700
C	-0.28517900	-1.04409500	1.28149900
O	-1.55863100	-0.90256500	1.29079000
C	0.33888000	-0.37010300	2.52105500
F	-0.15934600	-0.92722400	3.62911500
F	1.68446200	-0.46633900	2.61702000
F	0.06002900	0.94455700	2.57511100
C	2.52325000	-1.62523100	0.16369200
H	2.89694700	-1.25996800	1.11541700
C	3.68443300	-2.15694300	-0.68476200
O	3.44582200	-2.79418600	-1.69196300
C	5.09576500	-1.81934000	-0.31542100
C	6.10478300	-2.35168300	-1.12846900
C	5.44628400	-0.99389900	0.75849800
C	7.43888300	-2.07075900	-0.87118300
H	5.81463900	-2.98437200	-1.96010400



C	6.78470900	-0.70433400	1.00768900
H	4.69089300	-0.55115200	1.39698400
C	7.78070300	-1.24315200	0.19844200
H	8.21363200	-2.49164500	-1.50343600
H	7.04732500	-0.05626000	1.83698400
H	8.82327900	-1.01794300	0.39932600
C	-3.93227900	0.91451600	-1.39476300
C	-5.36046400	0.72953500	-1.81945800
C	-4.53190300	-1.29865200	-2.82216100
C	-3.43704300	-1.48147100	-1.77070400
C	-1.84661500	0.39939900	-1.03278700
H	-6.00840000	0.86673900	-0.94607000
H	-4.93145200	-2.27529500	-3.10217500
H	-2.57059200	-1.95795600	-2.22916200
N	-3.36692900	2.03382200	-1.03056600
N	-2.07016200	1.69080900	-0.80533600
N	-3.02908800	-0.10680300	-1.42301000
H	-4.09843200	-0.82683700	-3.71610900
H	-5.59252100	1.50504300	-2.56016600
O	-5.63081900	-0.55543600	-2.33644400
C	-3.83619500	-2.25440100	-0.49683900
H	-4.12705300	-3.25936300	-0.82090600
H	-2.92991600	-2.32888300	0.11305400
C	-4.94078500	-1.61417500	0.31490200
C	-6.28017200	-1.96404600	0.12051300
C	-4.63107700	-0.62461900	1.25427400
C	-7.29326600	-1.31746100	0.81954300
H	-6.53053900	-2.73413100	-0.60477800
C	-5.64692600	0.02816600	1.95297700
H	-3.58576900	-0.39273500	1.44401900
C	-6.97927800	-0.30958400	1.73243600
H	-8.32870000	-1.59687100	0.65228200
H	-5.39161800	0.79516100	2.67813400
H	-7.76990600	0.19722700	2.27678700
C	-1.11829800	2.67962400	-0.37212500
C	-0.11874500	3.09087900	-1.25521200
C	-1.20687200	3.10290100	0.95718400
C	0.84085200	3.96981400	-0.75553600
C	-0.22882800	3.98977200	1.39956100
C	0.80020000	4.42736900	0.56124900
H	1.65577700	4.27978700	-1.40526900
H	-0.25736800	4.32656800	2.43274600
C	-0.01457300	2.55645100	-2.65905900
H	0.56442000	1.62473900	-2.67506100

H	-0.99559800	2.35524500	-3.09724300
H	0.50558300	3.27298100	-3.29698500
C	1.84678300	5.38261500	1.07123400
H	2.74032500	5.35472700	0.44363500
H	1.46533700	6.40873000	1.07275100
H	2.13528900	5.13744900	2.09673200
C	-2.27185300	2.55369900	1.86757900
H	-3.27039100	2.84510400	1.52937100
H	-2.21498500	1.45851700	1.87892200
H	-2.12424600	2.91751600	2.88538100

**TS5SR**

C	-3.68044100	-0.73476400	1.63488900
C	-4.98981300	-0.48123200	2.31703800
C	-5.28456900	1.37243200	0.98297300
C	-3.92151800	1.36343200	0.27826100
C	-1.94985000	-0.30406300	0.38518700
H	-5.79739900	-1.02383300	1.80515000
H	-6.00895500	0.76976500	0.41893000
H	-3.29118100	2.18400600	0.62199700
N	-2.83596400	-1.68725100	1.89867400
N	-1.76668400	-1.40906400	1.10701200
N	-3.19549100	0.12476700	0.68246100
H	-5.63567600	2.40539900	1.01469600
H	-4.92570000	-0.82581400	3.34957500
O	-5.22646300	0.90426900	2.31641500
C	-4.09618800	1.48404900	-1.24578800
H	-4.65635600	2.41309600	-1.40306500
H	-3.10741700	1.62138600	-1.68525700
C	-4.82535800	0.32259700	-1.88222900
C	-6.20832400	0.35677400	-2.08915400
C	-4.12274000	-0.82472500	-2.26709800
C	-6.87846000	-0.73435000	-2.63744400
H	-6.76575800	1.25318900	-1.82641100
C	-4.79063800	-1.91857300	-2.81212700
H	-3.04100000	-0.82847400	-2.16989400
C	-6.17146200	-1.88025500	-2.99267400
H	-7.95163200	-0.68578900	-2.79242600
H	-4.22704900	-2.79803000	-3.11014800
H	-6.69126600	-2.73108000	-3.42115400
C	-0.65979500	-2.33186900	1.10542700
C	-0.45148500	-3.13698700	-0.01964400
C	0.08249000	-2.44717900	2.28297800
C	0.54508200	-4.10459000	0.07375800

C	1.06520400	-3.43518500	2.32087200
C	1.29793500	-4.27866700	1.23541200
H	0.73874200	-4.73947100	-0.78709100
H	1.66075000	-3.54617600	3.22361700
C	-1.26495900	-2.98336100	-1.27728000
H	-2.32932100	-2.85298500	-1.05455000
H	-0.93525500	-2.11359500	-1.85558000
H	-1.15416200	-3.86845200	-1.90568800
C	2.34299700	-5.36042500	1.30261200
H	1.87756900	-6.33928800	1.45511800
H	2.91162200	-5.40598100	0.36973700
H	3.04023900	-5.18930100	2.12588100
C	-0.17310100	-1.55087400	3.46615400
H	-0.28334200	-0.50405600	3.16602500
H	-1.09558900	-1.83802000	3.97906800
H	0.65117200	-1.62083900	4.17759000
C	-0.89124200	0.25346000	-0.56782100
O	-1.22063400	0.40864400	-1.74555400
C	0.32109500	0.63274600	0.04514700
C	1.54160000	0.70293700	-0.83715700
H	0.49545200	0.23529200	1.04260700
H	1.24420400	1.07230400	-1.82448300
C	2.19033500	-0.66396000	-1.00310400
C	2.78774100	-1.30813200	0.08561800
C	2.28334600	-1.25235600	-2.26573300
C	3.51446700	-2.47907500	-0.09507700
H	2.71188000	-0.87568400	1.08139200
C	2.98426000	-2.44422400	-2.44383000
H	1.82355800	-0.75542500	-3.11563400
C	3.61895900	-3.04975600	-1.36224500
H	3.99891300	-2.94851000	0.75653300
H	3.05346900	-2.88500200	-3.43350600
H	4.19270600	-3.96062500	-1.50553500
C	2.83463400	4.16172600	-0.76737100
C	1.99798100	5.24939100	-0.84795800
C	0.70048400	4.79940500	-0.51051200
C	0.79038700	3.45429300	-0.21621100
N	2.10317300	3.06797400	-0.37906500
H	3.88529900	4.07283500	-0.99534000
H	2.29236300	6.24965800	-1.12887500
H	-0.21277300	5.37267800	-0.44989000
C	-0.35073200	2.67369200	0.33836700
O	-1.48518100	2.88539100	-0.13145500
C	-0.30215200	2.50937400	1.86668100

F	-0.62714200	3.66881600	2.45236600
F	0.90030900	2.15098300	2.34977800
F	-1.19819000	1.59476100	2.30185100
C	2.59996200	1.70494900	-0.30227000
H	2.83337000	1.45298600	0.73694900
C	3.83708700	1.52536400	-1.20372100
O	3.77885200	1.85259900	-2.37002400
C	5.03609000	0.82984900	-0.65197400
C	5.79321700	0.05493200	-1.53545900
C	5.40411500	0.91409400	0.69344300
C	6.89391400	-0.65302100	-1.07080500
H	5.48452600	0.00202900	-2.57436600
C	6.52225400	0.22362900	1.15070700
H	4.83543100	1.53084800	1.38288400
C	7.25889000	-0.56851900	0.27272000
H	7.46852300	-1.27141400	-1.75243300
H	6.81622900	0.30039300	2.19219300
H	8.12099700	-1.11916400	0.63543100

**TS5SS**

C	0.28243400	0.65238100	-0.49059200
O	0.23217800	1.86375200	-0.67477500
C	-0.69372000	-0.07844300	0.28007100
C	-2.10712000	0.47986300	0.02396500
H	-0.64527600	-1.15920500	0.18505600
H	-2.04780000	1.14684600	-0.84219700
C	-3.10054100	-0.61458900	-0.30434200
C	-3.90490400	-0.49175200	-1.44038100
C	-3.23480200	-1.75319200	0.49915900
C	-4.81926800	-1.48681100	-1.78073800
H	-3.81345500	0.39553900	-2.06392300
C	-4.15175700	-2.74410000	0.16278300
H	-2.61406400	-1.86750700	1.38601600
C	-4.94284800	-2.61790300	-0.97860100
H	-5.43457600	-1.37528400	-2.66808100
H	-4.24955600	-3.62041900	0.79635300
H	-5.65599200	-3.39506400	-1.23646800
C	-3.64267700	0.09736300	3.19726800
C	-3.10213900	-0.80392200	4.08502000
C	-1.71146200	-0.90209500	3.81241300
C	-1.44621100	-0.04213500	2.76850400
N	-2.62095600	0.57159800	2.40906700
H	-4.65269100	0.43714800	3.05788600
H	-3.65061800	-1.32805500	4.85419400

H	-0.98513300	-1.51517000	4.32517400
C	-0.18642500	0.31563700	2.01523000
O	0.27367300	1.50452200	2.09914100
C	0.86604500	-0.78051500	2.27226100
F	1.30630800	-0.74389600	3.53294100
F	0.44641400	-2.03886300	2.03663600
F	1.95201200	-0.59426700	1.47765600
C	-2.59497600	1.38044100	1.20638400
H	-1.81896700	2.13774200	1.35809000
C	-3.89625300	2.05853700	0.82759600
O	-4.97238400	1.72089200	1.27860500
C	-3.81756200	3.15709600	-0.19480100
C	-5.02905400	3.63787200	-0.70428800
C	-2.61144300	3.71236300	-0.63938200
C	-5.04013300	4.65941800	-1.64443700
H	-5.95090900	3.19419600	-0.34397400
C	-2.62816500	4.73806100	-1.58102600
H	-1.65516100	3.35116700	-0.27210500
C	-3.83719000	5.21246000	-2.08297500
H	-5.98327100	5.02708800	-2.03511100
H	-1.69167300	5.16826700	-1.92006900
H	-3.84340400	6.01344200	-2.81552500
C	3.44956600	-0.31209400	-2.01061600
C	4.79970600	0.07248100	-2.54374700
C	4.25100200	2.29117300	-1.98899700
C	3.08636500	1.97814600	-1.04460900
C	1.49714900	-0.02798600	-1.08415500
H	5.52801800	-0.69942700	-2.28926300
H	4.74026800	3.20767600	-1.65342500
H	2.24036900	2.62094600	-1.28275700
N	2.83948500	-1.45784000	-2.14765000
N	1.62473800	-1.26329400	-1.56796400
N	2.65438200	0.59771000	-1.37425800
H	3.87242700	2.44503900	-3.01020100
H	4.72737900	0.14487600	-3.63919600
O	5.23950600	1.27949400	-1.97981100
C	3.40289700	2.10754700	0.45745300
H	3.42831400	3.18201400	0.66590500
H	2.55612200	1.70477500	1.02864700
C	4.72589000	1.49194900	0.84995600
C	5.84156500	2.31081400	1.03721200
C	4.88978400	0.10725500	0.96502500
C	7.09336000	1.76686200	1.31210500
H	5.72742500	3.38977500	0.96575500

C	6.14062100	-0.44060200	1.23276100
H	4.03310700	-0.54934900	0.85838600
C	7.24856500	0.38691200	1.40189300
H	7.94669300	2.42196100	1.45602600
H	6.24803200	-1.51741700	1.31995000
H	8.22284800	-0.04110300	1.61432500
C	0.64501000	-2.32057300	-1.55279000
C	-0.52351200	-2.16054500	-2.30209400
C	0.89929000	-3.43415700	-0.74521900
C	-1.49372800	-3.15495800	-2.18510500
C	-0.10055700	-4.40009900	-0.67453900
C	-1.30310600	-4.27235100	-1.37413800
H	-2.43137200	-3.03684700	-2.72254900
H	0.06009500	-5.27092900	-0.04398800
C	-0.76100600	-0.95680100	-3.17529900
H	-1.12961700	-0.10564400	-2.59139900
H	0.15098600	-0.64415100	-3.69184100
H	-1.51969800	-1.18470100	-3.92569400
C	-2.36220400	-5.33641800	-1.26108100
H	-2.56361900	-5.57269100	-0.21262100
H	-3.29592800	-5.01139500	-1.72354100
H	-2.03592400	-6.25949500	-1.75035000
C	2.19156400	-3.58870800	0.01074700
H	2.10388200	-4.39265100	0.74274200
H	3.01233500	-3.82639500	-0.67185400
H	2.45216400	-2.67214900	0.54377000

#### M6RR

C	3.68178900	0.06337900	1.73870600
C	5.07323700	-0.33955600	2.11606700
C	5.22665600	-1.62464900	0.19508700
C	3.81300100	-1.34143700	-0.35381800
C	1.83225800	-0.05194900	0.58945000
H	5.80570100	0.37351700	1.71165600
H	5.92973300	-0.87545900	-0.18957100
H	3.22465400	-2.25827800	-0.41275500
N	2.83992900	0.80371200	2.39782100
N	1.69676600	0.73542300	1.65546100
N	3.10797300	-0.47108000	0.61163900
H	5.53984700	-2.61084000	-0.15089400
H	5.16323000	-0.37187700	3.20206600
O	5.29092700	-1.63658700	1.60762400
C	3.87543100	-0.68712400	-1.75006900
H	4.45873700	-1.36528400	-2.38371100

