

**New Journal of Chemistry**

*Supporting Information*

**Mechanistic Study on the NHC-catalyzed [3+4] Annulation of Enals and  
Thiazolones**

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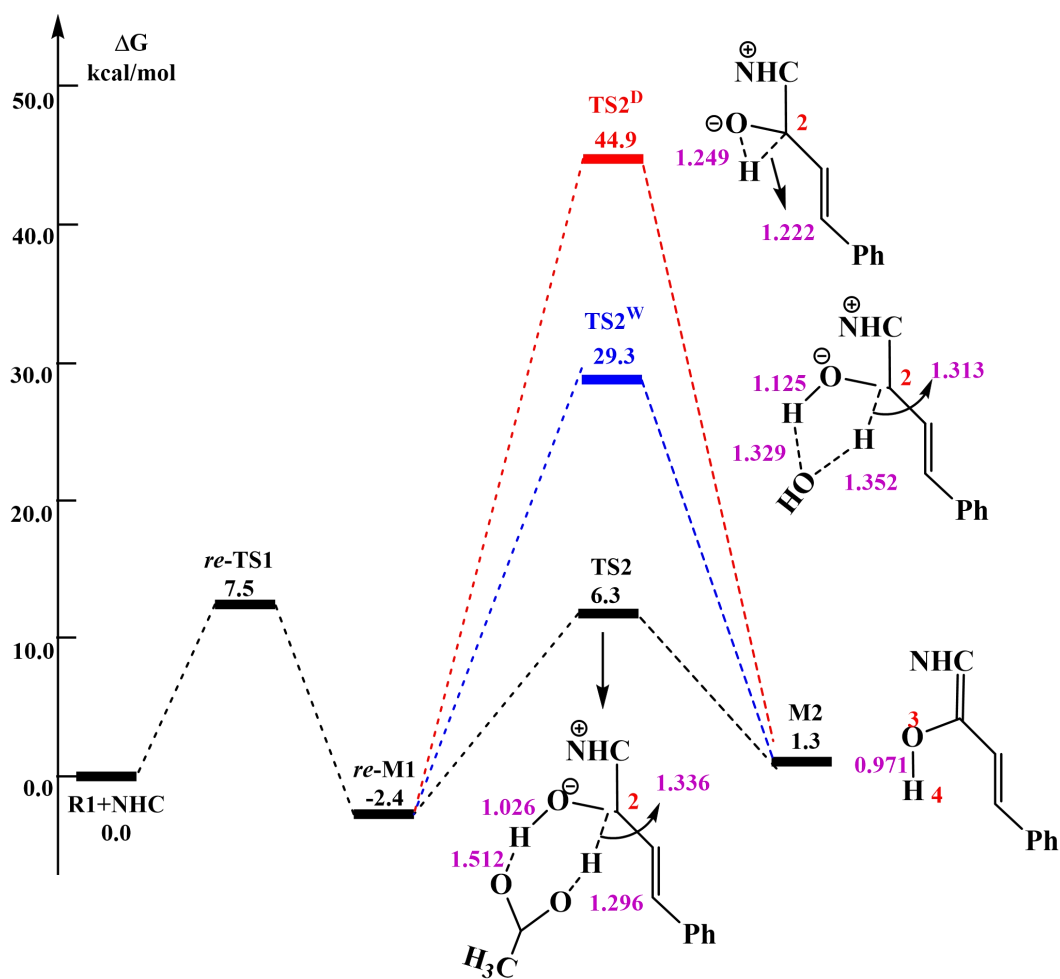
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Table S1. Comparison of the free energies of the stereoselective transition states calculated with M06-2X,  $\omega$ B97X-D and B3LYP-D3 methods in conjunction with 6-311++G(2df,2pd) basis set using IEF-PCM and SMD solvation models.

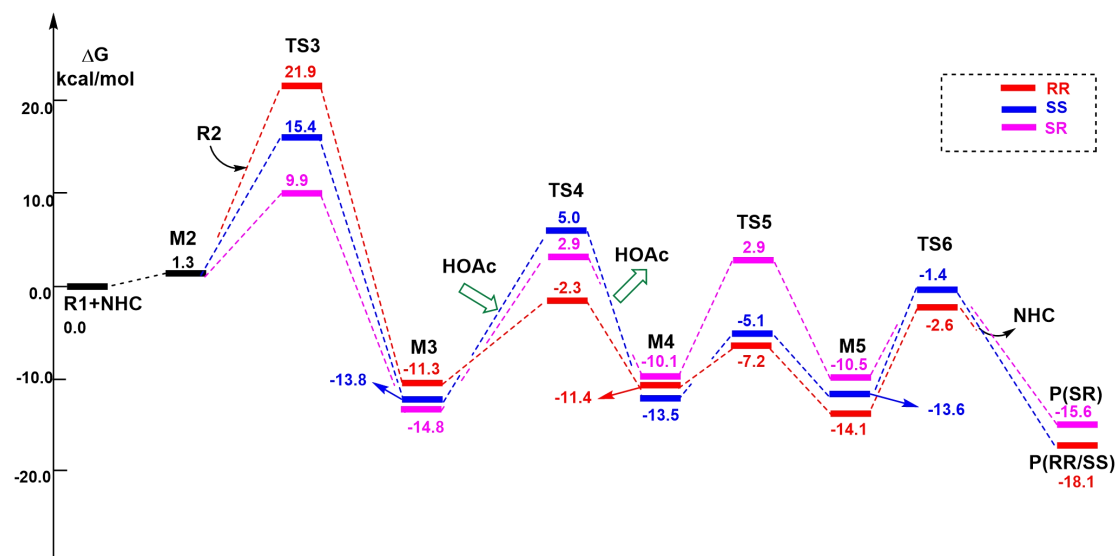
species	M06		$\omega$ B97XD		B3LYP-D3	
	SMD	IEFPCM	SMD	IEFPCM	SMD	IEFPCM
<b>TS3(RR)</b>	17.5	17.4	17.9	18.7	15.0	15.9
<b>TS3(RS)</b>	0.0	0.0	0.0	0.0	0.0	0.0
<b>TS3(SR)</b>	5.5	5.5	5.6	6.9	8.9	9.6
<b>TS3(SS)</b>	11.0	10.9	12.4	13.1	13.8	10.1



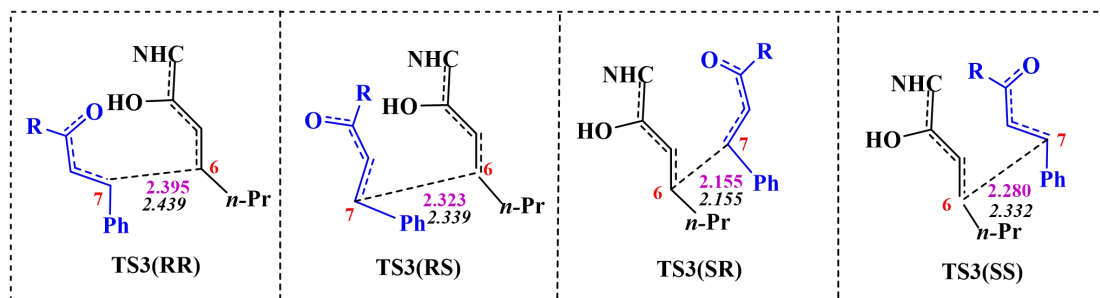
**Fig. S2** Free energy (kcal/mol) profiles of Step II.



**Fig. S3** Free energy (kcal/mol) profiles of the unfavored reaction pathways.



**Fig. S4** Optimized structures of stereoselective transition states in gas phase and in 1,4-dioxane (italic). Distances are given in Å.



## Cartesian Coordinates

### NHC

O	0.68055500	-1.89864400	1.17431500
N	-2.88201500	-2.08726500	-0.97295800
N	-2.73106300	-1.57853900	-2.25547100
N	-0.83656500	-2.00158300	-1.24951200
C	-4.83082600	-3.47925000	-0.63612300
H	-4.29391800	-4.26526400	-1.15661000
C	-6.11644700	-3.67980000	-0.15038500
H	-6.60771400	-4.63687600	-0.28787900
C	-6.75988300	-2.64039500	0.51423200
H	-7.76413900	-2.78104100	0.90096000
C	-6.12031600	-1.41794300	0.69330800
H	-6.64105700	-0.62493600	1.21947800
C	-4.82580400	-1.18869700	0.21751400
C	-4.20710500	-2.25056100	-0.45210600
C	-1.74475500	-2.34991100	-0.29474800
C	-1.44148400	-1.53184400	-2.37790100
C	-0.43527800	-1.05449900	-3.37621500
H	-0.63623100	-0.01839600	-3.66082900
H	-0.46222400	-1.65402900	-4.28833700
C	0.91834400	-1.23336700	-2.61201400
H	1.48444900	-0.30163500	-2.55392200
H	1.55640600	-1.94187800	-3.14132000
C	0.59943100	-1.80408800	-1.19520400
H	1.10204400	-2.76489400	-1.05162600
C	0.93499500	-1.01017600	0.10874700
C	2.43008100	-0.70831000	0.12760000
C	2.95609200	0.47666300	-0.38381500
C	3.30332500	-1.67867500	0.62282100
C	4.33367800	0.67780800	-0.41171000
H	2.30149100	1.26605600	-0.74227800
C	4.67592300	-1.45988700	0.59762100
H	2.89968800	-2.59474800	1.03934400
C	5.20682200	-0.28496000	0.07664600
C	0.09020500	0.25641100	0.29599500
C	-0.32727300	1.06724700	-0.75816000
C	-0.29211600	0.61200600	1.59103700
C	-1.10336600	2.19831400	-0.52651200
H	-0.06563600	0.83663900	-1.78259300
C	-1.06272500	1.74825200	1.81303300
H	0.00353600	-0.02018800	2.42162900
C	-1.47520200	2.55832100	0.76057900
H	6.27829700	-0.12131700	0.05798200



H	-2.08671000	3.43549200	0.93999400
H	-0.25058500	-2.20590700	1.08163600
C	5.59340100	-2.49015300	1.19738000
C	4.86810300	1.94069300	-1.02849700
C	-1.44140900	2.08861500	3.22898700
C	-1.49943900	3.03027100	-1.71323600
F	-2.48327900	3.88843400	-1.42023100
F	-1.91869600	2.25345300	-2.72696000
F	-0.46543000	3.74539400	-2.17802700
F	-1.97128300	1.03016500	3.85681000
F	-2.33901800	3.08351100	3.27851000
F	-0.37449400	2.47316200	3.94145400
F	5.12694500	-3.73152600	1.00654200
F	6.82104100	-2.42822100	0.66347700
F	5.72549600	-2.31682900	2.51896400
F	4.89462800	1.85236600	-2.36771200
F	6.11503800	2.20520000	-0.62212800
F	4.10134500	2.99638200	-0.72323000
C	-4.14719000	0.16193200	0.37329400
C	-4.52409400	0.86286200	1.67985400
C	-4.48336900	1.04989900	-0.83380700
H	-3.06074300	-0.00478000	0.38363600
H	-4.32178900	0.23324000	2.55030200
H	-3.95164300	1.78760200	1.78799500
H	-5.58125700	1.14567000	1.69320300
H	-4.12747100	0.60357200	-1.76607600
H	-5.56779900	1.18543000	-0.90844000
H	-4.02849700	2.03897500	-0.72167800

## R1

C	0.37519100	0.00565900	0.34743800
C	1.35679300	0.77152800	-0.13828400
H	0.63920800	-1.01099300	0.64299700
C	2.73720000	0.24713700	-0.25365000
H	1.17429400	1.79474600	-0.45925500
C	-1.05438100	0.41603900	0.49296700
C	-1.99716200	-0.47727500	-0.32522400
H	-1.17900100	1.46318800	0.19340500
H	-1.34105400	0.34819300	1.55161600
C	-3.45945300	-0.08156800	-0.14545400
H	-1.71683900	-0.41603900	-1.38258100
H	-1.85232100	-1.52199500	-0.02579100
H	-4.11979600	-0.71939000	-0.73775900
H	-3.76099400	-0.16557800	0.90322500