H	2.86008300	-0.65684000	-2.15369700
C	4.48338800	0.69671100	-1.75098900
C	5.84630400	0.90153900	-1.98786500
C	3.66915600	1.80738200	-1.49910700
C	6.39399000	2.18168700	-1.94195000
H	6.48368700	0.05308100	-2.22662200
C	4.21745800	3.08686800	-1.45079100
H	2.59608000	1.65666200	-1.38110600
C	5.58125400	3.27752500	-1.66368200
H	7.45330000	2.32233700	-2.13176100
H	3.57241200	3.94004100	-1.26082500
H	6.00576200	4.27571700	-1.62946500
C	0.48081400	1.39041400	2.06227900
C	-0.30768200	0.75767700	3.03105800
C	0.11703900	2.58739600	1.44090200
C	-1.54971500	1.32066200	3.31047900
C	-1.13632700	3.11191900	1.76257300
C	-1.98521700	2.48583300	2.67421000
H	-2.20154300	0.82790200	4.02734400
H	-1.45726300	4.03003100	1.27628500
C	0.17026100	-0.47627400	3.75177400
H	-0.66662900	-0.98148900	4.23666300
H	0.65830700	-1.19010900	3.08145300
H	0.90256700	-0.20707500	4.51928400
C	-3.33850000	3.06819300	2.98753500
H	-4.03687800	2.28503800	3.29231500
H	-3.26906500	3.79366300	3.80446800
H	-3.75362200	3.58465400	2.11782800
C	1.01777800	3.29156800	0.46477000
H	2.07139900	3.15678100	0.72724300
H	0.86839500	2.87217000	-0.53419100
H	0.79781200	4.36136000	0.45590800
C	0.70809100	-0.27637700	-0.44692100
O	0.57765500	0.76164100	-1.18952800
C	-0.54526800	-0.98159600	0.21958000
C	-1.85701600	-0.32371300	-0.17527700
H	-0.50497300	-1.10663500	1.30167300
H	-1.70096200	0.74872200	-0.01467600
C	-3.05476200	-0.75354500	0.64760400
C	-3.28639000	-2.08795800	0.99128500
C	-3.97590000	0.21540700	1.06011400
C	-4.40930500	-2.44070500	1.73713100
H	-2.58813100	-2.85936100	0.68045500
C	-5.09992300	-0.13602100	1.80128100

H	-3.80195300	1.25677700	0.79600700
C	-5.31834700	-1.46844300	2.14453600
H	-4.57372000	-3.48158500	1.99699800
H	-5.80504500	0.63063200	2.10871200
H	-6.19285100	-1.74706600	2.72376000
C	-2.88357600	-2.66493200	-2.87047800
C	-2.42107800	-3.96093600	-2.90203700
C	-1.30087600	-4.03637200	-2.03983800
C	-1.11516800	-2.77919000	-1.50741700
N	-2.09684000	-1.94530400	-2.01031100
H	-3.71645800	-2.20616700	-3.37213300
H	-2.85222500	-4.76544200	-3.47905600
H	-0.69881400	-4.90566500	-1.82156200
C	-0.11072300	-2.23665500	-0.55517800
O	1.00725200	-1.56214000	-1.15503900
C	0.45776300	-3.31844700	0.34917100
F	1.14801300	-4.23535000	-0.34139700
F	-0.48213600	-3.95321500	1.05705700
F	1.32552000	-2.78094300	1.23915600
C	-2.09538600	-0.51797600	-1.70504000
H	-1.24054800	-0.05796700	-2.21188800
C	-3.36300900	0.23239700	-2.09008000
O	-4.39907600	-0.32804800	-2.38241300
C	-3.30453400	1.73261000	-2.01054000
C	-4.52475800	2.41588100	-2.06462300
C	-2.11125200	2.45087500	-1.86028100
C	-4.55896400	3.80046000	-1.96318800
H	-5.43532500	1.83724200	-2.17857300
C	-2.15291400	3.84030300	-1.76609500
H	-1.15063300	1.94188900	-1.79846200
C	-3.37025300	4.51534200	-1.81327800
H	-5.50862000	4.32397700	-2.00089900
H	-1.22619500	4.39541800	-1.65531500
H	-3.39462800	5.59791100	-1.73603000

#### **M6RS**

C	-0.83173100	-0.60966600	-1.00754300
O	-0.64091000	-0.78915800	-2.24770400
C	0.39508000	-0.59057700	-0.00888700
C	1.76103000	-0.59509300	-0.68674600
H	0.31534500	0.17943500	0.76436400
H	1.59160200	-0.84100800	-1.74268700
C	2.53620000	0.70109300	-0.58016400
C	2.87216000	1.22860400	0.67044600



C	3.07351200	1.29019700	-1.72670700
C	3.76064100	2.29381800	0.77478800
H	2.45931700	0.78173800	1.57328400
C	3.94930500	2.36905900	-1.62655500
H	2.82378400	0.87579700	-2.70011300
C	4.30779400	2.86235700	-0.37413700
H	4.03118900	2.67801700	1.75372700
H	4.36718800	2.81020100	-2.52638900
H	5.01069000	3.68587100	-0.29223400
C	2.47965100	-4.22589700	-0.60086600
C	1.46341100	-5.14966200	-0.50857600
C	0.29523600	-4.46076000	-0.09155600
C	0.64055100	-3.13701900	0.05169500
N	1.96909500	-3.00019100	-0.26432900
H	3.50771500	-4.33468700	-0.90788200
H	1.55126200	-6.20237400	-0.73317600
H	-0.69042200	-4.86994500	0.07449000
C	-0.15356800	-1.94507700	0.47926100
O	-1.38801700	-1.81298100	-0.20096500
C	-0.38345000	-1.98544100	1.98095600
F	-1.06967900	-3.06519400	2.36152400
F	0.79089300	-1.98007700	2.63566500
F	-1.07379300	-0.91038600	2.41643100
C	2.65473500	-1.73261200	-0.11223300
H	2.82320400	-1.53993600	0.95220200
C	3.98161300	-1.69612400	-0.87910900
O	4.01659700	-2.05163400	-2.03874700
C	5.17944300	-1.10845200	-0.20825400
C	6.11817200	-0.46099700	-1.01769200
C	5.39113100	-1.18835400	1.17123100
C	7.24603300	0.11901800	-0.45173700
H	5.93406800	-0.41017800	-2.08584300
C	6.53395700	-0.62751200	1.73268300
H	4.68359200	-1.70691200	1.81036400
C	7.45503000	0.03433600	0.92435900
H	7.96359400	0.63571600	-1.08044000
H	6.70324700	-0.70435700	2.80146800
H	8.33855300	0.48325900	1.36691100
C	-3.90421500	1.35009700	-1.19554100
C	-5.30581300	1.45977700	-1.72968000
C	-4.79243400	-0.56114100	-2.86889200
C	-3.76961400	-1.04705500	-1.84383600
C	-1.95607300	0.42945800	-0.82320000
H	-5.98160300	1.76182700	-0.92543100

H	-5.31358900	-1.41347900	-3.30702800
H	-2.94513500	-1.56930200	-2.33638700
N	-3.17408700	2.30778000	-0.70307300
N	-1.96026800	1.71041000	-0.47159200
N	-3.19356000	0.18847500	-1.29117200
H	-4.28959800	-0.00059800	-3.66993000
H	-5.31046900	2.23409900	-2.50880900
O	-5.78110500	0.23216200	-2.23548400
C	-4.38899300	-1.92681300	-0.72815400
H	-5.12927300	-2.57831900	-1.20345500
H	-3.58700800	-2.55289200	-0.33334300
C	-5.01759500	-1.15533200	0.41096900
C	-6.38300100	-0.86201100	0.44708600
C	-4.20481600	-0.70465700	1.45661600
C	-6.92123200	-0.11797400	1.49442700
H	-7.02199100	-1.20359200	-0.36167200
C	-4.73985400	0.04287900	2.50285800
H	-3.14700800	-0.95381200	1.44024800
C	-6.10004400	0.34255500	2.52213700
H	-7.98445800	0.10062300	1.50891700
H	-4.09411000	0.37998300	3.30849800
H	-6.52050800	0.92243800	3.33747800
C	-0.87122900	2.52937700	-0.01215100
C	0.03973500	3.00371000	-0.95733000
C	-0.84205600	2.88490900	1.33871700
C	1.01869700	3.88581000	-0.50247400
C	0.16729800	3.75394500	1.74357600
C	1.09445400	4.27118700	0.83494900
H	1.74875300	4.26741500	-1.21066400
H	0.22260900	4.04474300	2.78978200
C	-0.05381800	2.59744300	-2.40397500
H	-0.00125400	1.50889900	-2.52531500
H	-1.00558200	2.92921400	-2.83400100
H	0.75847500	3.05042800	-2.97494100
C	2.14488100	5.24779900	1.29488600
H	2.95843800	5.31889300	0.56998200
H	1.71376100	6.24611400	1.42168200
H	2.56647400	4.94728700	2.25786400
C	-1.87279300	2.34873800	2.29532100
H	-2.87999000	2.65697700	1.99830100
H	-1.86116900	1.25494500	2.30846300
H	-1.68180100	2.70832500	3.30767100

**M6SR**

**S82/S123**

C	3.86819100	0.74263700	1.34064600
C	5.28254000	0.54979300	1.78928900
C	5.39674700	-1.42523700	0.59268700
C	3.95923600	-1.40612100	0.03340500
C	1.97380400	0.15324800	0.42958000
H	5.97981600	1.02625400	1.08529900
H	6.07353800	-0.90996400	-0.09975400
H	3.38594200	-2.25567700	0.40539900
N	3.03366900	1.67603800	1.68410100
N	1.85540900	1.29805700	1.09772800
N	3.26743300	-0.20443900	0.55364000
H	5.71341100	-2.46542200	0.68450000
H	5.41409300	0.98726800	2.77912500
O	5.51398600	-0.83807800	1.87418400
C	3.95988400	-1.43251700	-1.50938900
H	4.49062700	-2.34617400	-1.80136200
H	2.92492900	-1.52482000	-1.84929700
C	4.60993300	-0.22016200	-2.13684300
C	5.95762700	-0.22145900	-2.51040900
C	3.85783800	0.94306200	-2.33798400
C	6.55306300	0.92066300	-3.04107300
H	6.54491800	-1.12978600	-2.39425800
C	4.45363500	2.08635500	-2.86514900
H	2.79315400	0.91705000	-2.11377300
C	5.80355600	2.08201700	-3.21048900
H	7.59979900	0.90011100	-3.32750700
H	3.85554400	2.97971000	-3.02057600
H	6.26533800	2.97281000	-3.62422500
C	0.70649400	2.15106200	1.27622900
C	0.37652100	3.04145300	0.24871600
C	0.05827300	2.13690900	2.51537700
C	-0.65743000	3.94075300	0.49581400
C	-0.96919800	3.05954200	2.70715900
C	-1.33134600	3.97095900	1.71615900
H	-0.94292700	4.63618800	-0.28908600
H	-1.49010800	3.07081100	3.66146700
C	1.11196800	3.03464800	-1.06191600
H	2.19516600	3.08754000	-0.90229500
H	0.89969400	2.10507000	-1.60189400
H	0.80941200	3.88831600	-1.67088000
C	-2.41335600	4.98894200	1.96175900
H	-1.98225600	5.93415900	2.30727300
H	-2.97032200	5.19251600	1.04364400
H	-3.11597800	4.64545900	2.72481400

C	0.43086000	1.16459900	3.60435200
H	-0.00475400	0.17632400	3.42494400
H	1.51266500	1.03350500	3.67739900
H	0.06072900	1.52153400	4.56695000
C	0.89780600	-0.54747900	-0.43028800
O	0.90272300	-0.10301500	-1.62262700
C	-0.45882700	-0.80738300	0.34825100
C	-1.62996800	-0.69500600	-0.61800700
H	-0.62971500	-0.23526700	1.26508100
H	-1.25063600	-0.95288700	-1.61252500
C	-2.22594200	0.69552000	-0.69023200
C	-2.97035900	1.22003700	0.37021300
C	-2.14240000	1.42108200	-1.88065100
C	-3.68177500	2.40553500	0.21755600
H	-3.02980100	0.67985100	1.31321200
C	-2.83144100	2.62311200	-2.02615200
H	-1.53849900	1.02447000	-2.69170500
C	-3.62280300	3.10514200	-0.98571000
H	-4.28418400	2.78261400	1.03893400
H	-2.76588700	3.17180600	-2.96070800
H	-4.18635900	4.02540400	-1.10896800
C	-2.74296300	-4.23717300	-0.69356300
C	-1.85339900	-5.26797400	-0.49784200
C	-0.65428500	-4.70195800	0.00296100
C	-0.85105600	-3.34119000	0.09220500
N	-2.12767600	-3.06664200	-0.34246800
H	-3.75105900	-4.23884800	-1.07868900
H	-2.04309800	-6.31071200	-0.70466000
H	0.25694900	-5.21971100	0.26171400
C	0.05310300	-2.24309500	0.54713400
O	1.20507800	-2.03735800	-0.26309300
C	0.50389300	-2.50261400	1.97844500
F	1.13737000	-3.67318900	2.10853300
F	-0.53374800	-2.48911000	2.82807600
F	1.36819000	-1.55412100	2.40325700
C	-2.72308400	-1.74396800	-0.29753400
H	-3.13530700	-1.55944100	0.70055500
C	-3.80685800	-1.57406800	-1.37269200
O	-3.59878900	-1.95493000	-2.50454300
C	-5.04036400	-0.81241500	-1.01705500
C	-5.58396900	0.02713800	-1.99314400
C	-5.64288500	-0.90125700	0.24070400
C	-6.70576000	0.79373700	-1.70374200
H	-5.09698800	0.08389700	-2.96121900

C	-6.78354200	-0.15459900	0.51756900
H	-5.23940400	-1.56537700	0.99932800
C	-7.30700300	0.70143900	-0.44911900
H	-7.11310200	1.46285300	-2.45440900
H	-7.26072500	-0.23645100	1.48845600
H	-8.18651500	1.29651500	-0.22485700