H	-3.62484600	0.95440600	-0.45699000
H	3.48437900	0.95368200	-0.66873800
O	3.06848100	-0.87116700	0.07164000

**R2**

C	-1.64980600	0.51670400	-0.01536600
C	0.78344000	0.96279600	-0.07003400
C	-0.13513900	2.16177900	-0.07467500
N	-1.49730300	1.78735700	-0.04167300
O	0.25012700	3.30312900	-0.09988700
S	-0.17541000	-0.50310900	-0.03014500
C	2.11438000	1.13725000	-0.05737000
H	2.40768200	2.18724500	-0.04180900
C	-2.96872000	-0.13456100	0.02213000
C	-4.11272700	0.67276000	0.00249500
C	-3.09959700	-1.52504200	0.07816700
C	-5.37134800	0.08893200	0.03784200
H	-3.98673100	1.74904700	-0.04094000
C	-4.36215400	-2.10415700	0.11439000
H	-2.21893200	-2.16081200	0.09542300
C	-5.49784100	-1.29853200	0.09398900
H	-6.25672500	0.71565300	0.02239800
H	-4.45980200	-3.18350100	0.15945700
H	-6.48325500	-1.75250700	0.12283700
C	3.20115900	0.16068500	-0.03473800
C	3.03050700	-1.20240900	-0.31951100
C	4.48835300	0.62156600	0.28148300
C	4.11082500	-2.07420000	-0.26874000
H	2.05885200	-1.58442700	-0.61226600
C	5.56597800	-0.25211400	0.33903600
H	4.63268400	1.67775500	0.49084600
C	5.37908000	-1.60513600	0.06637900
H	3.96322800	-3.12462400	-0.49722600
H	6.55211700	0.12216300	0.59345500
H	6.21920300	-2.29070100	0.10808300

**H<sub>2</sub>O**

O	0.00000000	0.00000000	0.11778200
H	0.00000000	0.76046300	-0.47112900
H	0.00000000	-0.76046300	-0.47112900

**HOAc**

H	-1.71727300	-0.79993000	0.00003800
C	-0.09227300	0.12421400	-0.00000800

O	-0.77763900	-1.03785100	0.00006500
O	-0.63907000	1.19675400	-0.00008600
C	1.39241500	-0.11217200	0.00001800
H	1.67033800	-0.69422500	-0.88124000
H	1.90943300	0.84484600	-0.00000900
H	1.67032200	-0.69417200	0.88131500

**re-TS1**

O	1.23861900	-1.58180100	3.42992300
N	-2.82707400	-2.42367800	0.87916500
N	-2.70156100	-3.72457200	0.43959300
N	-0.95643700	-3.02650400	1.59267800
C	-4.95928700	-1.50343200	1.55174400
H	-4.77930600	-1.92968100	2.53363400
C	-6.10563400	-0.76488700	1.28186100
H	-6.84498200	-0.60386100	2.05849100
C	-6.29014200	-0.23885000	0.00691300
H	-7.18044600	0.33941000	-0.21798700
C	-5.33420500	-0.44166000	-0.98506200
H	-5.49053400	-0.00839700	-1.96772100
C	-4.16706500	-1.16907900	-0.74016200
C	-4.01675000	-1.69493800	0.54815300
C	-1.78334100	-1.94964600	1.58395000
C	-1.54041600	-4.05970600	0.90203100
C	-0.68764500	-5.28359000	0.91314800
H	-0.64401700	-5.77277400	-0.06049800
H	-1.08327500	-6.00221600	1.63754800
C	0.67028300	-4.70141700	1.36887700
H	1.24672700	-5.39849000	1.97782400
H	1.28220800	-4.46107700	0.49581700
C	0.34289700	-3.41570000	2.17434900
H	0.16906000	-3.67607700	3.22394600
C	1.42948400	-2.29768600	2.25118400
C	2.77775600	-3.02004000	2.41304200
C	3.59575900	-3.35384200	1.33396100
C	3.16793200	-3.40017700	3.69724600
C	4.77131100	-4.06992900	1.53917000
H	3.33058500	-3.05209400	0.32475800
C	4.34192300	-4.12218800	3.88725500
H	2.55646500	-3.10725800	4.54390300
C	5.15468800	-4.46728200	2.81448700
C	1.47133700	-1.36930100	1.03149500
C	1.04202500	-1.72888700	-0.24618700
C	2.03228400	-0.10379700	1.21479000

C	1. 19947500	-0. 85103200	-1. 31683800
H	0. 57200700	-2. 68701400	-0. 43725600
C	2. 18415700	0. 76244400	0. 13912400
H	2. 33703100	0. 19447000	2. 21273900
C	1. 78315000	0. 39541200	-1. 13987300
H	6. 07013900	-5. 02663400	2. 96941800
H	1. 90747700	1. 07432200	-1. 97592100
H	0. 48127300	-0. 91407600	3. 31339200
C	4. 69379100	-4. 56870100	5. 27929800
C	5. 66198300	-4. 36437300	0. 36448000
C	2. 74516600	2. 13534200	0. 38483500
C	0. 80113700	-1. 28105500	-2. 69854200
F	1. 82540400	-1. 82705500	-3. 36699300
F	0. 36485000	-0. 24429500	-3. 43283300
F	-0. 18220400	-2. 19850900	-2. 67326800
F	3. 82550900	2. 09446800	1. 17255600
F	1. 84722000	2. 92874900	0. 99376300
F	3. 09082000	2. 74321100	-0. 75930800
F	4. 49989500	-3. 59054900	6. 17250000
F	3. 92848000	-5. 60378700	5. 66217500
F	5. 97047000	-4. 96183500	5. 37171400
F	6. 43083700	-5. 43918500	0. 58370600
F	6. 48062500	-3. 33792900	0. 09703400
F	4. 94590000	-4. 59447400	-0. 74678900
C	-3. 10481600	-1. 36663800	-1. 80375600
C	-2. 95278400	-0. 14825600	-2. 71639100
C	-3. 40004000	-2. 62454000	-2. 63268300
H	-2. 14774600	-1. 51108800	-1. 28675300
H	-2. 83863900	0. 77182500	-2. 13551500
H	-2. 06812600	-0. 26770200	-3. 34636300
H	-3. 81531800	-0. 03264300	-3. 38088300
H	-3. 46451000	-3. 51055500	-1. 99754300
H	-4. 35212000	-2. 50817600	-3. 16170900
H	-2. 61132800	-2. 77666300	-3. 37470100
C	-1. 29087200	1. 71624300	0. 75306700
C	-2. 08825100	0. 78101100	1. 26897900
H	-0. 28819900	1. 81176200	1. 16753400
C	-1. 63520700	-0. 05016700	2. 42878200
H	-3. 11510100	0. 66949600	0. 92816800
C	-1. 68666800	2. 67104900	-0. 33133600
C	-0. 73111900	2. 63701600	-1. 52880900
H	-1. 69389300	3. 69304200	0. 07313500
H	-2. 71292800	2. 45937900	-0. 66046300
C	-1. 18318000	3. 56166000	-2. 65435200

H	0.27188400	2.92159300	-1.18589500
H	-0.65322200	1.60876100	-1.90235900
H	-0.48351100	3.54456600	-3.49379900
H	-2.16612400	3.25932700	-3.03117500
H	-1.26478500	4.59516100	-2.30337900
H	-2.45585000	-0.33592100	3.11188200
O	-0.48007500	0.12542700	2.88758000

**si-TS1**

O	-1.05953700	1.30728000	1.16895500
N	2.85031300	1.09343700	-1.62488800
N	2.40410400	0.85313700	-2.91213500
N	0.77604500	1.11430200	-1.45461700
C	4.97051900	2.15401100	-2.05540500
H	4.45021500	2.75908700	-2.79064300
C	6.32170300	2.32883400	-1.79834000
H	6.88478400	3.08285700	-2.33741400
C	6.93901800	1.53762800	-0.83153100
H	7.99217400	1.67382400	-0.60817000
C	6.21173600	0.56415600	-0.15919900
H	6.71107300	-0.05934200	0.57711900
C	4.85229700	0.34196900	-0.41478100
C	4.25251300	1.18349000	-1.35840300
C	1.88935000	1.26608100	-0.69960700
C	1.11714100	0.87120400	-2.75892800
C	-0.09923700	0.72192000	-3.61167100
H	-0.02358900	-0.11480800	-4.30724800
H	-0.25659600	1.63311400	-4.19650100
C	-1.21051500	0.52555500	-2.54581500
H	-1.44058700	-0.53693100	-2.44033700
H	-2.14407800	1.01749700	-2.82152000
C	-0.66463000	1.09804600	-1.20371800
H	-1.00388800	2.13007500	-1.05849900
C	-1.07925100	0.37404600	0.12903300
C	-2.55198100	-0.02974800	-0.02748400
C	-2.96039000	-1.30465200	-0.40664200
C	-3.52212800	0.95635100	0.17617400
C	-4.31392200	-1.58259200	-0.59474100
H	-2.23436900	-2.10081100	-0.54592100
C	-4.86629600	0.66686100	-0.01747100
H	-3.21383200	1.94425000	0.50003700
C	-5.27848600	-0.60426900	-0.40851900
C	-0.19718200	-0.83376900	0.46152900
C	0.36505800	-1.66166000	-0.50699300

C	0.04703500	-1.12516300	1.80788400
C	1.15607600	-2.75020400	-0.14209100
H	0.22844500	-1.46653400	-1.56598600
C	0.82462700	-2.21976900	2.15897100
H	-0.35849800	-0.47714600	2.57595400
C	1.39021700	-3.04604900	1.19060000
H	-6.32849800	-0.82511800	-0.56165700
H	2.01390000	-3.88782200	1.47180400
H	-0.13267400	1.47164500	1.51714400
C	-5.89546000	1.73070500	0.24840200
C	-4.70028600	-2.96445800	-1.04276300
C	1.05034100	-2.55304000	3.60828600
C	1.78330900	-3.55209900	-1.24532500
F	2.58051000	-4.52028400	-0.77978100
F	2.52043500	-2.76235900	-2.04560800
F	0.85542200	-4.12765400	-2.02440300
F	0.83886000	-1.50395900	4.40533400
F	2.30724500	-2.98163100	3.81548200
F	0.23556100	-3.53948300	4.01227500
F	-5.42018300	2.95283100	-0.03053900
F	-6.99776000	1.54394900	-0.49095500
F	-6.27710700	1.73909500	1.53226800
F	-4.31705100	-3.18583300	-2.31051800
F	-6.02257400	-3.16064900	-0.98245900
F	-4.10988000	-3.90276500	-0.29053100
C	4.13344000	-0.81098300	0.26767500
C	3.98139600	-0.59147800	1.77903100
C	4.86379800	-2.13028300	-0.01663000
H	3.13264000	-0.89205800	-0.16529700
H	3.23333700	0.17200700	2.01179500
H	3.66113700	-1.52026400	2.26035000
H	4.93704800	-0.30109600	2.22904700
H	5.01456400	-2.28179500	-1.08824800
H	5.84027600	-2.15959900	0.47744600
H	4.27613000	-2.97011000	0.36690300
C	0.36179400	4.17077000	0.99399500
C	1.49434300	3.57781600	0.61032900
H	-0.20920900	3.70934500	1.79969700
C	1.99205900	2.33326200	1.26160900
H	2.12399400	4.00460300	-0.16954300
C	-0.17449400	5.44866200	0.42659500
C	-0.30897100	6.54658200	1.48930500
H	-1.16729600	5.26301900	-0.00794500
H	0.47009500	5.79842300	-0.38903200