**M6SS**

C	0.33383800	0.80420700	0.22429600
O	-0.07482400	2.00340300	0.00724700
C	-0.66289000	-0.41592600	0.29962800
C	-2.11508800	0.03766000	0.20954000
H	-0.48742200	-1.24304900	-0.38913200
H	-2.15460600	0.73405800	-0.63517900
C	-3.10373500	-1.08016400	-0.05068600
C	-4.14197500	-0.87267700	-0.96479700
C	-3.02745800	-2.30910900	0.61049300
C	-5.09123700	-1.86149000	-1.20614200
H	-4.20650300	0.08007200	-1.48690300
C	-3.97395200	-3.30207200	0.36685700
H	-2.22597400	-2.49610800	1.31949500
C	-5.01124000	-3.08050700	-0.53599400
H	-5.89136800	-1.68026800	-1.91693400
H	-3.90240100	-4.25008700	0.89042800
H	-5.74975300	-3.85429700	-0.71989500
C	-2.99177700	-0.05345800	3.82036600
C	-2.29064200	-0.84494500	4.70175800
C	-1.07700700	-1.21522700	4.07324800
C	-1.07798600	-0.63426700	2.82423400
N	-2.25753800	0.06529500	2.66959100
H	-3.95577700	0.41347200	3.91358500
H	-2.62503600	-1.13063800	5.68800100
H	-0.29236100	-1.83897600	4.47524700
C	-0.09332700	-0.64892800	1.71262900
O	0.75658600	0.50715700	1.63249900
C	0.80385200	-1.87224300	1.77988800
F	1.61547400	-1.84061600	2.84307400
F	0.11741100	-3.01957100	1.81546100
F	1.60036200	-1.93028400	0.68591000
C	-2.48741800	0.87181800	1.47663300
H	-1.79778400	1.72222600	1.49883200
C	-3.91274900	1.38465000	1.31819300
O	-4.84945300	0.89997600	1.91933700
C	-4.13406000	2.48055900	0.31663500

C	-5.46274400	2.80619800	0.01981500
C	-3.09057300	3.16404200	-0.32079200
C	-5.75123100	3.80366600	-0.90165900
H	-6.25242500	2.26040700	0.52506000
C	-3.38825600	4.16354700	-1.24453100
H	-2.04873800	2.92005100	-0.12024800
C	-4.71164500	4.48477300	-1.53527300
H	-6.78303700	4.05143500	-1.12827200
H	-2.57897200	4.69242000	-1.73744900
H	-4.93496700	5.26509400	-2.25612200
C	3.49811400	1.15103100	-1.57787600
C	4.81511400	1.85895100	-1.71158300
C	3.93159500	3.27649300	0.02502100
C	3.10676700	2.15929200	0.66543900
C	1.59041900	0.60833700	-0.65812400
H	5.62343000	1.11937300	-1.68708300
H	4.32232800	3.93964500	0.79905800
H	2.17514600	2.56779800	1.06766400
N	2.91050100	0.39382900	-2.46100200
N	1.72359200	0.06132500	-1.86423300
N	2.72211600	1.30264800	-0.46334600
H	3.28782000	3.85900000	-0.64934700
H	4.83098100	2.37080600	-2.68164100
O	5.06162300	2.76779200	-0.65744300
C	3.83351200	1.33610800	1.74986000
H	4.18527400	2.04307100	2.50829200
H	3.07662600	0.69752400	2.21502800
C	4.97789400	0.49060200	1.23838100
C	6.29590400	0.95427500	1.25548300
C	4.72110500	-0.77417700	0.70080700
C	7.32682900	0.18838400	0.72129200
H	6.50898200	1.93573800	1.66987100
C	5.74942900	-1.54276700	0.15728700
H	3.70700800	-1.16436900	0.72282600
C	7.05503700	-1.05990700	0.16078800
H	8.34418300	0.56594500	0.73957100
H	5.52904300	-2.52127700	-0.25834700
H	7.85922500	-1.65575900	-0.25857600
C	0.75542700	-0.80260100	-2.48070600
C	-0.42087600	-0.21921500	-2.97199100
C	0.96422100	-2.18143700	-2.42641300
C	-1.45472500	-1.08170400	-3.32228900
C	-0.10509600	-2.99941000	-2.79892200
C	-1.32807100	-2.46960200	-3.20616900

H	-2.39237100	-0.66098200	-3.67675400
H	0.01775800	-4.07810200	-2.74071000
C	-0.56109100	1.27508300	-3.10723900
H	-0.49712600	1.77639500	-2.13458900
H	0.23508000	1.67505800	-3.74356100
H	-1.52143100	1.52066700	-3.56510200
C	-2.50541200	-3.36499500	-3.48127500
H	-3.12216200	-3.44783500	-2.57934200
H	-3.13608400	-2.95807500	-4.27528200
H	-2.18503300	-4.36870900	-3.76878800
C	2.27348300	-2.79069700	-1.99562500
H	2.81451000	-3.15700100	-2.87333100
H	2.92042100	-2.07502900	-1.48600900
H	2.10044700	-3.63665000	-1.32743900

**TS6RR**

C	3.74252800	0.23118700	2.09693000
C	5.08327800	-0.08759800	2.68849000
C	5.61306600	-1.14344300	0.68696600
C	4.20290600	-1.20871900	0.09960400
C	2.09892500	0.12176400	0.59512100
H	5.77156300	0.75477900	2.52734500
H	6.09868500	-0.19916600	0.40279800
H	3.80163600	-2.21463700	0.25336100
N	2.80346700	0.97228600	2.60148200
N	1.81064000	0.89472400	1.65328700
N	3.36317400	-0.28846300	0.88251900
H	6.20432100	-1.97545800	0.29863800
H	4.98559500	-0.26077000	3.76101000
O	5.58690200	-1.26513300	2.09793200
C	4.16418900	-0.89064400	-1.40447200
H	4.80263100	-1.63436500	-1.89530700
H	3.14321200	-1.06144400	-1.75650500
C	4.61875300	0.50414600	-1.76586200
C	5.96761300	0.78440500	-2.00723200
C	3.69013000	1.54530700	-1.86050600
C	6.38659400	2.07778900	-2.30778300
H	6.69655800	-0.02233200	-1.96927800
C	4.10797200	2.84044300	-2.15855800
H	2.63173700	1.33228200	-1.72465600
C	5.45640800	3.11221200	-2.37670300
H	7.43736300	2.27550800	-2.49451000
H	3.37342300	3.63733000	-2.22985100
H	5.77980400	4.12105900	-2.61213300

C	0.56301500	1.57102100	1.86456700
C	-0.36625600	1.00549100	2.74213300
C	0.30865500	2.75001900	1.15384800
C	-1.61697500	1.61786900	2.84498300
C	-0.95394300	3.32166000	1.29002500
C	-1.93663600	2.75611300	2.10664600
H	-2.36691300	1.17046900	3.49246600
H	-1.18236900	4.22929700	0.73632700
C	-0.05557600	-0.22940800	3.54909000
H	-0.96640200	-0.81098900	3.71461100
H	0.68194500	-0.87086100	3.05825100
H	0.35936500	0.04419300	4.52408200
C	-3.31680900	3.35823100	2.15599600
H	-3.95093300	2.83836200	2.87809600
H	-3.27797500	4.41631000	2.43082500
H	-3.79456400	3.29662300	1.17014900
C	1.34573400	3.36964700	0.25751600
H	2.35606900	3.22831600	0.65023500
H	1.30006400	2.90276900	-0.73024000
H	1.16080500	4.44077900	0.14955500
C	0.48386800	-0.15684500	-0.83567200
O	0.37665600	0.91881100	-1.39090900
C	-0.50257500	-0.91417800	0.07644000
C	-1.92741200	-0.39924700	-0.06865800
H	-0.21574200	-0.99074600	1.12161400
H	-1.86528400	0.68047200	0.11727200
C	-2.91404100	-0.99039400	0.91887100
C	-2.84292200	-2.31958900	1.33973700
C	-3.93921200	-0.18158800	1.42190600
C	-3.76714000	-2.82320700	2.25370300
H	-2.06549200	-2.97335800	0.95855400
C	-4.86412100	-0.68236500	2.33121200
H	-4.00245300	0.85614100	1.10107500
C	-4.77738900	-2.00759500	2.75356300
H	-3.69509900	-3.85816200	2.57198200
H	-5.64928800	-0.03687600	2.71243900
H	-5.49461900	-2.40151600	3.46631300
C	-3.10074100	-2.75230400	-2.70017500
C	-2.51303000	-3.98425000	-2.87648700
C	-1.28140900	-3.97415300	-2.17975300
C	-1.15668400	-2.73270300	-1.59730600
N	-2.28316500	-1.99118000	-1.90770800
H	-4.04068000	-2.36775200	-3.05446900
H	-2.93441400	-4.80421600	-3.43841300



H	-0.56562100	-4.77890400	-2.09933100
C	-0.07858500	-2.13838000	-0.76753600
O	0.87619300	-1.32652000	-1.51277900
C	0.71905000	-3.19870800	-0.01951300
F	1.46704800	-3.91821500	-0.86355800
F	-0.06720000	-4.04432900	0.65669600
F	1.55656900	-2.64437100	0.87590100
C	-2.38285600	-0.58171800	-1.54834400
H	-1.68786000	-0.01920100	-2.18122500
C	-3.76718200	0.03387500	-1.70393600
O	-4.77166200	-0.63837100	-1.80209400
C	-3.84778800	1.53381100	-1.65479200
C	-5.12913100	2.09215300	-1.56601500
C	-2.72757900	2.37428700	-1.69113200
C	-5.29439100	3.46998300	-1.52220600
H	-5.98177700	1.42216600	-1.53446800
C	-2.90081300	3.75636100	-1.65801300
H	-1.71659600	1.97617200	-1.73850400
C	-4.17768000	4.30541800	-1.57393400
H	-6.29015700	3.89489700	-1.45232400
H	-2.03040200	4.40318500	-1.70083100
H	-4.30426600	5.38307200	-1.54712200

**TS6RS**

C	-0.47989400	-0.87595900	-1.35712900
O	-0.47075000	-0.63304500	-2.54103500
C	0.60217200	-0.75730600	-0.26387600
C	2.03657200	-0.74878500	-0.79249800
H	0.41464300	0.04704700	0.44924800
H	2.02744300	-1.09581900	-1.83214300
C	2.70372100	0.61067500	-0.73689900
C	2.96064400	1.22562900	0.49252700
C	3.20225500	1.19435300	-1.90223700
C	3.75354800	2.36523100	0.56070400
H	2.56442500	0.79500000	1.41014200
C	3.97544700	2.35222400	-1.83884500
H	3.00165800	0.72230100	-2.86028300
C	4.27154300	2.92634600	-0.60526800
H	3.96820600	2.81602900	1.52482000
H	4.36365300	2.79122600	-2.75250100
H	4.89832800	3.81142800	-0.55187800
C	2.91084000	-4.30436700	-0.23922100
C	1.94599400	-5.28369900	-0.17075900
C	0.69594200	-4.63936000	0.00556600

C	0.94182000	-3.28525400	0.03248400
N	2.29415900	-3.08826000	-0.12494400
H	3.97703700	-4.37386600	-0.38713800
H	2.12262900	-6.34570700	-0.25282400
H	-0.27731800	-5.09990100	0.08899800
C	0.02640400	-2.12084500	0.18592500
O	-1.00542200	-2.07637400	-0.81921000
C	-0.60170300	-2.10119300	1.56907300
F	-1.33501900	-3.19648300	1.79167800
F	0.35514800	-2.03210000	2.50562800
F	-1.41125300	-1.04375400	1.74667800
C	2.90317900	-1.77629300	-0.01589800
H	2.94496800	-1.48338600	1.03828800
C	4.30041200	-1.73119700	-0.64994300
O	4.46648200	-2.19209100	-1.75950700
C	5.38177500	-0.99717500	0.06778100
C	6.32300000	-0.31481800	-0.70886400
C	5.47517800	-0.96657300	1.46229600
C	7.33497100	0.41241600	-0.09530800
H	6.23076500	-0.35132000	-1.78945000
C	6.50555500	-0.25940200	2.07296300
H	4.76380900	-1.51072000	2.07603100
C	7.42709100	0.43901200	1.29574800
H	8.05292100	0.95779400	-0.69867800
H	6.58668300	-0.24961000	3.15465000
H	8.22045500	1.00343400	1.77512800
C	-3.94645100	1.43579900	-1.26582600
C	-5.32850600	1.49807200	-1.84812500
C	-4.99009500	-0.72747500	-2.53471100
C	-3.82619400	-1.03313300	-1.59032800
C	-2.00993400	0.48323300	-0.69738100
H	-5.98323100	2.07912600	-1.19611900
H	-5.56407800	-1.63754600	-2.72144900
H	-3.05630300	-1.58546000	-2.13764000
N	-3.22431200	2.42208000	-0.82646700
N	-2.03862600	1.80346200	-0.48429000
N	-3.24744500	0.25882800	-1.21617700
H	-4.59928000	-0.35402600	-3.49321200
H	-5.27594100	1.99431600	-2.82865400
O	-5.88730400	0.21008900	-1.97003500
C	-4.21265500	-1.83469600	-0.33204200
H	-4.65460600	-2.77920700	-0.66724500
H	-3.28031900	-2.07864400	0.18562100
C	-5.15409800	-1.11657000	0.60541800

C	-6.52829100	-1.36414700	0.58500700
C	-4.65947300	-0.16636900	1.50398400
C	-7.39032700	-0.67020700	1.42806800
H	-6.92630800	-2.10058800	-0.10863000
C	-5.51890300	0.53604400	2.34520500
H	-3.58843600	0.01387600	1.54653400
C	-6.88848900	0.28718000	2.30774600
H	-8.45578900	-0.87517800	1.39768400
H	-5.11569500	1.26977100	3.03702200
H	-7.56049500	0.82933300	2.96523600
C	-0.96237900	2.61241800	0.00973600
C	-0.03050600	3.11189900	-0.90476000
C	-0.91716900	2.90758400	1.37431300
C	0.96595300	3.95197300	-0.41262800
C	0.10479000	3.74453700	1.82079900
C	1.04372600	4.28346700	0.94021900
H	1.70720700	4.34698100	-1.10257800
H	0.15918600	3.99054800	2.87879900
C	-0.11401000	2.75675900	-2.36461200
H	-0.00282800	1.67812200	-2.51773600
H	-1.08631800	3.04546900	-2.77712300
H	0.66943100	3.27023300	-2.92533700
C	2.10671500	5.22856100	1.43759400
H	2.96456300	5.24373600	0.76094600
H	1.71573600	6.24898300	1.50569500
H	2.45617500	4.94398000	2.43376600
C	-1.93653400	2.32921000	2.31987700
H	-2.95082100	2.46154200	1.93074600
H	-1.77280800	1.25478400	2.45340800
H	-1.87153300	2.80873000	3.29820600