C	-0.88179700	7.83763300	0.91255900
H	-0.94929200	6.18256300	2.30140600
H	0.67577000	6.73437300	1.93147800
H	-0.97678900	8.61034700	1.67920900
H	-0.23829400	8.22947600	0.11869500
H	-1.87381400	7.66729000	0.48259700
H	3.08620700	2.20024900	1.23077200
O	1.32309800	1.70144100	2.09522100

**re-M1**

O	1.35437800	-1.27542600	3.48728600
N	-2.87598000	-2.22572000	1.00014800
N	-2.72052400	-3.54280700	0.66719200
N	-0.95035700	-2.73928800	1.72994300
C	-5.07673400	-1.41310900	1.60068800
H	-4.89439100	-1.78276000	2.60468400
C	-6.26957500	-0.78349300	1.26619800
H	-7.04162500	-0.64929300	2.01530900
C	-6.45872700	-0.33198700	-0.03670100
H	-7.38673700	0.16013100	-0.30898200
C	-5.46274900	-0.49782000	-0.99530100
H	-5.62602500	-0.12605900	-2.00187300
C	-4.24833700	-1.11506500	-0.68783500
C	-4.09797900	-1.56665200	0.62673400
C	-1.81677100	-1.70708100	1.64438200
C	-1.54518800	-3.82436800	1.12997500
C	-0.71073000	-5.05359800	1.22618700
H	-0.69177100	-5.61703300	0.29293900
H	-1.11172900	-5.70408200	2.00987300
C	0.65391100	-4.45668400	1.61747100
H	1.23623100	-5.11292400	2.26438700
H	1.25350100	-4.27979400	0.72146800
C	0.36340900	-3.11634400	2.33840000
H	0.16871400	-3.29658500	3.40024100
C	1.50400100	-2.04263600	2.35175000
C	2.82613700	-2.81643700	2.50322300
C	3.60297400	-3.22997200	1.42102700
C	3.24022300	-3.14406900	3.79484200
C	4.75844800	-3.97672500	1.63163400
H	3.32967300	-2.95730800	0.40582700
C	4.39691800	-3.89121700	3.99119000
H	2.65560600	-2.79010100	4.63695600
C	5.16582000	-4.31882000	2.91513200
C	1.54348600	-1.17592900	1.08448700

C	1. 09901300	-1. 58080200	-0. 17213300
C	2. 10775300	0. 09493700	1. 21493900
C	1. 23646100	-0. 73908200	-1. 27619900
H	0. 62927100	-2. 54675300	-0. 32552200
C	2. 24399100	0. 92097400	0. 10873200
H	2. 41079400	0. 42552400	2. 20331700
C	1. 82181000	0. 51144800	-1. 15266700
H	6. 06951200	-4. 89697100	3. 07347600
H	1. 92791500	1. 16295100	-2. 01246300
H	0. 44836100	-0. 73068100	3. 30795200
C	4. 84973300	-4. 18771400	5. 39415400
C	5. 54481100	-4. 47323400	0. 45101900
C	2. 78906300	2. 30735100	0. 30786200
C	0. 80441000	-1. 22558100	-2. 62767300
F	1. 77683300	-1. 89957700	-3. 25618600
F	0. 44168500	-0. 21434100	-3. 43174600
F	-0. 24759100	-2. 06462800	-2. 53962300
F	3. 88044900	2. 30530300	1. 08159600
F	1. 88559300	3. 10147100	0. 90734300
F	3. 11118100	2. 88981600	-0. 85675400
F	3. 80823600	-4. 39066500	6. 21312500
F	5. 62393700	-5. 28187800	5. 44093000
F	5. 56259700	-3. 17597600	5. 90568600
F	5. 10923900	-5. 67936800	0. 04882300
F	6. 84522200	-4. 60394500	0. 74236500
F	5. 43812800	-3. 64903300	-0. 59921600
C	-3. 14496700	-1. 27800700	-1. 71438400
C	-2. 98767100	-0. 04425300	-2. 60554800
C	-3. 38518500	-2. 53848000	-2. 55580100
H	-2. 19968000	-1. 40209200	-1. 17259100
H	-2. 89450900	0. 86678500	-2. 00649100
H	-2. 08613700	-0. 14619000	-3. 21503200
H	-3. 83556500	0. 07352100	-3. 28803000
H	-3. 44384900	-3. 42857000	-1. 92414000
H	-4. 32588800	-2. 44807300	-3. 10939100
H	-2. 57322300	-2. 66904400	-3. 27575100
C	-1. 21637200	1. 68504200	0. 73173000
C	-2. 06429300	0. 72953800	1. 10158200
H	-0. 23916200	1. 70792400	1. 21037700
C	-1. 71110300	-0. 26179900	2. 21632400
H	-3. 07287800	0. 71183200	0. 69349000
C	-1. 55422900	2. 76040300	-0. 25987600
C	-0. 64021900	2. 77425100	-1. 48969000
H	-1. 48158000	3. 74063600	0. 23145300



H	-2.59951300	2.65173700	-0.58051800
C	-1.09261700	3.79550500	-2.52867200
H	0.38348900	2.99850800	-1.16794800
H	-0.61628800	1.77231800	-1.93647000
H	-0.42100600	3.81876500	-3.39068400
H	-2.09807600	3.55818500	-2.89265400
H	-1.12459300	4.80182300	-2.09912100
H	-2.58819700	-0.25213800	2.91472000
O	-0.54290000	-0.00334500	2.79294600

**si-M1**

O	-0.86073900	1.32245500	0.93045800
N	2.89794800	0.94589500	-1.65236000
N	2.52759400	0.17995000	-2.72166100
N	0.77797000	0.95060400	-1.61264300
C	5.04534500	1.82114500	-2.30617200
H	4.55998200	2.17656300	-3.20916800
C	6.39621000	2.03129200	-2.07902200
H	6.99418100	2.56518200	-2.80899800
C	6.96942800	1.55416800	-0.90106600
H	8.02416900	1.71843100	-0.70634700
C	6.19955500	0.86344100	0.02468600
H	6.66554700	0.48855600	0.93098800
C	4.83411200	0.62023400	-0.17564400
C	4.29125400	1.13454400	-1.35692500
C	1.85437000	1.43843600	-0.97611700
C	1.22883200	0.20640200	-2.66678400
C	0.11144600	-0.34821000	-3.47960200
H	0.19105800	-1.43523700	-3.55418400
H	0.14669000	0.05239700	-4.49495100
C	-1.14406500	0.13844300	-2.69892600
H	-1.80442800	-0.69249300	-2.44910900
H	-1.72831000	0.82143600	-3.31709500
C	-0.68401000	0.88407900	-1.40626500
H	-1.06946500	1.90527200	-1.36586700
C	-1.04274700	0.31859900	0.04216100
C	-2.54148200	-0.05275100	-0.00726600
C	-3.03838100	-1.31338200	-0.31847200
C	-3.44891900	0.97627000	0.27064700
C	-4.41629100	-1.53558400	-0.38160100
H	-2.36728800	-2.14932600	-0.49889100
C	-4.81376600	0.74522400	0.20085200
H	-3.05215300	1.94108900	0.56589800
C	-5.31535700	-0.51371900	-0.13079500

C	-0.17785700	-0.90756900	0.39864200
C	0.21050900	-1.88590000	-0.51323900
C	0.27585600	-1.01614700	1.71625300
C	1.05909800	-2.92472000	-0.13721800
H	-0.13320800	-1.85737100	-1.53987900
C	1.08726600	-2.07910600	2.09516200
H	-0.00385300	-0.24206500	2.42195900
C	1.49705200	-3.03971900	1.17349200
H	-6.38403300	-0.69230300	-0.18062500
H	2.16284500	-3.84459800	1.46745200
H	0.41275100	1.60086700	1.20285200
C	-5.79966400	1.84467500	0.47946900
C	-4.89149400	-2.90924500	-0.75882100
C	1.51710000	-2.22831400	3.52823400
C	1.48849600	-3.93104400	-1.16515200
F	2.72807500	-4.37886700	-0.92586700
F	1.48207300	-3.39773800	-2.40204900
F	0.68044800	-4.99874400	-1.19804600
F	1.47355900	-1.06832300	4.19136400
F	2.77856200	-2.69468700	3.61323300
F	0.74169700	-3.09921900	4.18805200
F	-5.19932200	2.99694800	0.79729700
F	-6.57887600	2.07638100	-0.59051900
F	-6.62166800	1.52136800	1.48873900
F	-4.51994800	-3.21936100	-2.01337000
F	-6.22342500	-3.02076000	-0.69542400
F	-4.36334100	-3.84818500	0.03892100
C	4.05574900	-0.19826000	0.84202000
C	4.12401200	0.42471500	2.24035500
C	4.58327400	-1.64021500	0.85676500
H	2.99589100	-0.22748900	0.56139000
H	3.72094300	1.43916500	2.24478000
H	3.51813700	-0.16648300	2.93155900
H	5.15138800	0.43619500	2.61939100
H	4.40226200	-2.14667100	-0.09598700
H	5.65975100	-1.66055900	1.05540900
H	4.08781500	-2.20282300	1.65110600
C	0.16234600	4.19711700	0.39347000
C	1.20312800	3.68254500	-0.25558500
H	-0.19898700	3.67640600	1.27811900
C	1.91837900	2.41835600	0.19285800
H	1.60355200	4.17068800	-1.14604600
C	-0.53866400	5.46449800	0.00610800
C	-0.43261000	6.54203700	1.09200300

H	-1.60213300	5.25072700	-0.17026100
H	-0.13022000	5.85088800	-0.93623400
C	-1.18567900	7.81475100	0.71702700
H	-0.82288700	6.14047100	2.03443800
H	0.62587200	6.76599200	1.26626700
H	-1.09387900	8.57758100	1.49407400
H	-0.79839500	8.23728100	-0.21559900
H	-2.25081200	7.60959500	0.57114000
H	2.99124900	2.65137100	0.29136700
O	1.46697900	1.84058200	1.34998300

**TS2**

O	-1.34216000	1.35255300	1.50914500
N	2.34290700	0.77440900	-1.62874200
N	1.68687300	0.31121300	-2.74974300
N	0.28291400	1.26145800	-1.32537900
C	4.50627600	1.86732700	-1.57696700
H	3.99007100	2.82104400	-1.61421200
C	5.89248400	1.81032100	-1.53177100
H	6.46869300	2.72883300	-1.52558800
C	6.52912000	0.57282100	-1.50947000
H	7.61260400	0.51767900	-1.48375700
C	5.78087100	-0.59798300	-1.52529600
H	6.29462000	-1.55432700	-1.52049500
C	4.38243600	-0.57929000	-1.54675400
C	3.77475900	0.68102900	-1.57241700
C	1.50471300	1.36542500	-0.74071400
C	0.45427000	0.62216200	-2.52878500
C	-0.83305000	0.45230800	-3.25436800
H	-1.01507600	-0.60304700	-3.46985400
H	-0.81216200	0.98284100	-4.20824100
C	-1.85807000	1.07181000	-2.26495100
H	-2.27236000	1.99026800	-2.68295700
H	-2.69696100	0.39888200	-2.08802000
C	-1.12489800	1.42519700	-0.92891000
H	-1.29464700	2.47129600	-0.66442200
C	-1.52224700	0.57995800	0.36447900
C	-3.03239500	0.30919200	0.32207400
C	-3.61255300	-0.94578600	0.18771100
C	-3.87023800	1.42631700	0.44216100
C	-5.00291000	-1.07823100	0.14121500
H	-3.00365500	-1.84147000	0.12793000
C	-5.24692200	1.28291400	0.38599800
H	-3.43298200	2.40714000	0.59709300