**TS6SR**

C	-3.80828000	-0.61499800	1.76894000
C	-5.07360300	-0.29021200	2.50258700
C	-5.44342600	1.39757500	0.95692400
C	-4.06767800	1.38229100	0.28632200
C	-2.17625800	-0.31098300	0.28203200
H	-5.89892900	-0.91290100	2.12749500
H	-6.11467600	0.68818000	0.45228600
H	-3.47210300	2.22349200	0.65515400
N	-2.97595500	-1.57757800	2.01237200
N	-1.97961900	-1.37085600	1.08215800
N	-3.37668700	0.15676700	0.71828900
H	-5.86667700	2.40108000	0.87737100

H	-4.94307200	-0.48251600	3.56818700
O	-5.36508400	1.07940900	2.33383000
C	-4.17965700	1.49652100	-1.24458900
H	-4.74366800	2.41547500	-1.44410600
H	-3.17846600	1.64095900	-1.65575000
C	-4.83805100	0.31990400	-1.92499400
C	-6.22328100	0.24913400	-2.10018900
C	-4.04640200	-0.72845300	-2.40387100
C	-6.80944800	-0.85692200	-2.71132900
H	-6.84911400	1.07462200	-1.76812900
C	-4.63022800	-1.83596600	-3.01373600
H	-2.96557000	-0.64854000	-2.31532900
C	-6.01365700	-1.90680900	-3.16302200
H	-7.88641400	-0.89407700	-2.84148400
H	-4.00043300	-2.64017600	-3.38306600
H	-6.46842200	-2.76832300	-3.64140900
C	-0.87617300	-2.28809700	1.07234500
C	-0.59006500	-3.01209400	-0.09362200
C	-0.15846000	-2.47583600	2.26113300
C	0.41643800	-3.97387400	-0.02639600
C	0.83144700	-3.45842100	2.27467700
C	1.11620100	-4.23146000	1.15127800
H	0.65149800	-4.54490100	-0.92140500
H	1.39140900	-3.62155800	3.19281500
C	-1.34221700	-2.78830800	-1.37751200
H	-2.42106200	-2.74156200	-1.20034500
H	-1.04625900	-1.84367400	-1.84628700
H	-1.13938500	-3.60208400	-2.07671900
C	2.14740900	-5.32790100	1.20375900
H	1.66867500	-6.30127000	1.35225900
H	2.71399900	-5.37611600	0.27023100
H	2.84916500	-5.17492700	2.02757400
C	-0.43112000	-1.65949000	3.49848700
H	-0.60620000	-0.60873400	3.25417300
H	-1.32307300	-2.01984600	4.01694100
H	0.41770400	-1.72304600	4.18243000
C	-0.79107900	0.83793500	-0.97474000
O	-0.95499500	0.48323600	-2.11658000
C	0.45722600	0.80756300	-0.06717600
C	1.76082900	0.73043000	-0.85925600
H	0.42473600	0.08334900	0.74972900
H	1.56385800	1.06356500	-1.88442500
C	2.36316100	-0.65668800	-0.91263400
C	2.81455400	-1.28606900	0.25062500

C	2.60326000	-1.26009600	-2.14807400
C	3.54790600	-2.46438200	0.17373100
H	2.62123100	-0.83949000	1.22434400
C	3.31564900	-2.45473400	-2.22465500
H	2.24702500	-0.77571900	-3.05297500
C	3.80849000	-3.04697900	-1.06504800
H	3.91533300	-2.92988500	1.08337900
H	3.50209800	-2.90986500	-3.19216700
H	4.39123900	-3.96122600	-1.12458600
C	2.83519300	4.25371400	-0.68766700
C	1.91300100	5.27040100	-0.58367200
C	0.68084500	4.68967100	-0.19340100
C	0.89203300	3.33401000	-0.07989700
N	2.20889400	3.07540100	-0.38712400
H	3.87308200	4.27119100	-0.98047000
H	2.10502400	6.31458700	-0.77995400
H	-0.25938400	5.19220900	-0.02151300
C	-0.01703500	2.22523700	0.32680300
O	-1.20010600	2.11176000	-0.48762700
C	-0.41330300	2.37893300	1.78722500
F	-1.03566800	3.54035600	2.00903400
F	0.67708600	2.32375100	2.56477400
F	-1.24594900	1.40789200	2.20057200
C	2.78561000	1.74718000	-0.29048300
H	2.98851300	1.50897500	0.75933300
C	4.05523900	1.60009500	-1.14020100
O	4.06417600	2.01267100	-2.28049800
C	5.19265400	0.81928100	-0.57495500
C	5.93533600	0.03017000	-1.45805000
C	5.52067400	0.84357600	0.78365000
C	6.98204100	-0.74866800	-0.98122100
H	5.66067300	0.02362300	-2.50779100
C	6.58761000	0.08445500	1.25290200
H	4.96467600	1.46966900	1.47486600
C	7.30966500	-0.71993400	0.37380000
H	7.54388200	-1.37770100	-1.66359700
H	6.85239800	0.11677500	2.30438700
H	8.13079800	-1.32456900	0.74528000

**TS6SS**

C	0.07181000	-0.09733900	-1.25978800
O	-0.10185900	-1.07605500	-1.95419700
C	-0.72989000	0.52500500	-0.10554400
C	-2.20529700	0.15094600	-0.17574900

H	-0.31908500	0.35894700	0.88970900
H	-2.22594500	-0.94492200	-0.19844400
C	-3.04722300	0.60494000	0.99902200
C	-4.02955800	-0.25770600	1.49790100
C	-2.90545400	1.86839900	1.57575900
C	-4.86593300	0.13812800	2.53633500
H	-4.14236200	-1.24699800	1.05853800
C	-3.73798000	2.26337600	2.62147100
H	-2.14783000	2.55469600	1.21105200
C	-4.72434500	1.40503800	3.09896900
H	-5.62502000	-0.54301800	2.90772300
H	-3.61748300	3.24995000	3.05712100
H	-5.37534100	1.71836100	3.90882500
C	-3.43248100	3.03858600	-2.16341700
C	-2.76526400	4.24195200	-2.16488300
C	-1.47141600	4.01516500	-1.63924900
C	-1.38924800	2.67507000	-1.33078400
N	-2.60108400	2.08326800	-1.64170400
H	-4.43345800	2.79260900	-2.46999200
H	-3.17307800	5.18340000	-2.50099600
H	-0.68762400	4.74256400	-1.49108900
C	-0.28860200	1.85863600	-0.75940300
O	0.49533700	1.13105500	-1.75783000
C	0.67780400	2.70218600	0.05883400
F	1.31790800	3.58491300	-0.71713000
F	0.04748500	3.37925600	1.02609700
F	1.61515400	1.94613000	0.64935200
C	-2.78546500	0.64193300	-1.53888800
H	-2.20677200	0.16758700	-2.33972300
C	-4.22741600	0.16156200	-1.65504100
O	-5.17418300	0.90557300	-1.51238400
C	-4.42979400	-1.30858000	-1.87916300
C	-5.73791200	-1.79028800	-1.75306100
C	-3.39133200	-2.19817800	-2.18553400
C	-6.00915400	-3.14042700	-1.92954100
H	-6.52567700	-1.08454200	-1.51236400
C	-3.66917700	-3.55103500	-2.36133100
H	-2.36253300	-1.86105300	-2.28501300
C	-4.97319400	-4.02305600	-2.23424700
H	-7.02527200	-3.50694800	-1.82886100
H	-2.86184500	-4.23556700	-2.59914900
H	-5.18285800	-5.07897600	-2.37188400
C	3.62191200	-2.22647200	-0.10712100
C	4.85872800	-2.87839700	-0.64937300

C	4.47358700	-1.70502800	-2.64842900
C	3.45181700	-0.70753800	-2.09365700
C	1.87739800	-0.83345700	-0.14403600
H	5.60613200	-2.98168300	0.13870500
H	5.03188100	-1.24633800	-3.46743200
H	2.59088000	-0.66100400	-2.76925900
N	2.99395100	-2.47872700	1.00343100
N	1.92644800	-1.60761900	0.94828800
N	2.96994900	-1.26019900	-0.82816900
H	3.95054300	-2.59335500	-3.03343400
H	4.60415000	-3.87926300	-1.02925400
O	5.42277300	-2.08563900	-1.66987900
C	3.98627500	0.72123500	-1.88018800
H	4.30538400	1.10410500	-2.85545500
H	3.13789600	1.33130600	-1.55091200
C	5.11422200	0.81125600	-0.88138200
C	6.44823400	0.82541200	-1.29302000
C	4.83507500	0.85012400	0.48791000
C	7.48040600	0.86141400	-0.36047600
H	6.67932900	0.79931500	-2.35516500
C	5.86435600	0.87954900	1.42500500
H	3.79889200	0.86711400	0.81505000
C	7.19142500	0.88278300	1.00249600
H	8.51206600	0.87177000	-0.69762300
H	5.62784300	0.91042300	2.48459800
H	7.99625300	0.91045900	1.73000200
C	0.93231300	-1.56488700	1.97989500
C	-0.24860800	-2.29156700	1.79267700
C	1.12844400	-0.71287400	3.06950400
C	-1.27782600	-2.09800600	2.71315300
C	0.07260300	-0.55896900	3.96758800
C	-1.14279800	-1.22171800	3.79144000
H	-2.21266800	-2.63718400	2.57952500
H	0.19848000	0.10832000	4.81714000
C	-0.40401600	-3.22860600	0.62344900
H	-0.35210400	-2.68985700	-0.32886700
H	0.39607700	-3.97531100	0.61962500
H	-1.36325700	-3.74841800	0.67666800
C	-2.28809400	-0.97271900	4.73628800
H	-2.72672000	0.01198400	4.54464700
H	-3.07775800	-1.71622300	4.60810100
H	-1.95328200	-0.99579800	5.77686200
C	2.41566900	0.05022000	3.24232500
H	2.56846900	0.30610300	4.29270600

H	3.27348500	-0.53104500	2.89440300
H	2.38626300	0.98287200	2.67015400

**M7RR**

C	1.00674700	-2.23775000	-1.06223700
O	0.34453900	-3.10945700	-1.53343800
C	1.07229300	-0.72043600	-1.16025600
C	-0.23626000	-0.05513700	-0.73204700
H	1.42830000	-0.34333000	-2.12085500
H	-1.02320100	-0.51666900	-1.33844800
C	-0.28623900	1.44177100	-0.96060700
C	0.80281900	2.27406000	-0.69085400
C	-1.47343000	2.00974100	-1.43156000
C	0.70237900	3.64833600	-0.89165900
H	1.73694000	1.85755500	-0.32672200
C	-1.57434600	3.38301200	-1.62907200
H	-2.32605900	1.36845800	-1.64449800
C	-0.48425000	4.20615600	-1.35897700
H	1.55635300	4.28338600	-0.68017700
H	-2.50232800	3.80788400	-1.99733300
H	-0.55856700	5.27745800	-1.51427500
C	0.56799100	0.60327800	2.82708500
C	1.87169900	0.73301300	3.24947900
C	2.70691400	0.19703400	2.24168400
C	1.88181100	-0.24241400	1.23004000
N	0.57189100	0.02014500	1.58822700
H	-0.35264500	0.89694300	3.29902400
H	2.18513200	1.17511100	4.18305200
H	3.78500600	0.14227900	2.24303000
C	2.16169000	-0.88174300	-0.06981700
O	1.95074600	-2.34240500	-0.08652500
C	3.57350900	-0.63432400	-0.57717600
F	4.49000600	-1.12065700	0.26201800
F	3.80141900	0.67445000	-0.73414100
F	3.75182000	-1.22540900	-1.76471500
C	-0.53082300	-0.43265700	0.75404300
H	-0.58474900	-1.52626300	0.83171300
C	-1.89848000	0.13128100	1.13175600
O	-2.01258200	1.13045500	1.80789600
C	-3.10007600	-0.55896700	0.56166700
C	-4.33170000	0.08660300	0.72454700
C	-3.04821200	-1.78464100	-0.11475600
C	-5.49408300	-0.48258800	0.22293100
H	-4.35069400	1.03613300	1.24835400



C	-4.21595600	-2.35259300	-0.61481700
H	-2.11146100	-2.31304500	-0.26549700
C	-5.43695800	-1.70453000	-0.44677600
H	-6.44462500	0.02388700	0.35188300
H	-4.16899500	-3.30277200	-1.13536400
H	-6.34470500	-2.15125900	-0.83912700

**M7RS**

C	-2.31007300	2.01555100	-0.89902400
O	-2.24060000	3.04073400	-1.49472100
C	-1.42064200	1.18774000	0.02264300
C	-0.15315400	0.63675200	-0.63861100
H	-1.21638600	1.66016400	0.98583000
H	-0.30952600	0.56488700	-1.72132800
C	1.07748800	1.47942200	-0.38142600
C	1.51831000	1.72907700	0.92130200
C	1.84954800	1.92061000	-1.45618300
C	2.71779300	2.39636600	1.14390800
H	0.93640600	1.38100900	1.77223900
C	3.04694900	2.59671700	-1.23500500
H	1.51578900	1.72068600	-2.47056200
C	3.48569900	2.83033600	0.06485500
H	3.05577000	2.57359000	2.15954900
H	3.63768200	2.93586300	-2.07958900
H	4.42233000	3.34967900	0.23864200
C	-1.13066800	-2.90552800	-1.00445700
C	-2.44733100	-3.26665900	-1.18385300
C	-3.24679000	-2.14961100	-0.84016400
C	-2.38762700	-1.13876300	-0.47139900
N	-1.09512700	-1.60731800	-0.57849800
H	-0.22034300	-3.45942500	-1.17162400
H	-2.79258000	-4.22742500	-1.53466500
H	-4.32399900	-2.07730900	-0.86495300
C	-2.63528600	0.23545300	0.02138600
O	-3.34135000	1.11349600	-0.90481400
C	-3.38692200	0.24942800	1.34339500
F	-4.57147700	-0.35427100	1.25096600
F	-2.65978700	-0.37913000	2.27703800
F	-3.59572300	1.50365200	1.76489900
C	0.05907500	-0.82642200	-0.16875600
H	0.14749600	-0.84275200	0.92284000
C	1.35455200	-1.30917400	-0.83754600
O	1.35353300	-1.54365900	-2.02752600
C	2.60346400	-1.33321200	-0.02605000

C	3.80490600	-1.06101700	-0.68859000
C	2.61021800	-1.60181500	1.34611700
C	4.99905300	-1.03549500	0.01934200
H	3.77643300	-0.85338000	-1.75319900
C	3.81152300	-1.59942200	2.04734700
H	1.68960500	-1.83935800	1.86975100
C	5.00260000	-1.30597400	1.38749600
H	5.92756100	-0.80542400	-0.49217700
H	3.81734200	-1.82313900	3.10868300
H	5.93642500	-1.28942400	1.94005400

**M7SR**

C	2.30991100	2.01571300	-0.89881200
O	2.24049000	3.04097300	-1.49439000
C	1.42042000	1.18771900	0.02264900
C	0.15308300	0.63652000	-0.63874800
H	1.21592100	1.66007400	0.98581700
H	0.30960500	0.56456500	-1.72143800
C	-1.07762700	1.47915500	-0.38180600
C	-1.51873800	1.72877600	0.92083100
C	-1.84939400	1.92046800	-1.45672000
C	-2.71819700	2.39618500	1.14319100
H	-0.93709100	1.38056000	1.77188300
C	-3.04676700	2.59670900	-1.23578800
H	-1.51542400	1.72055300	-2.47103100
C	-3.48578900	2.83032200	0.06398000
H	-3.05640500	2.57336600	2.15876300
H	-3.63726500	2.93596100	-2.08049300
H	-4.42238400	3.34979500	0.23757400
C	1.13114900	-2.90543200	-1.00498300
C	2.44787100	-3.26618200	-1.18470500
C	3.24713000	-2.14906900	-0.84073600
C	2.38777600	-1.13857700	-0.47146700
N	1.09537700	-1.60738000	-0.57853700
H	0.22093300	-3.45948600	-1.17219400
H	2.79328000	-4.22676700	-1.53585400
H	4.32431900	-2.07650100	-0.86560100
C	2.63519200	0.23560900	0.02156400
O	3.34131500	1.11379600	-0.90441700
C	3.38652900	0.24952200	1.34374600
F	4.57113700	-0.35409500	1.25156800
F	2.65922500	-0.37917100	2.27718200
F	3.59517500	1.50371100	1.76542900
C	-0.05892600	-0.82665200	-0.16877200

H	-0.14723800	-0.84293400	0.92283200
C	-1.35441300	-1.30962500	-0.83734900
O	-1.35350300	-1.54448900	-2.02725600
C	-2.60326700	-1.33343500	-0.02574000
C	-3.80477600	-1.06161700	-0.68830400
C	-2.60989500	-1.60142100	1.34655100
C	-4.99887000	-1.03585500	0.01971600
H	-3.77640800	-0.85444600	-1.75300600
C	-3.81113700	-1.59875300	2.04788400
H	-1.68922900	-1.83867600	1.87022100
C	-5.00228800	-1.30569200	1.38799500
H	-5.92743000	-0.80607800	-0.49183800
H	-3.81685600	-1.82197700	3.10932300
H	-5.93606800	-1.28894000	1.94062300

### M7SS

C	-1.00650500	-2.23735900	-1.06290400
O	-0.34403100	-3.10877500	-1.53424200
C	-1.07234100	-0.72005400	-1.16052600
C	0.23620000	-0.05463700	-0.73236100
H	-1.42849300	-0.34279300	-2.12100800
H	1.02305000	-0.51587500	-1.33911900
C	0.28581600	1.44235300	-0.96043700
C	1.47303600	2.01091100	-1.43062500
C	-0.80368000	2.27414100	-0.69100800
C	1.57351400	3.38426800	-1.62770100
H	2.32601700	1.37001400	-1.64331800
C	-0.70368400	3.64852800	-0.89137400
H	-1.73781100	1.85718000	-0.32742600
C	0.48296200	4.20692800	-1.35792500
H	2.50151800	3.80961400	-1.99536200
H	-1.55801600	4.28317500	-0.68013600
H	0.55696600	5.27830000	-1.51289300
C	-0.56748500	0.60200500	2.82732100
C	-1.87109800	0.73092400	3.25025500
C	-2.70643700	0.19545700	2.24228200
C	-1.88149700	-0.24283700	1.23000100
N	-0.57156400	0.01985400	1.58800200
H	0.35319700	0.89568800	3.29916800
H	-2.18440200	1.17221800	4.18425100
H	-3.78450900	0.14033700	2.24390600
C	-2.16158300	-0.88180800	-0.07002900
O	-1.95042500	-2.34239800	-0.08712500
C	-3.57359600	-0.63451300	-0.57692400

F	-4.48969600	-1.12180400	0.26213400
F	-3.80209100	0.67427700	-0.73295200
F	-3.75194400	-1.22480500	-1.76483800
C	0.53107300	-0.43261500	0.75351900
H	0.58516900	-1.52624200	0.83086000
C	1.89871700	0.13136800	1.13122300
O	2.01275700	1.13044800	1.80751700
C	3.10034700	-0.55884900	0.56118000
C	4.33206000	0.08636900	0.72478200
C	3.04842300	-1.78415600	-0.11590900
C	5.49448100	-0.48282400	0.22325600
H	4.35109200	1.03562300	1.24908400
C	4.21620500	-2.35209600	-0.61590200
H	2.11160600	-2.31227200	-0.26726000
C	5.43729900	-1.70440400	-0.44710700
H	6.44509700	0.02336600	0.35278200
H	4.16920100	-3.30198100	-1.13697900
H	6.34507500	-2.15113400	-0.83938800

#### TS7RR

C	-0.59929100	-0.42214500	-0.80754600
O	-1.02770500	0.64754900	-1.25349400
C	0.82185300	-0.94094900	-1.02546900
C	1.88684600	0.09888000	-0.68204200
H	0.95775100	-1.31372100	-2.04526600
H	1.59576000	1.00796900	-1.21766000
C	3.30246400	-0.26343700	-1.09263200
C	3.77925300	-1.57669600	-1.09159000
C	4.16626300	0.76585100	-1.48160500
C	5.09389000	-1.85053100	-1.46189600
H	3.13269500	-2.40477200	-0.81799800
C	5.47994600	0.49352300	-1.84671700
H	3.80261300	1.79065200	-1.50491700
C	5.94833500	-0.81789200	-1.83488600
H	5.44713500	-2.87627500	-1.46047900
H	6.13425200	1.30475700	-2.14768800
H	6.97150700	-1.03439800	-2.12294800
C	2.47622700	-1.00421200	2.80803400
C	2.24475500	-2.33727400	3.21534800
C	1.51481100	-2.95146900	2.22441700
C	1.31811600	-1.99588500	1.19125100
N	1.93933900	-0.80542100	1.60436200
H	3.00379100	-0.21836400	3.32426200
H	2.59603200	-2.76905700	4.13963800

H	1.16649600	-3.97359900	2.19360800
C	0.69362800	-2.07156800	-0.03024200
O	-1.19714900	-1.24743100	-0.03995300
C	0.22372800	-3.42528500	-0.52042000
F	-0.53978400	-4.03943400	0.38082500
F	1.29857600	-4.19867400	-0.74529200
F	-0.45147600	-3.33082100	-1.66168800
C	1.77064100	0.42969900	0.83468400
H	0.75474500	0.79100000	1.03607400
C	2.76402400	1.52636700	1.22041100
O	3.77330200	1.26265500	1.83854900
C	2.45879500	2.91239800	0.76160400
C	3.45541400	3.87559800	0.96237600
C	1.25060000	3.27832400	0.15273500
C	3.24903500	5.18843500	0.56292400
H	4.38394500	3.56997200	1.43222600
C	1.04958400	4.59624400	-0.24463300
H	0.45947000	2.55536400	-0.02832200
C	2.04447100	5.54943200	-0.04027600
H	4.02394800	5.93079700	0.71957800
H	0.11470600	4.87853600	-0.71600700
H	1.88199500	6.57531200	-0.35392500
C	-4.51492600	1.58362100	-1.16084300
C	-5.85752000	1.55863300	-0.90178900
C	-6.40129400	0.53055200	-0.07757000
C	-5.48395800	-0.43096900	0.43486500
C	-4.15313200	-0.33912100	0.12913300
N	-3.68298600	0.65378000	-0.65228300
H	-4.05982000	2.34419100	-1.78318200
H	-6.48216500	2.32686300	-1.33412800
H	-5.81373100	-1.24509800	1.06398100
H	-3.40488800	-1.04202700	0.47768400
N	-7.71227100	0.47263100	0.20013700
C	-8.23443500	-0.59155800	1.05084700
H	-7.79157600	-0.54665900	2.05056400
H	-9.31099300	-0.47074500	1.14604200
H	-8.03511300	-1.57517700	0.61498600
C	-8.62118500	1.47740400	-0.34103200
H	-8.60987800	1.46715500	-1.43507700
H	-9.63157500	1.25516400	-0.00635500
H	-8.35342100	2.47835000	0.01111000
H	-2.65730600	0.68926100	-0.87139100

TS7RS

S101/S123

C	0.93552200	0.25709300	0.87653900
O	1.33459200	-0.84605400	1.25870600
C	-0.48357300	0.78197300	1.11293700
C	-1.41954200	-0.00920200	0.17547200
H	-0.80486800	0.74737400	2.15730300
H	-0.84134600	-0.28299500	-0.71650800
C	-1.95868800	-1.27234800	0.81325300
C	-2.59163300	-1.24089400	2.05811600
C	-1.92147300	-2.47032200	0.09923300
C	-3.18374900	-2.38853900	2.57609800
H	-2.64354600	-0.31605100	2.62867700
C	-2.51762200	-3.61796300	0.61381200
H	-1.43522300	-2.49774200	-0.87251000
C	-3.15222100	-3.57815300	1.85210300
H	-3.67387700	-2.35230700	3.54333700
H	-2.48691000	-4.54184500	0.04605100
H	-3.61844400	-4.47143800	2.25392500
C	-2.54213900	2.83452900	-1.91012500
C	-1.79859900	4.03217000	-2.02491300
C	-0.81009000	3.99026900	-1.07077400
C	-0.93333000	2.74909600	-0.38261500
N	-2.02119900	2.07209500	-0.95502700
H	-3.41393100	2.52043400	-2.46659300
H	-1.99420600	4.81557600	-2.74062100
H	-0.04439800	4.72676300	-0.87594900
C	-0.21153300	2.18529300	0.63693800
O	1.55459100	1.12070300	0.17279700
C	0.60056400	3.11448800	1.52417800
F	1.49260400	3.81622800	0.82780400
F	-0.23670500	3.98546200	2.10676800
F	1.22942400	2.45704000	2.49596100
C	-2.58358100	0.85349700	-0.36468100
H	-3.24762500	1.15090000	0.45082900
C	-3.31450800	0.04033000	-1.45440000
O	-2.80898900	0.00920100	-2.55838600
C	-4.54787700	-0.71998500	-1.12784500
C	-5.02808800	-1.59155200	-2.11526000
C	-5.22623000	-0.61580500	0.09155800
C	-6.16508100	-2.35062000	-1.88457900
H	-4.48867500	-1.66000000	-3.05356000
C	-6.36607300	-1.37972500	0.31948300
H	-4.87858000	0.04647500	0.87595200
C	-6.83441400	-2.24593500	-0.66461200
H	-6.53088400	-3.02593000	-2.65026700

H	-6.88735500	-1.29865600	1.26689700
H	-7.72269400	-2.84157100	-0.48173100
C	4.38532700	-0.05682400	-0.27153600
C	5.67059500	-0.10118100	-0.74244100
C	6.46151900	-1.26736900	-0.54228000
C	5.84556800	-2.34828100	0.15149500
C	4.55594600	-2.22562400	0.59274300
N	3.84450300	-1.10184700	0.38425700
H	3.72756600	0.79729600	-0.39105700
H	6.06020600	0.76148800	-1.26363800
H	6.37443800	-3.27069500	0.34382000
H	4.04956100	-3.02014700	1.12722300
N	7.72689300	-1.34609300	-0.98502500
C	8.50220300	-2.56315500	-0.77554100
H	8.02212700	-3.42176800	-1.25524500
H	9.48843100	-2.43240700	-1.21489600
H	8.62424900	-2.77269700	0.29178100
C	8.32873300	-0.21583100	-1.68244900
H	8.32935900	0.67756500	-1.05075300
H	9.35915100	-0.46183500	-1.92837000
H	7.79328600	0.00486100	-2.61131700
H	2.84775400	-1.02567200	0.73862700

**TS7SR**

C	-0.93577300	0.25557600	0.87596900
O	-1.33411800	-0.84821600	1.25704000
C	0.48318700	0.78089500	1.11283300
C	1.41985200	-0.00972500	0.17557100
H	0.80403200	0.74602800	2.15732500
H	0.84185300	-0.28450300	-0.71622900
C	1.96041100	-1.27203400	0.81385000
C	2.59320100	-1.23938700	2.05876300
C	1.92502200	-2.47023900	0.10012600
C	3.18690900	-2.38604100	2.57711400
H	2.64369800	-0.31433800	2.62910000
C	2.52276900	-3.61689300	0.61505800
H	1.43896200	-2.49860700	-0.87168300
C	3.15717300	-3.57588000	1.85341200
H	3.67690200	-2.34884400	3.54438400
H	2.49348200	-4.54094000	0.04749300
H	3.62468900	-4.46838200	2.25547300
C	2.53947100	2.83449300	-1.91100200
C	1.79526000	4.03176200	-2.02546100
C	0.80753200	3.98959800	-1.07054600

C	0.93189000	2.74859400	-0.38224600
N	2.01966600	2.07202200	-0.95533100
H	3.41094300	2.52069800	-2.46812900
H	1.98992600	4.81509000	-2.74151500
H	0.04162100	4.72575100	-0.87530400
C	0.21076900	2.18432700	0.63747700
O	-1.55538400	1.11949300	0.17313900
C	-0.60142000	3.11291000	1.52526300
F	-1.49385700	3.81463600	0.82937400
F	0.23570100	3.98392300	2.10801000
F	-1.22986200	2.45486500	2.49691200
C	2.58306000	0.85383700	-0.36508300
H	3.24718000	1.15179700	0.45016400
C	3.31416000	0.04110200	-1.45501600
O	2.80813200	0.00940500	-2.55875800
C	4.54816700	-0.71834400	-1.12887900
C	5.02855400	-1.58970400	-2.11639400
C	5.22668700	-0.61390300	0.09041000
C	6.16585100	-2.34837100	-1.88589600
H	4.48901800	-1.65834600	-3.05460900
C	6.36682100	-1.37744100	0.31814900
H	4.87899500	0.04833400	0.87482200
C	6.83529700	-2.24350500	-0.66600700
H	6.53178100	-3.02354600	-2.65164300
H	6.88820200	-1.29621600	1.26549700
H	7.72377800	-2.83887500	-0.48323900
C	-4.38564200	-0.05785300	-0.27013000
C	-5.67096200	-0.10138700	-0.74094500
C	-6.46200900	-1.26776400	-0.54239300
C	-5.84625700	-2.34956900	0.15016300
C	-4.55656800	-2.22770200	0.59146400
N	-3.84494800	-1.10376800	0.38435800
H	-3.72778300	0.79635100	-0.38851400
H	-6.06062900	0.76229200	-1.26043200
H	-6.37527600	-3.27215900	0.34125100
H	-4.05029100	-3.02300900	1.12487700
N	-7.72727900	-1.34575700	-0.98554700
C	-8.50392500	-2.56184500	-0.77524200
H	-8.62416100	-2.77172500	0.29221000
H	-9.49090800	-2.42951600	-1.21251100
H	-8.02600300	-3.42096100	-1.25622700
C	-8.32816000	-0.21480100	-1.68265800
H	-7.78918900	0.00878300	-2.60875500
H	-9.35701400	-0.46201300	-1.93363800