C	-5.83155600	0.02612300	0.22943400
C	-0.67920700	-0.69465000	0.42646600
C	-0.65806800	-1.60537900	-0.63069000
C	0.14950400	-0.92599900	1.52337100
C	0.15550000	-2.73089500	-0.58399300
H	-1.28649700	-1.45112600	-1.50419700
C	0.94927500	-2.06696100	1.56592900
H	0.16208500	-0.21157000	2.34013100
C	0.95172900	-2.98584200	0.52535800
H	-6.90896200	-0.08318300	0.17864900
H	1.57492700	-3.87013500	0.56983500
H	-0.50210100	1.88663100	1.42235300
C	-6.13836200	2.48278300	0.55284100
C	-5.57517200	-2.46202000	0.00666200
C	1.86592700	-2.27294200	2.74047100
C	0.18418900	-3.63450500	-1.78238900
F	-0.96446100	-4.30309500	-1.93978400
F	1.17376500	-4.53494500	-1.70632100
F	0.37533800	-2.91871400	-2.90631700
F	2.32518300	-3.52969600	2.79932000
F	1.25200600	-2.00511100	3.89933100
F	2.93830300	-1.46409400	2.66788400
F	-5.51314300	3.61713300	0.21351200
F	-7.23830300	2.37825600	-0.20711800
F	-6.54793700	2.61579600	1.82111900
F	-5.03293100	-3.10856300	-1.03720500
F	-6.90120000	-2.44146200	-0.17187800
F	-5.32199800	-3.20150700	1.09456100
C	3.59318900	-1.87456000	-1.59526900
C	4.08824300	-2.89237500	-0.56390300
C	3.63648500	-2.46210600	-3.01211000
H	2.54729200	-1.64390900	-1.36255100
H	4.01332200	-2.50142700	0.45548700
H	3.49018700	-3.80512300	-0.63704800
H	5.12863200	-3.17803600	-0.74428100
H	3.22698100	-1.75292400	-3.73487100
H	4.66876200	-2.69397000	-3.29547000
H	3.05198700	-3.38474900	-3.05760900
C	2.80151400	1.91827800	2.69702500
C	2.78388100	1.57415800	1.40737600
H	2.08786900	2.66270800	3.04775200
C	1.85109500	2.16096500	0.41754700
H	3.48929300	0.83074500	1.03901000
C	3.73842500	1.33171800	3.71117700

C	3.00588700	0.78950400	4.94270000
H	4.45609500	2.09590500	4.04340300
H	4.32619200	0.52960800	3.24887000
C	3.94526200	0.06252200	5.89890600
H	2.50979100	1.62051900	5.45886700
H	2.21318300	0.10845000	4.61787600
H	3.42225000	-0.27993500	6.79547600
H	4.38446400	-0.81342900	5.41045600
H	4.76649700	0.71377200	6.21572100
H	2.37944100	3.27612200	-0.23563300
O	0.71797200	2.75712500	1.00993300
C	1.48097300	4.86609400	-1.22256100
O	2.58927500	4.32858800	-0.84671000
O	0.35681900	4.49497200	-0.83923500
H	0.47703900	3.53474300	0.41894000
C	1.61585700	6.02143400	-2.18486200
H	0.63420600	6.36556300	-2.50553500
H	2.15021900	6.83419400	-1.68725300
H	2.21569900	5.71496700	-3.04411100

**TS2<sup>D</sup>**

O	0.96603400	-1.89513600	0.82277700
N	-2.58518400	-1.09824600	-2.10161700
N	-2.02812600	-0.35147100	-3.12063100
N	-0.47839700	-1.43344400	-1.96355800
C	-4.67275100	-2.18376200	-2.64365400
H	-4.10190300	-2.85739700	-3.27443800
C	-6.05038300	-2.30300700	-2.51394100
H	-6.58302200	-3.08121900	-3.04909300
C	-6.73352200	-1.41608100	-1.68696800
H	-7.80976400	-1.50000800	-1.57490400
C	-6.04732800	-0.42307000	-0.99399900
H	-6.60127500	0.25219000	-0.35017500
C	-4.66162900	-0.28014200	-1.10475200
C	-4.00425300	-1.18116800	-1.94901400
C	-1.65664000	-1.78533600	-1.38763600
C	-0.76270000	-0.58311900	-3.00341100
C	0.48203900	-0.15285000	-3.70099700
H	0.52527700	0.93500000	-3.79235700
H	0.51572700	-0.56588500	-4.71154300
C	1.60094900	-0.74829100	-2.79516500
H	2.19890400	-1.46618700	-3.35786600
H	2.28816500	0.02682700	-2.45625300
C	0.93395200	-1.48245100	-1.58386600

H	1. 24884300	-2. 52691400	-1. 53023800
C	1. 21498400	-0. 91623200	-0. 12653000
C	2. 72529300	-0. 62151800	-0. 04658600
C	3. 28960600	0. 64752500	-0. 16066800
C	3. 57300200	-1. 71678500	0. 13560500
C	4. 67340200	0. 80877400	-0. 11397100
H	2. 66505400	1. 52936900	-0. 26751100
C	4. 95075200	-1. 54356300	0. 17626900
H	3. 13863400	-2. 70140000	0. 27239700
C	5. 51817900	-0. 27975000	0. 04978000
C	0. 38949900	0. 33530800	0. 20001200
C	0. 17645000	1. 36506400	-0. 71134400
C	-0. 10090900	0. 48709400	1. 50306200
C	-0. 51013100	2. 52024900	-0. 34192400
H	0. 56953700	1. 30871900	-1. 71941800
C	-0. 74457500	1. 66203300	1. 87497000
H	0. 05715700	-0. 31588900	2. 21431500
C	-0. 96561400	2. 68779900	0. 95590000
H	6. 59307900	-0. 14548100	0. 08781900
H	-1. 46480700	3. 60446100	1. 25411500
H	0. 31595100	-2. 61640300	0. 48509200
C	5. 82857300	-2. 73919300	0. 42469400
C	5. 24800600	2. 18553000	-0. 29965400
C	-1. 16527600	1. 90011100	3. 30191300
C	-0. 64926600	3. 61142000	-1. 36469700
F	0. 50684400	4. 26945100	-1. 53496400
F	-1. 57677000	4. 51270800	-1. 02002900
F	-0. 98624800	3. 11082000	-2. 56582400
F	-0. 74794000	3. 10459500	3. 72028000
F	-0. 66942500	0. 98326700	4. 13755600
F	-2. 50333500	1. 89312500	3. 44492200
F	5. 35936300	-3. 82720600	-0. 20191700
F	7. 08184100	-2. 53094900	-0. 00277700
F	5. 89825900	-3. 03524900	1. 72926200
F	5. 31031100	2. 51495400	-1. 59998100
F	6. 48976800	2. 27811700	0. 19224100
F	4. 49553100	3. 11633400	0. 30225000
C	-3. 90473100	0. 81855900	-0. 38178800
C	-4. 48953000	1. 13960800	0. 99330700
C	-3. 86236700	2. 06947200	-1. 27002000
H	-2. 87136900	0. 47530600	-0. 22618900
H	-4. 58061500	0. 24068600	1. 61285800
H	-3. 83463500	1. 84049500	1. 51504600
H	-5. 47611900	1. 60733300	0. 91474000

H	-3.32861600	1.87244600	-2.20404500
H	-4.88057800	2.38970500	-1.51559800
H	-3.36631600	2.89307100	-0.74964300
C	-2.46023500	-2.94804300	2.00122000
C	-2.72380700	-2.52139300	0.76379300
H	-1.55561000	-3.52871100	2.17044200
C	-1.83426600	-2.77442900	-0.37745300
H	-3.62187100	-1.93408600	0.57597400
C	-3.28227000	-2.53538600	3.18759600
C	-2.64882100	-1.31710500	3.87050200
H	-3.37650400	-3.35540700	3.91024600
H	-4.29954000	-2.27507500	2.86576500
C	-3.45062900	-0.79164900	5.05470300
H	-1.62881800	-1.56929600	4.18612200
H	-2.54979000	-0.53130400	3.11231500
H	-2.96286700	0.07669100	5.50422500
H	-4.45424700	-0.48701100	4.73941600
H	-3.56284000	-1.55796500	5.82824300
H	-1.59662400	-3.89213500	-0.81181100
O	-0.61963100	-3.53454300	-0.12006600

#### TS2<sup>w</sup>

O	0.96848100	-1.72120100	1.03987300
N	-2.59834300	-1.12697000	-1.93243100
N	-2.03706500	-0.47550300	-3.00655800
N	-0.50686600	-1.45896800	-1.74638100
C	-4.71028000	-2.26205300	-2.22507500
H	-4.16073600	-3.06340400	-2.70991000
C	-6.08752600	-2.32209700	-2.05127900
H	-6.64435600	-3.17898000	-2.41375000
C	-6.73956000	-1.27470100	-1.40623700
H	-7.81538900	-1.31086400	-1.26827900
C	-6.02301000	-0.18452500	-0.92108600
H	-6.55105200	0.61107100	-0.40575400
C	-4.63629400	-0.09953000	-1.06946600
C	-4.01750800	-1.15500300	-1.74785500
C	-1.68844500	-1.74522600	-1.15507000
C	-0.77274400	-0.70889500	-2.86382800
C	0.47402400	-0.38276800	-3.61119300
H	0.55698400	0.69184800	-3.78990800
H	0.47073900	-0.87541700	-4.58583900
C	1.58416800	-0.95244500	-2.67936200
H	2.12225700	-1.75425900	-3.18589700
H	2.32357900	-0.19156900	-2.43039700

C	0.91507600	-1.53486800	-1.38999900
H	1.18613900	-2.58286100	-1.24828400
C	1.23968500	-0.84224000	-0.00181300
C	2.75977100	-0.59030600	0.03917700
C	3.36084100	0.63309200	-0.24073800
C	3.57725900	-1.68123100	0.35360900
C	4.75088000	0.75476900	-0.23171500
H	2.76426400	1.51253200	-0.46515600
C	4.95848200	-1.54724000	0.35932400
H	3.11580800	-2.62742200	0.61333400
C	5.56326000	-0.32829000	0.06163000
C	0.46046100	0.46508500	0.20373700
C	0.28724700	1.40313900	-0.80932900
C	-0.02965700	0.76733100	1.48040700
C	-0.36490900	2.61039100	-0.56968900
H	0.68988500	1.23459200	-1.80064800
C	-0.64149000	1.99331800	1.72062400
H	0.10040100	0.03973100	2.27382700
C	-0.82641600	2.92445700	0.69773900
H	6.64247000	-0.22804300	0.05883400
H	-1.30026200	3.88125700	0.89306300
H	0.28585000	-2.42369900	0.77684600
C	5.81942200	-2.71818300	0.74727900
C	5.34190400	2.09418000	-0.57110400
C	-1.08084900	2.38901100	3.10647400
C	-0.46002400	3.58599500	-1.70735900
F	0.73187500	4.13921900	-1.97339700
F	-1.31899800	4.58015000	-1.45313100
F	-0.85858600	2.97324200	-2.83605800
F	-0.66752100	3.63145000	3.39633000
F	-0.59978600	1.57038000	4.04645400
F	-2.42095900	2.39723800	3.22539300
F	5.22909200	-3.88409600	0.45517000
F	7.00002900	-2.68683300	0.11227600
F	6.07948300	-2.72166200	2.06165600
F	4.97677200	2.47964300	-1.80514200
F	6.67893900	2.08045100	-0.53028500
F	4.91621000	3.04540800	0.27102100
C	-3.83703500	1.07504200	-0.53477500
C	-4.38222400	1.60387100	0.79246900
C	-3.77735500	2.18887000	-1.58801500
H	-2.81021000	0.72719000	-0.34954600
H	-4.47643500	0.80674700	1.53744100
H	-3.70234000	2.35774200	1.19500800