H	-8.33282700	0.67718600	-1.04894700
H	-2.84790600	-1.02830100	0.73803700

**TS7SS**

C	0.58903100	-0.42708600	-0.80472500
O	1.02528500	0.63483800	-1.26118600
C	-0.83207800	-0.94347700	-1.02411900
C	-1.89591800	0.10180900	-0.69267000
H	-0.96565000	-1.32515500	-2.04099900
H	-1.60310600	1.00640400	-1.23529900
C	-3.31094200	-0.26547200	-1.10174600
C	-4.19352200	0.76335300	-1.44777300
C	-3.76770600	-1.58489400	-1.14507200
C	-5.50553900	0.48384300	-1.81274600
H	-3.84645800	1.79411600	-1.43831200
C	-5.08107900	-1.86607900	-1.51482100
H	-3.10685800	-2.41254700	-0.90664400
C	-5.95400600	-0.83431300	-1.84422300
H	-6.17446700	1.29504300	-2.07970300
H	-5.41834500	-2.89664300	-1.54741200
H	-6.97604700	-1.05608500	-2.13227700
C	-2.52034200	-0.97566700	2.79592400
C	-2.29977300	-2.30783600	3.21206300
C	-1.56021500	-2.92991200	2.23307400
C	-1.34717400	-1.98018200	1.19802000
N	-1.96761400	-0.78527700	1.59805400
H	-3.05034100	-0.18453000	3.30140300
H	-2.66482900	-2.73405500	4.13358400
H	-1.21685000	-3.95396300	2.21091300
C	-0.71106400	-2.06534800	-0.01717100
O	1.17828600	-1.24550900	-0.02270300
C	-0.23712400	-3.42487800	-0.48771100
F	0.53308300	-4.02041900	0.42016000
F	-1.30900400	-4.20776800	-0.69429500
F	0.43254700	-3.34574000	-1.63347100
C	-1.78027100	0.44299400	0.82226500
H	-0.75935100	0.78971700	1.02359400
C	-2.75515400	1.55759000	1.20159200
O	-3.77352300	1.31222400	1.81260000
C	-2.42002000	2.93838400	0.74766200
C	-3.39358600	3.92340300	0.95611100
C	-1.20517400	3.27965400	0.13761800
C	-3.15751200	5.23338200	0.56393700
H	-4.32767200	3.63703200	1.42710800

C	-0.97456200	4.59481400	-0.25269800
H	-0.43113500	2.53988200	-0.04940800
C	-1.94627200	5.56981700	-0.04012100
H	-3.91445800	5.99267200	0.72715700
H	-0.03441200	4.85778500	-0.72477300
H	-1.76063700	6.59354700	-0.34787600
C	4.51489500	1.56069300	-1.16557700
C	5.85751000	1.53004700	-0.90734800
C	6.39708000	0.50118200	-0.08134000
C	5.47563100	-0.45490600	0.43395400
C	4.14495400	-0.35718900	0.12944000
N	3.67897000	0.63606000	-0.65405500
H	4.06294900	2.32182700	-1.78954200
H	6.48543800	2.29431800	-1.34193700
H	5.80208900	-1.26909500	1.06472200
H	3.39357500	-1.05524900	0.48105200
N	7.70797600	0.43772700	0.19540200
C	8.22606400	-0.62763100	1.04716900
H	8.02233100	-1.61091000	0.61255800
H	9.30315900	-0.51119700	1.14162100
H	7.78399300	-0.57964900	2.04708800
C	8.62078700	1.43816800	-0.34728000
H	8.35706900	2.44054100	0.00385900
H	9.63039100	1.21229900	-0.01265300
H	8.60912000	1.42675000	-1.44130500
H	2.65365200	0.67492800	-0.87368100

**PRR**

C	1.35812300	0.12509900	-1.42874300
C	-0.04406300	0.09751600	-0.87997900
H	1.50970500	0.51804300	-2.42776200
H	-0.72820000	-0.17561200	-1.68947700
C	-0.47201700	1.46781400	-0.36969900
C	0.31494100	2.18000800	0.53998700
C	-1.69359300	2.00614900	-0.77953400
C	-0.11999100	3.40614500	1.03242600
H	1.27009600	1.77518000	0.86210900
C	-2.12659800	3.23598700	-0.28935500
H	-2.31295000	1.45468700	-1.48318700
C	-1.34042700	3.93750000	0.61947600
H	0.49734500	3.94899700	1.74072200
H	-3.07665100	3.64369900	-0.61940900
H	-1.67501100	4.89543900	1.00418400
C	1.00050300	-1.48611500	2.40221800

C	2.32259000	-1.52418700	2.78190200
C	3.09639700	-1.06102900	1.68891700
C	2.21521700	-0.75429600	0.67261100
N	0.93261600	-0.99216700	1.12445000
H	0.10708500	-1.74444900	2.94481700
H	2.68823200	-1.83629800	3.74864800
H	4.16924700	-0.94543600	1.64352500
C	2.39673100	-0.25737200	-0.67797000
C	3.80335000	-0.17316500	-1.18839900
F	4.40463800	-1.37301700	-1.17725100
F	4.55177700	0.63910400	-0.42247800
F	3.86263100	0.29331200	-2.44180300
C	-0.19477800	-1.01323700	0.20692800
H	-0.19721300	-1.98329900	-0.30666100
C	-1.53629400	-0.81309700	0.91428300
O	-1.59698300	-0.38517500	2.04625000
C	-2.78005100	-1.07489400	0.12246900
C	-3.96242900	-0.49073600	0.59044900
C	-2.80589500	-1.84355000	-1.04587700
C	-5.15217400	-0.66561800	-0.10327200
H	-3.91891600	0.10647600	1.49494600
C	-4.00151200	-2.02359800	-1.73571500
H	-1.90595200	-2.31902800	-1.42274500
C	-5.17252100	-1.43290200	-1.26793900
H	-6.06410400	-0.20365200	0.25975300
H	-4.01765400	-2.62680300	-2.63705100
H	-6.10197700	-1.57052200	-1.81087600

**PRS**

C	-1.68173500	1.18805300	-0.44736400
C	-0.34120500	0.59228500	-0.79437400
H	-1.81054100	2.26189200	-0.53179000
H	-0.37131300	0.26587800	-1.84480600
C	0.81216600	1.55415100	-0.60434900
C	0.87490200	2.36479400	0.53170400
C	1.87520900	1.56937700	-1.50876200
C	1.98903200	3.16556700	0.76747200
H	0.04972700	2.35907200	1.24056800
C	2.99147500	2.36692900	-1.27376200
H	1.83446400	0.93573600	-2.39161600
C	3.05222200	3.16331700	-0.13278800
H	2.02735200	3.78976500	1.65446400
H	3.81475300	2.36352900	-1.98053500
H	3.92293300	3.78391100	0.05196800

C	-1.32193500	-2.91119500	0.13038500
C	-2.64502700	-3.27182200	0.25956600
C	-3.41886000	-2.08730500	0.19121500
C	-2.53764100	-1.03780400	0.01939200
N	-1.26153100	-1.55458600	-0.03532600
H	-0.42731500	-3.51375600	0.11326100
H	-3.01324300	-4.28076700	0.36964200
H	-4.49432200	-2.00072500	0.23745400
C	-2.70246300	0.39857100	-0.09312200
C	-4.05806800	0.95897600	0.21298700
F	-4.99974900	0.42313600	-0.58204200
F	-4.42586000	0.69389600	1.47625100
F	-4.10745100	2.28720400	0.05209900
C	-0.08920000	-0.69556700	0.04182500
H	0.06385400	-0.40764800	1.08765200
C	1.14185400	-1.41040100	-0.53253100
O	1.00285100	-2.07311400	-1.54122600
C	2.48450000	-1.23480000	0.09781500
C	3.56811300	-1.84569500	-0.54610500
C	2.70972900	-0.47504900	1.25052700
C	4.85484100	-1.69855100	-0.04848900
H	3.37502500	-2.42685700	-1.44118500
C	4.00196500	-0.32289400	1.74321800
H	1.89466000	0.02175400	1.76316000
C	5.07350100	-0.93301000	1.09695700
H	5.68905900	-2.17458800	-0.55284500
H	4.17014200	0.27575800	2.63200000
H	6.07996800	-0.81161900	1.48443300

**PSR**

C	1.68165100	1.18809000	-0.44715200
C	0.34116200	0.59218200	-0.79407400
H	1.81029500	2.26195500	-0.53150800
H	0.37132600	0.26566200	-1.84448500
C	-0.81231200	1.55392900	-0.60417000
C	-0.87513800	2.36472100	0.53179400
C	-1.87532000	1.56895600	-1.50859600
C	-1.98934700	3.16539700	0.76744300
H	-0.04995000	2.35917700	1.24064500
C	-2.99169500	2.36641300	-1.27370800
H	-1.83444700	0.93523300	-2.39137800
C	-3.05254300	3.16291200	-0.13283300
H	-2.02773900	3.78971900	1.65434500
H	-3.81494900	2.36284600	-1.98050700

H	-3.92333700	3.78340800	0.05185400
C	1.32222000	-2.91114900	0.13096700
C	2.64538800	-3.27168600	0.25971000
C	3.41911000	-2.08713300	0.19099500
C	2.53773700	-1.03769200	0.01948800
N	1.26165400	-1.55455000	-0.03472300
H	0.42763500	-3.51377200	0.11432600
H	3.01366800	-4.28061000	0.36976600
H	4.49457700	-2.00044100	0.23688000
C	2.70249800	0.39868200	-0.09306100
C	4.05813400	0.95916300	0.21276300
F	4.99961000	0.42357000	-0.58270200
F	4.42636500	0.69396000	1.47586200
F	4.10730300	2.28740600	0.05200100
C	0.08920500	-0.69564900	0.04217900
H	-0.06411200	-0.40772500	1.08796700
C	-1.14174300	-1.41060400	-0.53231000
O	-1.00265000	-2.07339800	-1.54092300
C	-2.48447400	-1.23489900	0.09785800
C	-3.56805100	-1.84563300	-0.54626500
C	-2.70980900	-0.47510800	1.25052300
C	-4.85486200	-1.69826300	-0.04891300
H	-3.37489200	-2.42683700	-1.44130200
C	-4.00211700	-0.32270300	1.74292900
H	-1.89474900	0.02152300	1.76334400
C	-5.07363200	-0.93264400	1.09645200
H	-5.68904800	-2.17418900	-0.55342900
H	-4.17036800	0.27600200	2.63166200
H	-6.08016200	-0.81103900	1.48369900

**PSS**

C	-1.35812200	0.12509200	-1.42874400
C	0.04406300	0.09751800	-0.87997800
H	-1.50970500	0.51802600	-2.42776600
H	0.72820100	-0.17561500	-1.68947400
C	0.47201500	1.46782100	-0.36970700
C	1.69359600	2.00614800	-0.77953500
C	-0.31495100	2.18002600	0.53996300
C	2.12660000	3.23598900	-0.28936300
H	2.31295900	1.45467900	-1.48317800
C	0.11998000	3.40616700	1.03239500
H	-1.27011100	1.77520500	0.86207900
C	1.34042200	3.93751400	0.61945400
H	3.07665900	3.64369400	-0.61941000

H	-0.49736200	3.94902800	1.74067900
H	1.67500600	4.89545500	1.00415700
C	-1.00050100	-1.48609100	2.40223100
C	-2.32258900	-1.52416900	2.78191100
C	-3.09639600	-1.06102100	1.68892200
C	-2.21521600	-0.75428900	0.67261700
N	-0.93261400	-0.99215100	1.12446000
H	-0.10708300	-1.74441500	2.94483300
H	-2.68823200	-1.83627600	3.74865800
H	-4.16924700	-0.94543400	1.64352700
C	-2.39673000	-0.25737800	-0.67796900
C	-3.80334900	-0.17318200	-1.18839800
F	-4.40463300	-1.37303700	-1.17723600
F	-4.55177600	0.63909400	-0.42248600
F	-3.86263000	0.29328100	-2.44180700
C	0.19477800	-1.01322900	0.20693700
H	0.19721000	-1.98329300	-0.30664800
C	1.53629600	-0.81309100	0.91428800
O	1.59698900	-0.38516400	2.04625400
C	2.78005200	-1.07489600	0.12247400
C	3.96243300	-0.49074400	0.59045300
C	2.80589100	-1.84355300	-1.04587100
C	5.15217600	-0.66563300	-0.10326800
H	3.91892300	0.10646900	1.49494900
C	4.00150600	-2.02360800	-1.73571000
H	1.90594500	-2.31902700	-1.42273800
C	5.17251900	-1.43291700	-1.26793500
H	6.06411000	-0.20367100	0.25975600
H	4.01764500	-2.62681400	-2.63704500
H	6.10197400	-1.57054300	-1.81087300

**TS6RR-Decar**

C	3.53478400	0.09073000	1.83258900
C	4.82782800	-0.37905300	2.42458100
C	5.23969900	-1.59390700	0.50026700
C	3.91390300	-1.30878600	-0.22828000
C	1.87406800	0.08510600	0.41818400
H	5.63785900	0.32578400	2.18889900
H	5.97687100	-0.82084800	0.24680000
H	3.32643700	-2.22010800	-0.34319100
N	2.64985600	0.88767200	2.35575900
N	1.62930800	0.89290600	1.45289900
N	3.10946400	-0.40879000	0.62935900
H	5.61519300	-2.56160600	0.16403900