H	-5.36046000	2.07837200	0.66643500
H	-3.29542700	1.84138600	-2.50550900
H	-4.78965300	2.52581400	-1.83552200
H	-3.22008600	3.04816500	-1.20364500
C	-2.46775900	-2.51072300	2.33285900
C	-2.75239300	-2.23485400	1.06047200
H	-1.56962000	-3.08453300	2.55418600
C	-1.92972700	-2.70257100	-0.08469800
H	-3.64752600	-1.65958200	0.82354200
C	-3.26005900	-1.96384600	3.48468900
C	-2.57286500	-0.72003400	4.05726900
H	-3.37842600	-2.71763400	4.27328700
H	-4.26967900	-1.69237600	3.14922200
C	-3.33267300	-0.07260800	5.20833500
H	-1.55592400	-0.98180100	4.37570200
H	-2.46295900	-0.00190300	3.23736600
H	-2.80876800	0.81442300	5.57291200
H	-4.33349300	0.23586700	4.88838600
H	-3.44967100	-0.76850800	6.04503000
H	-2.37331100	-3.75771500	-0.72867700
O	-0.74227300	-3.37063100	0.25270500
O	-1.84467100	-4.94340700	-1.10504100
H	-0.98626900	-4.31431700	-0.30888300
H	-2.28171300	-5.64705800	-0.61254800

**M2**

O	-1.29703200	-2.16719500	-0.36996200
N	2.23177300	0.13719400	1.90917200
N	1.50978200	1.08001300	2.67004800
N	0.18954000	-0.64478100	2.13316500
C	4.01774800	-0.78795000	3.27428100
H	3.25255000	-1.31394700	3.83781600
C	5.36302400	-0.91651500	3.59425600
H	5.66889400	-1.54468600	4.42407200
C	6.31003900	-0.22728700	2.84174200
H	7.36478500	-0.31805800	3.08128100
C	5.91262100	0.57352300	1.77561900
H	6.66678500	1.09246200	1.19269300
C	4.56542400	0.71205800	1.42992500
C	3.62981800	0.02149600	2.20959800
C	1.43599200	-0.97404600	1.61528400
C	0.32855600	0.59248900	2.73561400
C	-0.98229900	1.08922500	3.24043000
H	-1.16186700	2.10711200	2.88798700

H	-0.99647700	1.11205500	4.33219400
C	-1.98292100	0.04752300	2.67018900
H	-2.78663700	0.52886900	2.11239000
H	-2.45661900	-0.50640600	3.48225800
C	-1.19161700	-0.95974000	1.76957200
H	-1.42244300	-1.99056700	2.05333300
C	-1.49063900	-0.90117500	0.20346900
C	-2.98745500	-0.63907600	-0.00697200
C	-3.52058500	0.49112700	-0.61640400
C	-3.86558600	-1.63128800	0.44728900
C	-4.90412100	0.64040600	-0.73591200
H	-2.87821900	1.27199800	-1.00760100
C	-5.23693900	-1.46708000	0.33397500
H	-3.46542500	-2.54154800	0.88039200
C	-5.77408800	-0.32448400	-0.25581700
C	-0.58847200	0.14576200	-0.44776500
C	-0.61452700	1.47712600	-0.03870800
C	0.34495300	-0.23761700	-1.41072700
C	0.26799800	2.40808300	-0.57826700
H	-1.33800200	1.81431400	0.69953400
C	1.22353000	0.70013200	-1.94407700
H	0.38840500	-1.27325300	-1.73060900
C	1.19340100	2.03210900	-1.54062800
H	-6.84768700	-0.19181000	-0.33287600
H	1.88009900	2.75741000	-1.96298700
H	-0.52694600	-2.61967300	0.03070900
C	-6.16880000	-2.54846400	0.80690800
C	-5.44476100	1.85508200	-1.43937100
C	2.27654800	0.23953100	-2.91338800
C	0.16757300	3.82363300	-0.08840400
F	1.11306400	4.61172000	-0.61140800
F	0.27708000	3.87892200	1.24946000
F	-1.02343400	4.35950600	-0.39738200
F	1.80203200	-0.68687800	-3.75666400
F	3.32519000	-0.31524800	-2.27722500
F	2.75858600	1.25380400	-3.64525000
F	-5.58779000	-3.33941600	1.71939800
F	-7.27350100	-2.02810000	1.36136400
F	-6.56899900	-3.33193900	-0.20316200
F	-6.70533600	2.11829100	-1.07076100
F	-5.44338500	1.69245400	-2.76943400
F	-4.70546700	2.94195600	-1.17587400
C	4.10598300	1.56842200	0.26812800
C	5.15415300	1.70981800	-0.83501500

C	3. 64873700	2. 94468300	0. 76994400
H	3. 23468100	1. 05970500	-0. 15989500
H	5. 55918900	0. 73907000	-1. 13497100
H	4. 70068800	2. 17048500	-1. 71809100
H	5. 98486600	2. 35095100	-0. 52156400
H	2. 81196400	2. 85590200	1. 46854300
H	4. 47385200	3. 44875000	1. 28481300
H	3. 34074600	3. 57812600	-0. 06763900
C	3. 11282600	-3. 31383000	-0. 74283200
C	2. 92880500	-2. 28561400	0. 10119700
H	2. 35047100	-4. 09016500	-0. 82201800
C	1. 77270300	-2. 10934500	0. 94572200
H	3. 68160900	-1. 50138300	0. 14463400
C	4. 29188300	-3. 44484200	-1. 66013100
C	3. 88307000	-3. 57603800	-3. 13171300
H	4. 89072900	-4. 32628900	-1. 38659800
H	4. 94724900	-2. 57289700	-1. 53867300
C	5. 08730200	-3. 72116200	-4. 05688900
H	3. 22178600	-4. 44480300	-3. 24339300
H	3. 29373900	-2. 69849000	-3. 41525300
H	4. 78130400	-3. 82153200	-5. 10136300
H	5. 74221400	-2. 84713500	-3. 98278900
H	5. 68044300	-4. 60292500	-3. 79369800
O	0. 78628100	-3. 10448600	0. 93570500
H	1. 20000700	-3. 95085900	1. 14646500

**TS3(RR)**

O	-0. 53873300	-0. 87786900	1. 31012000
N	2. 39205400	1. 82461300	-1. 86661300
N	1. 46096200	2. 01291400	-2. 86652400
N	0. 52330200	1. 12184900	-1. 05050900
C	4. 01343000	3. 57062700	-2. 21986100
H	3. 18253300	4. 26908600	-2. 19861500
C	5. 32417100	4. 00471500	-2. 37893900
H	5. 53910300	5. 06208400	-2. 48908500
C	6. 35105800	3. 06697400	-2. 38176700
H	7. 38115000	3. 39056500	-2. 49050900
C	6. 06795400	1. 70893000	-2. 25513400
H	6. 88646500	0. 99827500	-2. 27398000
C	4. 76017800	1. 23890500	-2. 11227500
C	3. 75117800	2. 21189900	-2. 07638300
C	1. 83666600	1. 35536900	-0. 71300900
C	0. 36559000	1. 57797700	-2. 34148300
C	-1. 06466600	1. 62610600	-2. 74160000

H	-1.33187300	0.76026100	-3.35193300
H	-1.27791600	2.52658000	-3.31825200
C	-1.75229800	1.62525200	-1.35596000
H	-2.70929900	1.10462800	-1.37081600
H	-1.95490800	2.65509900	-1.05200700
C	-0.76082200	0.99732100	-0.32041600
H	-0.68480800	1.61548700	0.57974700
C	-1.18042800	-0.45826600	0.13855400
C	-2.67954300	-0.44537700	0.49251700
C	-3.60786100	-1.37745000	0.04461300
C	-3.08185600	0.48121700	1.46687500
C	-4.92021300	-1.35248400	0.52347500
H	-3.32837200	-2.14935300	-0.66453400
C	-4.38249300	0.48548800	1.94464100
H	-2.36483200	1.18207700	1.89147700
C	-5.32456900	-0.42525500	1.46848100
C	-0.74669600	-1.42131100	-0.95621000
C	-1.42206300	-1.55145000	-2.16667000
C	0.47309200	-2.08481500	-0.79018200
C	-0.88895600	-2.32897100	-3.19357500
H	-2.36499100	-1.03787400	-2.33635500
C	0.98197400	-2.87113300	-1.81640300
H	1.01721600	-1.95074300	0.14015400
C	0.31371500	-3.00104400	-3.03047400
H	-6.34503300	-0.41319600	1.83316500
H	0.72873700	-3.59964800	-3.83306200
H	-0.54238300	-0.15817900	1.96606100
C	-4.75324400	1.43514600	3.05143400
C	-5.87952600	-2.38683200	0.00352500
C	2.26143500	-3.62373900	-1.57900400
C	-1.66274100	-2.42514300	-4.47686300
F	-2.06198700	-1.20427500	-4.88613000
F	-2.77169400	-3.16086900	-4.33050900
F	-0.94150700	-2.96666800	-5.46272200
F	2.05284800	-4.74898700	-0.88666500
F	3.14087400	-2.88830300	-0.88005700
F	2.85664300	-3.97223600	-2.73236600
F	-4.06176000	2.57831100	2.97485000
F	-6.05840400	1.74116300	3.01945700
F	-4.50277900	0.90025600	4.25620000
F	-5.88746600	-2.40674400	-1.33843300
F	-7.13323000	-2.16128100	0.41405000
F	-5.53484500	-3.61707600	0.40713900
C	4.42565900	-0.24241800	-2.06056000

C	5. 63579500	-1. 12665400	-1. 76536300
C	3. 76868300	-0. 66785100	-3. 38345300
H	3. 70179400	-0. 40091500	-1. 25238500
H	6. 14440500	-0. 82123000	-0. 84626100
H	5. 30511200	-2. 15987100	-1. 64535800
H	6. 35798000	-1. 10295700	-2. 58841100
H	2. 85936100	-0. 09717800	-3. 59230900
H	4. 46375700	-0. 51031000	-4. 21481300
H	3. 51322800	-1. 73031200	-3. 35292200
C	3. 77852400	2. 02373300	2. 39465000
C	3. 49568500	1. 95907800	1. 03925700
H	3. 32279600	1. 27083100	3. 03273400
C	2. 43877600	1. 18068200	0. 55189300
H	4. 00454800	2. 65266200	0. 37188300
C	5. 01826600	2. 69075400	2. 91129000
C	6. 23802600	1. 75808000	2. 87913800
H	4. 85799700	3. 03143200	3. 94345400
H	5. 23823100	3. 59017700	2. 31896000
C	7. 48420500	2. 41900200	3. 46116900
H	6. 00631400	0. 84053200	3. 43267400
H	6. 41906100	1. 45421600	1. 84069700
H	8. 34914300	1. 75169900	3. 42238000
H	7. 73594300	3. 33010400	2. 90912000
H	7. 32346200	2. 69992600	4. 50686900
O	1. 82563400	0. 28781000	1. 36673400
H	1. 18518000	0. 77273300	1. 96820700
C	-0. 21047200	2. 57775200	5. 82844400
C	1. 21375700	3. 10539400	3. 89652800
C	0. 17890500	2. 13133400	3. 69485100
N	-0. 60572200	1. 88989500	4. 80217900
O	-0. 02006200	1. 53297900	2. 59366400
S	1. 16897900	3. 63681200	5. 56365900
C	1. 98815800	3. 55344800	2. 82983400
H	1. 58759800	3. 21336100	1. 87773600
C	-0. 88020100	2. 51458000	7. 13357200
C	-2. 13637000	1. 89918200	7. 20970900
C	-0. 29767900	3. 04843700	8. 28735000
C	-2. 79557100	1. 82392300	8. 42915100
H	-2. 57703800	1. 49920100	6. 30275500
C	-0. 96261700	2. 96856400	9. 50463600
H	0. 68307000	3. 51384200	8. 23680100
C	-2. 21158600	2. 35625800	9. 57760800
H	-3. 77018600	1. 35029400	8. 48541200
H	-0. 50426500	3. 37996800	10. 39776800