H	4.72461900	-0.45767000	3.50721100
O	5.10045400	-1.65978300	1.90535200
C	4.16961800	-0.69744300	-1.62112900
H	4.85000200	-1.38618300	-2.13559100
H	3.22336700	-0.71518500	-2.16761100
C	4.75337500	0.69591800	-1.59759100
C	6.13514400	0.91031700	-1.62521800
C	3.90685200	1.80934700	-1.54611100
C	6.66124100	2.19889300	-1.57232900
H	6.80746500	0.05957200	-1.70704000
C	4.43038800	3.09881500	-1.49238200
H	2.82881000	1.66562400	-1.58023000
C	5.80913600	3.29737500	-1.49789800
H	7.73649100	2.34344000	-1.59869000
H	3.75720000	3.95043900	-1.46045200
H	6.21652900	4.30233400	-1.46021100
C	0.40699300	1.59647400	1.73498200
C	-0.44745100	1.06714800	2.70759800
C	0.12562100	2.77367200	1.03267600
C	-1.68422100	1.68993500	2.87728900
C	-1.11492400	3.36505000	1.25788500
C	-2.04602100	2.81680100	2.14095800
H	-2.38951800	1.26441200	3.58672700
H	-1.36714100	4.27433300	0.71840300
C	-0.08070200	-0.11290000	3.57108200
H	-0.96066200	-0.73794200	3.74355000
H	0.70113400	-0.73533100	3.13218800
H	0.28515200	0.23543300	4.54192200
C	-3.40896700	3.44225100	2.28201100
H	-3.34173200	4.43698700	2.73308400
H	-3.87585400	3.55863100	1.29731600
H	-4.06366600	2.82788500	2.90435700
C	1.11043300	3.40823400	0.08804000
H	2.14125600	3.16846400	0.36310600
H	0.94582200	3.04994800	-0.93157100
H	0.99541200	4.49447500	0.10746700
C	0.98413300	-0.19693300	-0.79434700
O	0.57180800	0.79888800	-1.38688000
C	-0.62701400	-1.15078700	0.37462400
C	-1.92883500	-0.47606400	0.03196000
H	-0.39806100	-1.22188900	1.42905300
H	-1.81947600	0.60610000	0.20082300
C	-3.11565500	-0.94761100	0.86243700
C	-3.26658300	-2.29030800	1.21721700

C	-4.09096500	-0.03291100	1.27278500
C	-4.36955900	-2.70744700	1.95840700
H	-2.50415500	-3.00617800	0.92223600
C	-5.19135100	-0.44533800	2.01885100
H	-3.98001400	1.01509300	1.00126100
C	-5.33410800	-1.78754600	2.36314500
H	-4.47372300	-3.75502100	2.22351100
H	-5.93573800	0.28121600	2.33119200
H	-6.18995200	-2.11419000	2.94538100
C	-2.78369400	-2.74768000	-2.81170700
C	-2.15356300	-3.96623600	-2.97331600
C	-1.01974300	-3.97371300	-2.13313000
C	-0.99868200	-2.75835900	-1.47156500
N	-2.09163900	-2.02431300	-1.88522800
H	-3.67474000	-2.35401900	-3.26887500
H	-2.48863500	-4.76268700	-3.62080700
H	-0.30589400	-4.77277000	-2.00038900
C	-0.13544400	-2.20938700	-0.43665200
O	1.18833500	-1.39576800	-1.35520200
C	0.72067800	-3.23793700	0.26578200
F	1.51563800	-3.92992100	-0.56126800
F	-0.04583900	-4.12634400	0.91411700
F	1.52386500	-2.66950000	1.18950300
C	-2.20175400	-0.62212100	-1.49948000
H	-1.40468500	-0.08104900	-2.01793700
C	-3.53723400	0.01786600	-1.83250900
O	-4.53560700	-0.63436700	-2.05967900
C	-3.59889000	1.51874800	-1.80060400
C	-4.87295000	2.09945800	-1.79466900
C	-2.46422600	2.33765300	-1.78342200
C	-5.01603600	3.48013700	-1.77460600
H	-5.73689800	1.44324200	-1.80364300
C	-2.61392700	3.72316400	-1.78355400
H	-1.46257700	1.91458200	-1.76773000
C	-3.88297400	4.29569900	-1.77551500
H	-6.00631400	3.92349100	-1.76524000
H	-1.73108200	4.35527200	-1.79077800
H	-3.99147700	5.37579600	-1.77198200

**TS6RS-Decar**

C	0.97503800	-0.84201500	0.95288400
O	0.42633200	-1.10181100	2.00720500
C	-0.73245000	-0.27982400	-0.49946800
C	-2.01247900	-0.45703700	0.27156100



H	-0.58494200	0.65440100	-1.02883700
H	-1.79808700	-0.76670200	1.31006700
C	-2.87054900	0.79248000	0.29874100
C	-3.20438700	1.44689400	-0.89218900
C	-3.43635900	1.24744900	1.49045500
C	-4.09766200	2.51297200	-0.89356200
H	-2.76003200	1.10492100	-1.82442600
C	-4.32108400	2.32530300	1.49710900
H	-3.19353900	0.73690600	2.41978000
C	-4.65953100	2.95743200	0.30333000
H	-4.35771900	2.99971200	-1.82899000
H	-4.75609800	2.66037900	2.43360500
H	-5.35894300	3.78771100	0.30368000
C	-2.51295200	-4.07475300	-0.62341000
C	-1.47551100	-4.85810500	-1.08411600
C	-0.37349900	-4.00315700	-1.30756800
C	-0.77370300	-2.72136600	-0.97919500
N	-2.07997700	-2.78384800	-0.54731500
H	-3.51526300	-4.34076800	-0.32514100
H	-1.50933400	-5.92836700	-1.22431800
H	0.61656700	-4.27722900	-1.63882800
C	-0.06768900	-1.43373000	-1.01591600
O	1.30172200	-1.71198500	-0.01406900
C	0.70732200	-1.19561000	-2.29626500
F	1.56902700	-2.17701900	-2.59664900
F	-0.12961400	-1.07021400	-3.33457300
F	1.42786700	-0.05718400	-2.23042900
C	-2.90267000	-1.60964800	-0.30566600
H	-3.32109600	-1.27793000	-1.26068700
C	-3.99654200	-1.92209600	0.71543800
O	-3.72415100	-2.60870200	1.68121200
C	-5.35709900	-1.30894200	0.58080400
C	-6.20863700	-1.41476600	1.68780000
C	-5.80298800	-0.64063000	-0.56314300
C	-7.47791900	-0.85523800	1.65672600
H	-5.84620100	-1.93814400	2.56591700
C	-7.07672800	-0.07966300	-0.59277900
H	-5.16765400	-0.54202000	-1.43519900
C	-7.91353200	-0.18338000	0.51434800
H	-8.12867700	-0.93825100	2.52101900
H	-7.41270500	0.44117300	-1.48328800
H	-8.90472800	0.25819300	0.48843700
C	3.91998900	1.20204200	1.59722900
C	5.26796000	1.29174300	2.25730200

C	4.69083000	-0.75978100	3.28522900
C	3.68904200	-1.19828000	2.21715200
C	2.00316800	0.31123600	1.03030300
H	6.00362300	1.65412800	1.53585100
H	5.17823100	-1.63746200	3.71220500
H	2.84172100	-1.69778900	2.69416900
N	3.25955000	2.15983000	1.01686200
N	2.06755100	1.58702000	0.66453200
N	3.17686300	0.05747200	1.64218500
H	4.17184200	-0.21585400	4.08801500
H	5.19623700	2.01004600	3.08574500
O	5.71204900	0.03583400	2.71593500
C	4.28177600	-2.10702500	1.11331400
H	4.91587100	-2.84641200	1.61333600
H	3.44354300	-2.63570800	0.65285400
C	5.05206700	-1.38025500	0.03248300
C	6.42815800	-1.15437700	0.12110600
C	4.36345300	-0.91907800	-1.09394500
C	7.09820200	-0.46477800	-0.88621400
H	6.97319400	-1.50937000	0.99048300
C	5.03320600	-0.23003800	-2.10309500
H	3.29967800	-1.12145100	-1.17867100
C	6.40177700	0.00413200	-1.99920300
H	8.16781800	-0.29865700	-0.80477500
H	4.47992300	0.11102400	-2.97332000
H	6.92676500	0.53802800	-2.78482300
C	1.07096400	2.42216200	0.04971800
C	-0.06421900	2.74917900	0.79288800
C	1.32591400	2.91312300	-1.23209500
C	-1.00337100	3.57698700	0.18318800
C	0.34952100	3.73154200	-1.79707200
C	-0.81773700	4.06740000	-1.10934500
H	-1.91572100	3.81949600	0.72340300
H	0.50986300	4.11895800	-2.80063100
C	-0.27368700	2.21744300	2.18421200
H	-0.46716100	1.13911000	2.16966500
H	0.60947100	2.38866400	2.80933900
H	-1.12866500	2.71022600	2.64968200
C	-1.85693500	4.94144300	-1.76122900
H	-2.27303900	4.44982600	-2.64637800
H	-2.68011500	5.15223800	-1.07561300
H	-1.42213000	5.89077900	-2.08729700
C	2.60649100	2.61530600	-1.96506900
H	3.36030300	3.37456900	-1.73465600

H	3.02223500	1.64630600	-1.68591200
H	2.43416700	2.61889500	-3.04335700

**TS6SR-Decar**

C	-3.67628700	-0.93084400	1.51981400
C	-4.89930300	-0.77567500	2.37072300
C	-5.29960500	1.26055000	1.35873100
C	-4.01729600	1.34824700	0.51396100
C	-2.07191400	-0.29214300	0.18876700
H	-5.76943600	-1.23412500	1.87972300
H	-6.08647700	0.74551700	0.79210700
H	-3.37560800	2.15382000	0.87004500
N	-2.84807400	-1.93232300	1.48590200
N	-1.86347900	-1.53048300	0.63437400
N	-3.25436700	0.09286800	0.71575200
H	-5.63235900	2.27595200	1.57995600
H	-4.73403300	-1.26183600	3.33268100
O	-5.10536200	0.59919600	2.59213900
C	-4.35678600	1.59338000	-0.97051100
H	-4.99390400	2.48532300	-0.98987900
H	-3.43130200	1.85643800	-1.48813900
C	-5.05044400	0.44303500	-1.66222300
C	-6.44543900	0.35129100	-1.70745300
C	-4.29652200	-0.55921000	-2.28204100
C	-7.07207200	-0.72667600	-2.32778000
H	-7.04879600	1.14234300	-1.26832800
C	-4.92012300	-1.63854800	-2.90316900
H	-3.21223200	-0.47736800	-2.30696100
C	-6.30981100	-1.72930200	-2.92138700
H	-8.15577500	-0.77699600	-2.35520800
H	-4.31694500	-2.40174200	-3.38571900
H	-6.79591600	-2.56792100	-3.40889900
C	-0.74725300	-2.41523500	0.42576200
C	-0.65711200	-3.12259600	-0.77818100
C	0.10319400	-2.64018100	1.51115600
C	0.37689400	-4.04845700	-0.89106400
C	1.11235100	-3.58751200	1.34622800
C	1.26511900	-4.29586400	0.15707100
H	0.47277600	-4.61169100	-1.81621500
H	1.79939600	-3.76755600	2.16874000
C	-1.65693000	-2.94643100	-1.88820800
H	-2.67157100	-2.84267800	-1.49075400
H	-1.43080000	-2.04879500	-2.46913000
H	-1.63779200	-3.81360700	-2.55106000

C	2.33529800	-5.34596300	0.01408300
H	2.81003100	-5.28992100	-0.96905600
H	3.10854900	-5.22396800	0.77530200
H	1.90715200	-6.34835600	0.11777100
C	-0.07985600	-1.95368400	2.83928500
H	-0.68330100	-2.57742900	3.50633600
H	0.89359000	-1.79286900	3.30919500
H	-0.58306000	-0.98922200	2.74720500
C	-1.22601500	0.55482100	-0.75276800
O	-0.83842700	0.05179800	-1.78671800
C	0.62816200	0.83113100	0.67278200
C	1.82560300	0.54076100	-0.18308000
H	0.55607900	0.35031200	1.63879100
H	1.51924800	0.35118500	-1.22667900
C	2.65338800	-0.63082700	0.30070100
C	3.02853100	-0.73124000	1.64459300
C	3.18388600	-1.54494900	-0.61069300
C	3.92441600	-1.71049600	2.06422600
H	2.63151600	-0.01500500	2.36054600
C	4.09343100	-2.51599100	-0.19871500
H	2.90398900	-1.46976700	-1.65877300
C	4.46828100	-2.60111500	1.13959800
H	4.21121500	-1.76860400	3.11032800
H	4.51468100	-3.20381100	-0.92586900
H	5.18213000	-3.35407500	1.46007600
C	2.48328600	4.10695400	-1.17137000
C	1.48484200	5.05719900	-1.13783400
C	0.36684000	4.46601900	-0.50765900
C	0.71891900	3.17211300	-0.17311800
N	2.01215100	2.96274500	-0.59757300
H	3.48137700	4.15062100	-1.57919100
H	1.55390000	6.05749000	-1.53893200
H	-0.60160200	4.91027800	-0.33504400
C	-0.01802400	2.09662800	0.51259100
O	-1.35504500	1.86828500	-0.51330500
C	-0.75318300	2.57431300	1.74830200
F	-1.62155000	3.57054500	1.50604900
F	0.10263700	3.01363900	2.67638700
F	-1.47086800	1.57793200	2.31506700
C	2.78872000	1.77691400	-0.27008300
H	3.24657600	1.92062200	0.71316500
C	3.83467600	1.50376600	-1.34936600
O	3.53172400	1.64806600	-2.51822800
C	5.18272200	0.96442200	-0.97668600

C	5.97893100	0.48132300	-2.02266300
C	5.66218100	0.89684500	0.33448200
C	7.22506900	-0.07065500	-1.76296200
H	5.59017900	0.54222200	-3.03337900
C	6.91266600	0.34237700	0.59369800
H	5.06931100	1.26086100	1.16510400
C	7.69300300	-0.14419500	-0.45076500
H	7.83229500	-0.44759900	-2.57947900
H	7.27404200	0.28832400	1.61531600
H	8.66557900	-0.57962100	-0.24414700