H	-2. 72951700	2. 29378800	10. 52932300
C	2. 80658800	4. 76436700	2. 75488300
C	3. 40298000	5. 37774000	3. 86501300
C	3. 04701100	5. 31224500	1. 48346400
C	4. 20074600	6. 50636400	3. 70646100
H	3. 27209700	4. 95951300	4. 85762800
C	3. 84358900	6. 43645000	1. 32611700
H	2. 60168300	4. 83150100	0. 61532300
C	4. 42371400	7. 04122800	2. 44119800
H	4. 65642900	6. 96550100	4. 57776800
H	4. 01345400	6. 84379000	0. 33428500
H	5. 04825400	7. 92070800	2. 32312000

**TS3(RS)**

O	-1. 16987800	0. 56983100	-2. 09893200
N	1. 65054900	1. 04512700	1. 52622400
N	0. 72788200	0. 96412200	2. 55169900
N	-0. 06260900	0. 08407900	0. 67969600
C	3. 80338400	1. 05512400	2. 61515600
H	3. 50601500	0. 12408700	3. 08427700
C	5. 06196800	1. 60085200	2. 82562200
H	5. 76438500	1. 10741800	3. 48910600
C	5. 41050900	2. 77883200	2. 16809000
H	6. 39669700	3. 20960600	2. 30734200
C	4. 49047400	3. 41623500	1. 34566000
H	4. 76870700	4. 34739800	0. 86051700
C	3. 20518200	2. 90327200	1. 13105100
C	2. 90414600	1. 68931300	1. 75831800
C	1. 21922400	0. 44040400	0. 38256600
C	-0. 28187700	0. 37003200	2. 00388200
C	-1. 57749200	-0. 19947000	2. 47855700
H	-2. 30210200	0. 58834900	2. 69458600
H	-1. 42421200	-0. 77954500	3. 39269100
C	-1. 97468200	-1. 10256800	1. 27932200
H	-3. 04805100	-1. 11736900	1. 08818100
H	-1. 66095500	-2. 12712200	1. 48577200
C	-1. 17291900	-0. 63213300	0. 03630500
H	-0. 75645400	-1. 49303400	-0. 48869300
C	-1. 96070900	0. 25053500	-0. 99307700
C	-3. 13453600	-0. 59716000	-1. 52193600
C	-4. 43912000	-0. 12588400	-1. 62803400
C	-2. 84520200	-1. 87078400	-2. 03240200
C	-5. 43948100	-0. 92161300	-2. 18795300
H	-4. 69791200	0. 87637700	-1. 30531900

C	-3.84961000	-2.65518600	-2.58002700
H	-1.82794200	-2.25425500	-2.03498200
C	-5.16130100	-2.19278500	-2.65975000
C	-2.40072800	1.56495600	-0.33398500
C	-3.37978800	1.63960700	0.65563300
C	-1.76755100	2.74858800	-0.72433100
C	-3.68143300	2.85292300	1.27165700
H	-3.93272600	0.75609600	0.95979000
C	-2.09977400	3.95747600	-0.12627000
H	-1.03044500	2.70369800	-1.51722400
C	-3.04745900	4.02491900	0.89084100
H	-5.93821300	-2.80428700	-3.10436900
H	-3.29091900	4.96828200	1.36693700
H	1.22276900	-1.48974100	-1.79097900
C	-3.53606200	-4.04699200	-3.05716700
C	-6.84180900	-0.38231200	-2.23491000
C	-1.49327200	5.23727400	-0.62655800
C	-4.67848300	2.84221000	2.39421000
F	-4.18097500	2.19769300	3.46710600
F	-5.80145400	2.19937400	2.04874200
F	-5.01192200	4.07515400	2.78772400
F	-0.36577600	5.01919100	-1.32264000
F	-1.19060200	6.06709900	0.38455800
F	-2.33576600	5.89589100	-1.43167000
F	-2.26490500	-4.16530800	-3.45112900
F	-3.73760600	-4.94890400	-2.08345400
F	-4.32267700	-4.39922600	-4.08458300
F	-7.42594700	-0.44079400	-1.02786400
F	-7.61318000	-1.06953200	-3.08597700
F	-6.85986600	0.90379800	-2.61130200
C	2.22172700	3.67870400	0.27307300
C	2.71638100	3.80455700	-1.17279000
C	1.97289200	5.05937800	0.89585900
H	1.26612300	3.14100300	0.25968300
H	2.87729600	2.82131300	-1.62346100
H	1.98067900	4.34550100	-1.77271200
H	3.65831400	4.36179100	-1.21455600
H	1.57531800	4.96726300	1.91023800
H	2.90155100	5.63629800	0.94806800
H	1.26096000	5.62525900	0.29387000
C	3.98243100	-0.53168600	-1.92790700
C	3.31360200	0.19334700	-0.95516300
H	3.36924000	-0.97731500	-2.70911500
C	1.92863600	0.10137700	-0.80397100

H	3.90627400	0.70310300	-0.20014000
C	5.40880600	-0.23641500	-2.29489100
C	5.51143200	0.89720500	-3.32494500
H	5.88900400	-1.13462500	-2.70513300
H	5.98087000	0.03728500	-1.39893100
C	6.95492400	1.16138600	-3.74389900
H	4.90583700	0.64557300	-4.20363400
H	5.06958900	1.80485400	-2.89591500
H	7.02014100	1.97644100	-4.46922400
H	7.56856300	1.42981100	-2.87820800
H	7.39789500	0.26991100	-4.19881900
O	1.17643200	-0.43522600	-1.80891700
H	-0.26874900	0.16009300	-2.04348000
C	1.34750400	-2.71390900	1.96515600
C	3.00878700	-2.61028700	0.15986400
C	1.65007300	-2.81621000	-0.23799300
N	0.75677700	-2.91267900	0.82833200
O	1.25084000	-2.84275600	-1.43993300
S	3.07211800	-2.43189100	1.90120900
C	4.07419300	-2.52327100	-0.73546400
H	3.86793600	-2.99060300	-1.69598500
C	0.62738700	-2.72232500	3.24730000
C	-0.50733700	-3.53371700	3.37579300
C	1.01804900	-1.90519300	4.31267600
C	-1.24418700	-3.51906900	4.55293900
H	-0.78971600	-4.16784000	2.54118000
C	0.27622300	-1.89403700	5.49028500
H	1.87697100	-1.24891500	4.20739300
C	-0.85531800	-2.69692000	5.61137800
H	-2.12016400	-4.15234200	4.64835600
H	0.57586500	-1.24787600	6.30845200
H	-1.43400500	-2.68423600	6.52920700
C	5.48192300	-2.48544600	-0.30752000
C	5.91954000	-1.63873200	0.72166100
C	6.42820000	-3.28113700	-0.96443600
C	7.25725600	-1.61029700	1.09597600
H	5.21426500	-0.96019100	1.19614100
C	7.76616400	-3.25640100	-0.58507700
H	6.10405500	-3.92941200	-1.77396200
C	8.18545500	-2.42359700	0.44890800
H	7.57894300	-0.93966100	1.88692700
H	8.48323400	-3.88723200	-1.10058100
H	9.23000700	-2.40063300	0.74187700



**TS3(SR)**

O	2.28300000	1.83570300	-0.41116900
N	-0.81448100	-0.79165800	2.45281000
N	0.06154000	-1.57108700	3.16180800
N	1.12380200	-0.02630800	1.99446000
C	-3.15617200	-0.55989100	3.10878600
H	-2.88105600	0.31219400	3.69138700
C	-4.45961900	-1.03847600	3.11346900
H	-5.22851400	-0.51310800	3.66894400
C	-4.75756200	-2.20794000	2.41909100
H	-5.77171000	-2.59682800	2.40941000
C	-3.76418100	-2.87850800	1.71688000
H	-4.02245100	-3.78543600	1.18004500
C	-2.44880300	-2.41154200	1.66626100
C	-2.18423300	-1.23718600	2.38004000
C	-0.19413500	0.17368200	1.75424700
C	1.22155000	-1.07939900	2.86136300
C	2.62279700	-1.34462700	3.27942600
H	2.94650900	-2.32456400	2.91890300
H	2.70817300	-1.34892500	4.36721900
C	3.38989900	-0.16428700	2.62765700
H	4.27060600	-0.51297100	2.08960400
H	3.74549500	0.52321600	3.39663200
C	2.42152800	0.61007700	1.67145300
H	2.35685600	1.66348400	1.95628500
C	2.78988800	0.65791200	0.12514600
C	4.31559000	0.80841900	0.02294500
C	5.18018700	-0.19601600	-0.40358300
C	4.85407700	2.04302700	0.39592400
C	6.55672900	0.02689800	-0.43001600
H	4.80051900	-1.15880800	-0.72913600
C	6.22751500	2.24780200	0.37717100
H	4.18620200	2.85295600	0.67085900
C	7.09623000	1.24177700	-0.03328100
C	2.26422300	-0.58306100	-0.59769600
C	2.47509800	-1.86174600	-0.09024800
C	1.52386700	-0.44489600	-1.77358800
C	1.94774200	-2.97992600	-0.73184800
H	3.06322700	-2.01112100	0.81014100
C	0.99875300	-1.56422800	-2.40489800
H	1.34391500	0.54381300	-2.17808800
C	1.20603500	-2.84301600	-1.89520500
H	8.16730200	1.40607500	-0.05200400
H	0.78342800	-3.70972600	-2.39213800

H	1. 27363800	1. 78545300	-0. 35629600
C	6. 76729200	3. 56644600	0. 85872200
C	7. 45251600	-1. 06318000	-0. 95071800
C	0. 21152800	-1. 43330600	-3. 68256200
C	2. 23006600	-4. 33027500	-0. 14330800
F	1. 34822100	-5. 25398000	-0. 54905700
F	2. 18056200	-4. 28736200	1. 20396900
F	3. 45152700	-4. 77245000	-0. 46781600
F	-0. 07150700	-0. 16377300	-3. 97521800
F	-0. 92945400	-2. 12653300	-3. 62347500
F	0. 91428700	-1. 93631200	-4. 71498000
F	6. 01638800	4. 58849100	0. 43150900
F	6. 77604100	3. 62199900	2. 20075000
F	8. 02298700	3. 77390800	0. 44439800
F	7. 05753300	-2. 26798500	-0. 51168900
F	8. 72350100	-0. 88621800	-0. 56846700
F	7. 43814400	-1. 11060700	-2. 28899400
C	-1. 37584300	-3. 21600400	0. 95218900
C	-1. 78821700	-3. 64016300	-0. 46005200
C	-1. 02215200	-4. 44145400	1. 80918900
H	-0. 47468400	-2. 59550900	0. 85285500
H	-1. 95399500	-2. 77602100	-1. 10691500
H	-0. 99950400	-4. 26985100	-0. 88204400
H	-2. 70327900	-4. 24124200	-0. 44441400
H	-0. 67903500	-4. 14293400	2. 80285200
H	-1. 90357400	-5. 08083400	1. 92693400
H	-0. 23856700	-5. 02935500	1. 32639200
C	-2. 16935300	3. 24156900	0. 71398400
C	-1. 74177000	2. 05598100	1. 42232600
H	-1. 35103900	3. 79708300	0. 25195500
C	-0. 75321600	1. 26329600	0. 92476200
H	-2. 23154400	1. 78787100	2. 35224500
C	-3. 23327500	4. 08820500	1. 35902800
C	-2. 75198600	4. 77428900	2. 64503000
H	-4. 11052000	3. 46385100	1. 58683400
H	-3. 56968100	4. 85880000	0. 65618200
C	-3. 83391300	5. 65122800	3. 26899400
H	-2. 42388400	4. 01711500	3. 36830800
H	-1. 86738200	5. 37987800	2. 41339800
H	-3. 48137800	6. 13615400	4. 18310200
H	-4. 14916100	6. 43361400	2. 57196100
H	-4. 71867100	5. 05850000	3. 52205400
O	-0. 17560000	1. 42841800	-0. 23875100
H	-1. 07528300	0. 51777100	-1. 20806000

C	-4.96306500	-0.63838000	-0.65223200
C	-3.55897200	1.33529400	-1.05719200
C	-2.96318700	0.09309800	-1.22826900
N	-3.76804100	-0.99162500	-1.02605800
O	-1.70461400	-0.13647900	-1.63058400
S	-5.18772400	1.08175700	-0.50298900
C	-2.88715900	2.60645500	-1.21594900
H	-1.89333800	2.45141200	-1.63041400
C	-6.05147400	-1.59155000	-0.40531200
C	-5.88111700	-2.92528400	-0.79604800
C	-7.23020900	-1.21419000	0.24490000
C	-6.86527900	-3.86525600	-0.51936900
H	-4.96239600	-3.19923200	-1.30551800
C	-8.21628400	-2.15717400	0.51441000
H	-7.37010500	-0.18352300	0.56078400
C	-8.03474900	-3.48664500	0.14007100
H	-6.72404400	-4.89759400	-0.82394000
H	-9.12568500	-1.85428900	1.02346500
H	-8.80304800	-4.22276800	0.35333000
C	-3.50248300	3.85210300	-1.71685400
C	-4.87066700	4.15053900	-1.66899600
C	-2.63695600	4.83991400	-2.21762100
C	-5.34860000	5.38463700	-2.10241900
H	-5.58198600	3.42187200	-1.29889500
C	-3.11250100	6.07122100	-2.64579700
H	-1.57219400	4.62525600	-2.26760700
C	-4.47669600	6.35224600	-2.59000000
H	-6.41428300	5.58695400	-2.05796600
H	-2.41802600	6.81127300	-3.03114600
H	-4.85405300	7.31189700	-2.92757200

### TS3(SS)

O	1.93581600	0.04451000	2.03502300
N	-0.73604000	-3.83523400	0.10003600
N	0.29070600	-4.65020800	-0.33845300
N	1.07821000	-2.69468100	0.38986800
C	-2.85926200	-4.94834200	0.49607100
H	-2.48340100	-5.21891400	1.47784000
C	-4.10870500	-5.36857200	0.06120700
H	-4.73571800	-5.97310500	0.70750300
C	-4.53732600	-5.01622500	-1.21785700
H	-5.50788300	-5.34497300	-1.57624700
C	-3.72563000	-4.24666200	-2.04148700
H	-4.07598400	-3.97993400	-3.03431000

C	-2.45641800	-3.81498600	-1.63366100
C	-2.05746900	-4.17534400	-0.34208600
C	-0.28505800	-2.63399900	0.58138800
C	1.34671100	-3.94330900	-0.13456000
C	2.80781000	-4.21927800	-0.21217000
H	3.10702300	-4.61887200	-1.18185400
H	3.07467500	-4.95325500	0.55414400
C	3.40203000	-2.83390000	0.09151600
H	3.62547500	-2.30694800	-0.83949700
H	4.33139600	-2.88891700	0.65799900
C	2.32614700	-2.05182500	0.89195900
H	2.40373600	-2.29857200	1.95827100
C	2.48739000	-0.49270600	0.86462300
C	3.99737000	-0.22397900	0.98499000
C	4.81067500	0.01903600	-0.12057400
C	4.57549100	-0.25355500	2.25467800
C	6.17972300	0.20881900	0.04408000
H	4.38238100	0.08718400	-1.11661000
C	5.94542600	-0.06472200	2.40454500
H	3.94168000	-0.39396200	3.12386500
C	6.76264900	0.16503300	1.30418300
C	1.93295000	0.20618400	-0.37839800
C	1.68987900	-0.42727300	-1.59473000
C	1.72961600	1.58566100	-0.28729600
C	1.26016100	0.31217600	-2.69529100
H	1.82279300	-1.49633000	-1.71534000
C	1.28866700	2.30592900	-1.38749700
H	1.90563800	2.08330100	0.66088300
C	1.05011000	1.67941900	-2.60472000
H	7.82682100	0.32818400	1.42924500
H	0.69682000	2.24559600	-3.45950800
H	0.95692000	-0.02776400	1.92673700
C	6.53991600	-0.15689900	3.78280100
C	7.03352400	0.42162300	-1.17499600
C	1.15187800	3.79941700	-1.29315900
C	1.11998200	-0.36550100	-4.02634700
F	0.12108100	0.14871200	-4.75525700
F	0.88585500	-1.68583800	-3.89138500
F	2.23768300	-0.24763300	-4.75820000
F	0.82865900	4.20252600	-0.05977600
F	0.22880300	4.27114900	-2.14171200
F	2.31278600	4.40308900	-1.60850600
F	5.77058800	0.45474500	4.69131300
F	6.66205600	-1.43645400	4.17156000

F	7.75974800	0.39278600	3.83784500
F	7.29849800	-0.74229500	-1.79061800
F	8.20830500	0.98433700	-0.86790300
F	6.42233400	1.20546700	-2.07209900
C	-1.57390700	-3.04023200	-2.59583900
C	-2.14161600	-1.64205100	-2.87312800
C	-1.38376000	-3.83635800	-3.89337500
H	-0.58364700	-2.91416800	-2.14314200
H	-2.02725800	-0.98194300	-2.00799200
H	-1.61069200	-1.17999400	-3.70870800
H	-3.20326100	-1.69378500	-3.13876700
H	-0.99770500	-4.83838300	-3.68639500
H	-2.32862200	-3.93954500	-4.43616800
H	-0.68016700	-3.31624600	-4.54617800
C	-3.02810600	-0.67736900	2.24301900
C	-2.30192000	-1.74623500	1.73390900
H	-2.49379700	0.26373200	2.34165500
C	-1.03558000	-1.58959500	1.15937500
H	-2.75853500	-2.73327400	1.73848300
C	-4.18020300	-0.88692200	3.18421200
C	-3.72011700	-1.08238000	4.63506200
H	-4.77261400	-1.75738600	2.86915700
H	-4.85735100	-0.02305000	3.14098800
C	-4.89374300	-1.24261900	5.59709900
H	-3.06767300	-1.96248800	4.68440700
H	-3.10398100	-0.22661400	4.93547900
H	-4.55317400	-1.39158300	6.62510100
H	-5.53518200	-0.35597400	5.58076900
H	-5.51156100	-2.10225900	5.31858300
O	-0.43818800	-0.36731900	1.19042700
H	-0.80647500	0.21966100	0.39267300
C	-3.11152200	3.77881900	0.04972000
C	-3.57666800	1.36899800	0.15621800
C	-2.27948100	1.75181200	-0.32249200
N	-2.08406000	3.12332500	-0.39005700
O	-1.36934600	0.93433900	-0.64888700
S	-4.47397800	2.80265300	0.59078900
C	-3.92839000	0.02427700	0.26959100
H	-3.22166900	-0.61359400	-0.25319800
C	-3.17911800	5.24641700	0.10802400
C	-2.06563700	5.98930300	-0.30274100
C	-4.32145700	5.91242500	0.56490200
C	-2.10118800	7.37668400	-0.25418700
H	-1.18833300	5.45959400	-0.65302700

C	-4.35092300	7.30033100	0.61130300
H	-5.19425800	5.34863600	0.88271300
C	-3.24089900	8.03587700	0.20218500
H	-1.23434100	7.94682500	-0.57210000
H	-5.24150700	7.80849400	0.96618700
H	-3.26485800	9.12029000	0.23934200
C	-5.26601400	-0.56412700	0.41586700
C	-6.40099900	0.13410600	0.84703700
C	-5.39384500	-1.93457300	0.14005400
C	-7.62339500	-0.51710900	0.98497200
H	-6.34408500	1.19038700	1.08389000
C	-6.61174400	-2.58337400	0.27935300
H	-4.51200600	-2.48845400	-0.17405000
C	-7.73578400	-1.87471700	0.70287500
H	-8.49172900	0.04260200	1.31749000
H	-6.68235500	-3.64441000	0.06112000
H	-8.69073700	-2.37787200	0.81496400

**M3(RR)**

O	0.24426600	-0.87331600	2.00187600
N	1.52873400	2.35486300	-1.51853200
N	0.34692400	2.45156500	-2.19826500
N	0.08848000	1.41310300	-0.25669300
C	2.71595300	4.33569300	-2.18818500
H	1.82070500	4.88752200	-1.92011400
C	3.85292700	4.97995000	-2.65884200
H	3.86072300	6.05839400	-2.76969000
C	4.97743200	4.22365500	-2.97157600
H	5.87865100	4.71213800	-3.32753900
C	4.95712500	2.83768300	-2.83958000
H	5.84550200	2.27340500	-3.09827400
C	3.82646300	2.15377900	-2.38225300
C	2.72622600	2.95306700	-2.04885300
C	1.38815800	1.76181700	-0.32822100
C	-0.50389000	1.87263700	-1.40419000
C	-1.98070800	1.70254200	-1.37774300
H	-2.28212700	0.89043200	-2.04392000
H	-2.48203300	2.61343100	-1.70727000
C	-2.22622600	1.39511300	0.12221000
H	-3.01338000	0.65555500	0.26515800
H	-2.54407800	2.30373600	0.64033200
C	-0.88183300	0.92512300	0.76296900
H	-0.69419800	1.47616200	1.68981500
C	-0.78366400	-0.60837200	1.10718000

C	-2.09182400	-1.02303500	1.81164100
C	-2.86424700	-2.12108900	1.44959800
C	-2.43052300	-0.31580500	2.97526500
C	-3.97876600	-2.48269700	2.20982900
H	-2.60169700	-2.73488900	0.59486600
C	-3.54158100	-0.68692300	3.71853600
H	-1.80340500	0.50695100	3.32322100
C	-4.33305900	-1.77072400	3.34237500
C	-0.48364300	-1.37224300	-0.17931400
C	-1.41018800	-1.49518700	-1.21300700
C	0.80462200	-1.87709600	-0.36931700
C	-1.05291300	-2.09561700	-2.41830200
H	-2.42878800	-1.13524100	-1.09135400
C	1.13654300	-2.50356200	-1.56582500
H	1.53403600	-1.75292700	0.42402600
C	0.22079000	-2.61294200	-2.60797700
H	-5.18871800	-2.06657600	3.93859900
H	0.49349500	-3.08594900	-3.54437100
H	0.46209300	-0.11632800	2.61827200
C	-3.92616200	0.10027300	4.94008600
C	-4.81508400	-3.64512800	1.75302200
C	2.50255300	-3.11769400	-1.69713100
C	-2.08705300	-2.15024100	-3.50516000
F	-2.46666300	-0.90735400	-3.86682300
F	-3.19554400	-2.78078100	-3.09654900
F	-1.64018900	-2.76805100	-4.60128900
F	2.55816700	-4.32673800	-1.12923100
F	3.43739300	-2.35767600	-1.10550400
F	2.86250300	-3.26869400	-2.98396000
F	-4.82015200	1.06202600	4.63367400
F	-4.49863900	-0.67494700	5.86869800
F	-2.87297500	0.70683900	5.49548000
F	-5.62057300	-3.29308800	0.73806600
F	-5.59389000	-4.11560000	2.73471500
F	-4.05261400	-4.65440300	1.31157800
C	3.76717200	0.63515200	-2.31899900
C	5.14106600	-0.02297000	-2.44069000
C	2.83577500	0.12090000	-3.42947300
H	3.35314200	0.33375900	-1.34743400
H	5.83967600	0.35670900	-1.68894700
H	5.03650900	-1.09908900	-2.29583700
H	5.57325600	0.13913600	-3.43376000
H	1.81072200	0.48715900	-3.31687900
H	3.20401600	0.45129200	-4.40606200