**TS6SS-Decar**

C	0.68066900	0.76128800	0.79318300
O	0.09659000	1.84556200	0.95502200
C	-0.71945500	-0.68290100	0.15134300
C	-2.10476200	-0.08724900	0.17012000
H	-0.43704300	-1.14760800	-0.78539500
H	-2.08704500	0.83771500	-0.42129100
C	-3.17878000	-0.98369300	-0.43080200
C	-4.17881300	-0.42975900	-1.23704900
C	-3.20516300	-2.35849700	-0.18282200
C	-5.19084300	-1.22327700	-1.77103200
H	-4.16096100	0.63858300	-1.44558300
C	-4.21879700	-3.15459400	-0.71172300
H	-2.41824500	-2.80747500	0.41700500
C	-5.21695100	-2.59022200	-1.50358600
H	-5.95663100	-0.77470000	-2.39634500
H	-4.22758400	-4.22021100	-0.50484800
H	-6.00461700	-3.21283300	-1.91588000
C	-2.87867900	-1.05498500	3.70596200
C	-2.13587000	-2.01563800	4.37055600
C	-0.97931400	-2.25917300	3.60706700
C	-1.05331400	-1.44581000	2.48522600
N	-2.23178500	-0.72682300	2.55503500
H	-3.82079200	-0.60110200	3.96053700
H	-2.41465800	-2.48931500	5.29979000
H	-0.18417700	-2.95693200	3.82205700
C	-0.21868700	-1.31742400	1.31617200
O	1.09726400	-0.03548100	1.78142200
C	0.75922400	-2.44714000	1.10416400
F	1.56594200	-2.66860500	2.14628700
F	0.09113800	-3.59007600	0.87187700
F	1.54113200	-2.23140000	0.03068200
C	-2.46818000	0.36789700	1.61984100

H	-1.77039400	1.16810100	1.88114500
C	-3.88435900	0.91535700	1.64158900
O	-4.81417900	0.30854900	2.13283700
C	-4.10470000	2.23329300	0.95767300
C	-5.42881700	2.59717000	0.69070400
C	-3.06034000	3.08321900	0.57260300
C	-5.71078400	3.79248700	0.04238300
H	-6.21996400	1.92039100	0.99569600
C	-3.34902800	4.28234200	-0.07405800
H	-2.02275500	2.82429400	0.76891700
C	-4.66917400	4.63703000	-0.34119600
H	-6.73951000	4.06719800	-0.16612400
H	-2.53799500	4.94062500	-0.36820200
H	-4.88745200	5.57170500	-0.84802600
C	3.59573400	1.68903200	-1.22003700
C	4.88841500	2.45498700	-1.27858000
C	4.19468300	3.36157800	0.79665500
C	3.33310800	2.16932400	1.21021800
C	1.74805300	0.90388500	-0.34211600
H	5.68619300	1.79855500	-1.63457600
H	4.63025500	3.82629700	1.68244500
H	2.43548800	2.51926100	1.72650000
N	2.95993500	1.14160300	-2.21464200
N	1.80966400	0.66212100	-1.65009100
N	2.88010500	1.57906000	-0.06131300
H	3.58269300	4.10748400	0.26861800
H	4.76393900	3.28305400	-1.98968000
O	5.27533800	2.93272200	-0.00976100
C	4.07389800	1.13072500	2.08644200
H	4.70273100	1.68744500	2.78868600
H	3.30676300	0.59954600	2.65460100
C	4.88920200	0.12214300	1.31019000
C	6.23493600	0.31605900	0.99054500
C	4.25290100	-1.04444000	0.87863400
C	6.92328500	-0.63253500	0.23674900
H	6.73909500	1.21973300	1.31928700
C	4.93721800	-1.99190000	0.12151900
H	3.21519100	-1.19560600	1.15633000
C	6.27546400	-1.78492900	-0.20579200
H	7.96994600	-0.47249200	-0.00286600
H	4.42182300	-2.89172600	-0.20182600
H	6.81519700	-2.52093600	-0.79308300
C	0.81164500	0.02486500	-2.46238800
C	-0.37950300	0.72056200	-2.69819100

C	1.04152600	-1.27943600	-2.89810200
C	-1.41282200	0.01476600	-3.30407500
C	-0.03075700	-1.94113800	-3.50081900
C	-1.27114400	-1.32744700	-3.66981100
H	-2.36494800	0.51280000	-3.46881400
H	0.10294300	-2.97249700	-3.81720600
C	-0.54407200	2.16129400	-2.28911400
H	-0.43801100	2.28824200	-1.20633800
H	0.21106900	2.78824600	-2.77502000
H	-1.53167800	2.52523300	-2.58123100
C	-2.45452500	-2.09739700	-4.18927100
H	-3.09945600	-1.46665200	-4.80601200
H	-2.14187400	-2.96178600	-4.77909500
H	-3.05566200	-2.45680000	-3.34588400
C	2.37727300	-1.95359900	-2.73317500
H	3.00419700	-1.76127000	-3.60951500
H	2.91792000	-1.58980700	-1.85759500
H	2.24895900	-3.03329200	-2.63465200

#### TS7RR-D

C	1.01350400	-2.22282500	-1.16422800
O	-0.02766600	-2.74192900	-1.55661100
C	1.12110800	-0.64147800	-1.15428500
C	-0.20089500	0.00151300	-0.75440600
H	1.45925900	-0.29125300	-2.13321400
H	-0.95024500	-0.45540100	-1.40729100
C	-0.28134000	1.51089100	-0.89825600
C	0.82943000	2.34839300	-0.76728900
C	-1.52485800	2.09098000	-1.17480000
C	0.69628100	3.72935600	-0.89550400
H	1.81602400	1.93661600	-0.57984100
C	-1.66045700	3.46908800	-1.29926300
H	-2.39556900	1.45176200	-1.30254400
C	-0.54780600	4.29444100	-1.15604000
H	1.57200800	4.36216300	-0.79497400
H	-2.63377900	3.89669000	-1.51638500
H	-0.64872200	5.37007600	-1.25624600
C	0.54492700	0.19305100	2.87702400
C	1.87450200	0.29803300	3.35590000
C	2.71271400	0.01686700	2.30557500
C	1.89487900	-0.24023400	1.16769200
N	0.55777200	-0.11007000	1.58322200
H	-0.38214100	0.33115000	3.41042000
H	2.14547000	0.55646900	4.36781900

H	3.79281900	0.00510600	2.29893800
C	2.19267200	-0.52514900	-0.13705900
O	2.05564500	-2.72108100	-0.65997800
C	3.64604000	-0.51649300	-0.56014900
F	4.40592800	-1.27147600	0.22917600
F	4.10251900	0.75109100	-0.46005600
F	3.81087900	-0.89802000	-1.81881000
C	-0.54166400	-0.48371500	0.68525600
H	-0.57697500	-1.57854500	0.66482300
C	-1.89835500	0.04181400	1.14326500
O	-1.98223200	0.94381700	1.95208100
C	-3.10560200	-0.57743600	0.52285800
C	-4.34159900	0.00925300	0.82308100
C	-3.04781000	-1.69248000	-0.32476600
C	-5.51006700	-0.51143200	0.28613000
H	-4.35924800	0.87301300	1.47906400
C	-4.22536300	-2.20954600	-0.85769600
H	-2.10480000	-2.16518800	-0.59247200
C	-5.45161400	-1.62358200	-0.55447800
H	-6.46560000	-0.05420900	0.51970800
H	-4.17994500	-3.07228500	-1.51312600
H	-6.36461300	-2.03236400	-0.97532500

**TS7RS-D**

C	2.15431700	-1.59222300	-1.50580500
O	1.50014900	-2.36935300	-2.17623800
C	1.47118900	-1.03479900	-0.14496200
C	0.09649000	-0.45688200	-0.52537800
H	1.41569100	-1.85867200	0.56987400
H	0.10369400	-0.26525000	-1.60438000
C	-1.03466200	-1.41736000	-0.22308200
C	-1.18407800	-1.96873200	1.05173600
C	-1.99818400	-1.68639100	-1.19463300
C	-2.28847200	-2.75872200	1.35592100
H	-0.44103500	-1.76997100	1.82143200
C	-3.10623500	-2.47264000	-0.89215000
H	-1.88068400	-1.26917800	-2.19114900
C	-3.25656300	-3.00568300	0.38528300
H	-2.39349500	-3.17965600	2.35071200
H	-3.85067200	-2.67038800	-1.65626200
H	-4.11992300	-3.61896000	0.62159300
C	1.03568900	3.11058800	-0.11426200
C	2.37535800	3.54143800	-0.01179600
C	3.15560800	2.41739800	0.15182900



C	2.28926200	1.29266400	0.12065700
N	0.98745300	1.78076500	-0.05616900
H	0.13695100	3.69998000	-0.21900700
H	2.70131700	4.56870600	-0.06424600
H	4.23038700	2.35967300	0.23719600
C	2.50928700	-0.06140600	0.20433300
O	3.27581200	-1.04789900	-1.67749200
C	3.78920700	-0.54073200	0.86053900
F	4.87733500	0.02171700	0.33988800
F	3.73796100	-0.18122300	2.15933600
F	3.91940000	-1.86116600	0.82663100
C	-0.18511300	0.91910300	0.13331100
H	-0.33358300	0.79964700	1.21069200
C	-1.41432200	1.54333200	-0.54959100
O	-1.24365200	2.17439500	-1.57359000
C	-2.77756400	1.30162600	-0.00154300
C	-3.85634200	1.63258200	-0.83211800
C	-3.02191700	0.75554900	1.26245800
C	-5.15855400	1.40884700	-0.41017000
H	-3.64734600	2.05368900	-1.80943900
C	-4.32891200	0.53251800	1.68263500
H	-2.20784900	0.48928300	1.92615500
C	-5.39563100	0.85478100	0.84804800
H	-5.98968800	1.65929300	-1.06054500
H	-4.51223800	0.10252400	2.66134100
H	-6.41360000	0.67369600	1.17751000

**TS7SR-D**

C	-2.15631900	-1.59322500	-1.50352900
O	-1.50410700	-2.37344800	-2.17233900
C	-1.47193100	-1.03463000	-0.14399600
C	-0.09714100	-0.45772600	-0.52571600
H	-1.41606700	-1.85733700	0.57214500
H	-0.10504000	-0.26599400	-1.60470500
C	1.03390000	-1.41863100	-0.22408600
C	1.18276400	-1.97188100	1.04998500
C	1.99829300	-1.68574200	-1.19534900
C	2.28719800	-2.76205100	1.35364300
H	0.43933100	-1.77449400	1.81963500
C	3.10646600	-2.47198700	-0.89332700
H	1.88128500	-1.26705000	-2.19131200
C	3.25601200	-3.00720100	0.38329000
H	2.39171300	-3.18445600	2.34786400
H	3.85151300	-2.66819200	-1.65724100

H	4.11937400	-3.62063400	0.61918400
C	-1.03368500	3.11034700	-0.11733200
C	-2.37305400	3.54223800	-0.01418100
C	-3.15386000	2.41899300	0.15163000
C	-2.28823100	1.29356700	0.12113600
N	-0.98625500	1.78063900	-0.05754200
H	-0.13467300	3.69906900	-0.22357800
H	-2.69836600	4.56965200	-0.06776000
H	-4.22860500	2.36207500	0.23800600
C	-2.50920000	-0.06017300	0.20516900
O	-3.27664600	-1.04690100	-1.67649600
C	-3.78973300	-0.53837400	0.86104300
F	-4.87730200	0.02448100	0.33966100
F	-3.73889400	-0.17813900	2.15968000
F	-3.92070700	-1.85874400	0.82783700
C	0.18565300	0.91819200	0.13263700
H	0.33351500	0.79888100	1.21011000
C	1.41537200	1.54137900	-0.55027900
O	1.24506900	2.17072900	-1.57542100
C	2.77838400	1.30093500	-0.00119500
C	3.85750200	1.63350700	-0.83070600
C	3.02224800	0.75438000	1.26267700
C	5.15958900	1.41095900	-0.40778900
H	3.64886100	2.05491900	-1.80796400
C	4.32913800	0.53243300	1.68377600
H	2.20793400	0.48666500	1.92546200
C	5.39620300	0.85636700	0.85029800
H	5.99100500	1.66267400	-1.05731400
H	4.51211800	0.10207900	2.66238800
H	6.41408900	0.67620500	1.18052600

**TS7SS-D**

C	-1.01259500	-2.22315100	-1.16334900
O	0.02835200	-2.74394800	-1.55360000
C	-1.12054700	-0.64154000	-1.15440700
C	0.20114400	0.00203400	-0.75469800
H	-1.45900300	-0.29169200	-2.13337800
H	0.95067900	-0.45483300	-1.40741600
C	0.28094500	1.51137500	-0.89892100
C	1.52396100	2.09197300	-1.17655100
C	-0.83013100	2.34834500	-0.76708100
C	1.65882200	3.47014300	-1.30119900
H	2.39485000	1.45310800	-1.30487300
C	-0.69771300	3.72936000	-0.89544300

H	-1.81641600	1.93605300	-0.57905500
C	0.54591400	4.29498500	-1.15705100
H	2.63175500	3.89818700	-1.51918500
H	-1.57363800	4.36178300	-0.79422100
H	0.64625900	5.37066200	-1.25738400
C	-0.54466100	0.19606800	2.87630000
C	-1.87417700	0.30079000	3.35504700
C	-2.71230700	0.01749700	2.30510300
C	-1.89443500	-0.24060500	1.16763700
N	-0.55743500	-0.10887600	1.58282000
H	0.38237000	0.33562200	3.40935000
H	-2.14530200	0.56046800	4.36660500
H	-3.79240400	0.00497200	2.29851900
C	-2.19247100	-0.52694900	-0.13696200
O	-2.05591900	-2.71996600	-0.65952600
C	-3.64593600	-0.51858600	-0.55959100
F	-4.40555100	-1.27362000	0.22992100
F	-4.10246500	0.74901900	-0.45915800
F	-3.81125200	-0.89976400	-1.81828800
C	0.54202200	-0.48272800	0.68505900
H	0.57754000	-1.57756100	0.66497500
C	1.89878500	0.04292700	1.14263600
O	1.98293500	0.94546600	1.95081600
C	3.10591100	-0.57703100	0.52262800
C	4.34210600	0.00917700	0.82298300
C	3.04786100	-1.69237400	-0.32458900
C	5.51049400	-0.51229500	0.28661700
H	4.35998000	0.87317500	1.47864600
C	4.22532800	-2.21022900	-0.85694300
H	2.10470700	-2.16466500	-0.59251300
C	5.45177300	-1.62476100	-0.55355300
H	6.46617600	-0.05545000	0.52032800
H	4.17969300	-3.07320400	-1.51204900
H	6.36470800	-2.03416800	-0.97393300