H	2. 81324900	-0. 97074500	-3. 42849400
C	3. 94692900	2. 70398600	2. 34333700
C	3. 04010900	2. 73861300	1. 15253600
H	4. 04695400	1. 66115400	2. 66327500
C	2. 41557800	1. 63736300	0. 71426200
H	2. 84460900	3. 69840300	0. 67548300
C	5. 33598700	3. 23819200	1. 96708900
C	6. 00586800	2. 41343100	0. 86844500
H	5. 96896600	3. 25232200	2. 86270500
H	5. 23897300	4. 28209600	1. 63125600
C	7. 35924100	2. 97896000	0. 44989800
H	6. 11817500	1. 37871000	1. 21582100
H	5. 34300400	2. 37459900	-0. 00569300
H	7. 82321200	2. 36886800	-0. 33060000
H	7. 24995900	3. 99586700	0. 05844000
H	8. 05026800	3. 02053300	1. 29749900
O	2. 53868700	0. 40891400	1. 24084400
H	2. 21497800	0. 53900400	2. 21538100
C	-0. 58503100	3. 80879900	3. 56710800
C	1. 82680200	3. 36550400	3. 62303900
C	1. 02303700	2. 24288200	3. 50360300
N	-0. 33997600	2. 53015700	3. 48593000
O	1. 40747900	0. 99804600	3. 37125800
S	0. 83753900	4. 78547400	3. 71062000
C	3. 32678000	3. 50909800	3. 53429400
H	3. 53340100	4. 56741800	3. 32011300
C	-1. 93560500	4. 39115800	3. 52150200
C	-3. 04573000	3. 56497500	3. 72885200
C	-2. 13756200	5. 74909600	3. 25227000
C	-4. 33198200	4. 08621900	3. 66357500
H	-2. 87893900	2. 52208300	3. 96711900
C	-3. 42518500	6. 26894500	3. 19344500
H	-1. 28454000	6. 39926300	3. 07684300
C	-4. 52619900	5. 43969700	3. 39466800
H	-5. 17944200	3. 43226200	3. 83965600
H	-3. 56972400	7. 32417500	2. 98507700
H	-5. 53056100	5. 84807600	3. 34765100
C	4. 04305700	3. 16473000	4. 82933100
C	3. 76876900	1. 96166500	5. 48868200
C	4. 99896200	4. 02898400	5. 36273500
C	4. 44692000	1. 63785800	6. 65878000
H	3. 01676500	1. 29099300	5. 07714200
C	5. 67792300	3. 70380300	6. 53519400
H	5. 21036700	4. 96838900	4. 85664200



C	5. 40301200	2. 50577200	7. 18537300
H	4. 22604600	0. 70374200	7. 16590800
H	6. 41602600	4. 38911900	6. 94027200
H	5. 92788900	2. 24917400	8. 10011200

**M3(RS)**

O	-0. 64120200	-0. 43617700	-1. 53593500
N	1. 48826600	2. 23130000	1. 76746400
N	0. 50332200	2. 38145700	2. 70823500
N	-0. 00616400	0. 81829900	1. 23493900
C	3. 39109700	2. 80364700	3. 11116200
H	2. 95643600	2. 16387800	3. 87199200
C	4. 60173200	3. 44917600	3. 31425500
H	5. 13468600	3. 32163400	4. 24983200
C	5. 12226800	4. 25033100	2. 30035500
H	6. 07387100	4. 75302800	2. 43889500
C	4. 42538100	4. 41003700	1. 10943100
H	4. 84135800	5. 04492900	0. 33273200
C	3. 19671500	3. 78077000	0. 87194200
C	2. 71595500	2. 97096800	1. 90373200
C	1. 21165500	1. 26419200	0. 88008100
C	-0. 39072000	1. 51034600	2. 35089000
C	-1. 68865300	1. 01312800	2. 88693000
H	-2. 48241900	1. 73787600	2. 68805700
H	-1. 63564100	0. 85772300	3. 96520000
C	-1. 86068900	-0. 31590200	2. 10283600
H	-2. 89594800	-0. 49595100	1. 81154400
H	-1. 55671300	-1. 15774200	2. 73105400
C	-0. 91860700	-0. 28120500	0. 86054800
H	-0. 32538000	-1. 19602800	0. 79495200
C	-1. 56573800	-0. 08316300	-0. 55900900
C	-2. 72228600	-1. 08459300	-0. 70078400
C	-3. 97541100	-0. 74426900	-1. 20327100
C	-2. 47180300	-2. 42346900	-0. 37869800
C	-4. 96966700	-1. 71267500	-1. 33809700
H	-4. 19844000	0. 27441700	-1. 50070000
C	-3. 47747700	-3. 37403500	-0. 50316400
H	-1. 48075400	-2. 74042000	-0. 05457400
C	-4. 73922900	-3. 03199500	-0. 97828900
C	-2. 00514300	1. 37756200	-0. 69470200
C	-3. 04992900	1. 89865100	0. 06815500
C	-1. 30121200	2. 23999800	-1. 53801200
C	-3. 36731300	3. 25298500	0. 01352400
H	-3. 64703100	1. 25025000	0. 70409700

C	-1.64736700	3.58662300	-1.60328800
H	-0.47088200	1.86255500	-2.12607100
C	-2.67226900	4.11329200	-0.82353400
H	-5.51938400	-3.77821700	-1.07530600
H	-2.92227800	5.16708800	-0.86921300
H	0.23008300	-1.98362600	-2.00217700
C	-3.19633200	-4.78194100	-0.05865800
C	-6.29534900	-1.31391800	-1.92524600
C	-0.94406600	4.47986300	-2.58705400
C	-4.46191100	3.74957300	0.91354600
F	-4.10676700	3.62453000	2.20847900
F	-5.58413400	3.03619000	0.75749300
F	-4.75436800	5.03483700	0.70137800
F	0.31746100	4.07955900	-2.80488900
F	-0.89852000	5.74963900	-2.15329600
F	-1.56486900	4.49036900	-3.77255400
F	-1.95469200	-5.16337900	-0.38118200
F	-3.29995300	-4.89673000	1.28092000
F	-4.05208100	-5.65925200	-0.59424000
F	-6.65724900	-0.08697000	-1.52201400
F	-7.26854400	-2.16373200	-1.57098000
F	-6.25388100	-1.29026700	-3.26394100
C	2.46675200	4.02848900	-0.43637000
C	3.31860900	3.60958700	-1.63943100
C	2.06115200	5.50541100	-0.53121700
H	1.55342100	3.42397200	-0.46341600
H	3.60168500	2.55718200	-1.56787400
H	2.74892000	3.74969900	-2.56049700
H	4.22771000	4.21654200	-1.70543800
H	1.41365400	5.79446100	0.30153400
H	2.94418200	6.15215800	-0.51116200
H	1.52916700	5.69071100	-1.46560100
C	4.34268600	-0.21457800	-0.75796600
C	3.32439700	0.42901900	0.14218400
H	4.54465400	0.45835200	-1.60628700
C	2.07054800	0.76522800	-0.23200600
H	3.59934900	0.57126300	1.18352300
C	5.66487500	-0.37835600	0.00291500
C	6.25466000	0.97220600	0.41657000
H	6.39162600	-0.91038300	-0.61984900
H	5.50665500	-0.99787900	0.89932100
C	7.55110200	0.83077100	1.20812500
H	6.43302200	1.56772000	-0.48889300
H	5.52666200	1.54073700	1.00942200

H	7.95576900	1.80730800	1.48878200
H	7.38463600	0.26073500	2.12790300
H	8.31369000	0.30406900	0.62622400
O	1.51728300	0.69860000	-1.40702000
H	0.28918000	0.08002500	-1.45434100
C	1.46541100	-3.12801700	1.30652600
C	2.87836700	-2.31211600	-0.52808400
C	1.57985000	-2.61827300	-0.83999800
N	0.79403500	-3.07071600	0.18857400
O	1.06763200	-2.48429600	-2.07365900
S	3.13438600	-2.67035300	1.14943400
C	3.78358200	-1.52551200	-1.42863100
H	3.09463700	-1.17408000	-2.20603600
C	0.83509100	-3.48270100	2.58675400
C	-0.40853500	-4.12759800	2.56784600
C	1.41000300	-3.13576400	3.81327600
C	-1.07024200	-4.40424200	3.75777400
H	-0.82979000	-4.42592700	1.61443000
C	0.74970200	-3.42693800	5.00209700
H	2.36801400	-2.62291800	3.83665000
C	-0.49399400	-4.05426400	4.97813500
H	-2.03320300	-4.90361800	3.72589100
H	1.20375600	-3.15474500	5.94949200
H	-1.00911600	-4.27487600	5.90744400
C	4.88913300	-2.30770900	-2.11173700
C	5.42081200	-3.48543600	-1.58610800
C	5.43800800	-1.79518400	-3.29134700
C	6.48343300	-4.12913500	-2.21708200
H	4.99605800	-3.91112000	-0.68155500
C	6.49968500	-2.43357800	-3.92236300
H	5.02039700	-0.88663200	-3.71919800
C	7.02954300	-3.60415600	-3.38378800
H	6.88214300	-5.04655900	-1.79520400
H	6.90880100	-2.02227100	-4.83996000
H	7.85566900	-4.10722500	-3.87589100

**M3(SR)**

O	-2.36035700	1.80428400	0.25783600
N	0.63192700	-0.95153700	-2.46541000
N	-0.23032700	-1.84218600	-3.04188800
N	-1.31795000	-0.22325800	-2.00645300
C	2.90787600	-0.64091700	-3.29014300
H	2.51602800	0.06548000	-4.01409500
C	4.26507000	-0.92328500	-3.23222400

H	4.95349000	-0.41673900	-3.89985700
C	4.72503400	-1.86010500	-2.30917800
H	5.78629200	-2.07750400	-2.23076800
C	3.83141100	-2.52329000	-1.47827800
H	4.21595100	-3.24762500	-0.76834100
C	2.45748000	-2.26081400	-1.50498400
C	2.03852300	-1.28142000	-2.41249200
C	-0.00695800	0.05656100	-1.84683400
C	-1.40131500	-1.37132700	-2.74440100
C	-2.80621500	-1.74869500	-3.05184000
H	-3.04885700	-2.70830500	-2.58777100
H	-2.95238600	-1.85669700	-4.12789900
C	-3.60661700	-0.55699300	-2.46057400
H	-4.42160300	-0.90180000	-1.82463000
H	-4.06299900	0.02432200	-3.26304100
C	-2.63018600	0.36961400	-1.66274900
H	-2.65219800	1.38733400	-2.05994400
C	-2.88245600	0.57018200	-0.10793500
C	-4.40027300	0.70013100	0.08600500
C	-5.21189400	-0.29818000	0.61892800
C	-4.99182600	1.89674800	-0.32655200
C	-6.58990700	-0.10745100	0.71189500
H	-4.78811500	-1.23186600	0.97458100
C	-6.36741500	2.06956600	-0.23901800
H	-4.36133000	2.70227900	-0.68870000
C	-7.18369500	1.06951400	0.27845100
C	-2.27205000	-0.57583600	0.70216400
C	-2.43558600	-1.90610900	0.32863900
C	-1.48243700	-0.28979900	1.81856400
C	-1.81107400	-2.92901300	1.03941300
H	-3.05304500	-2.17342400	-0.52312800
C	-0.85525000	-1.31384600	2.51455700
H	-1.33499800	0.74118300	2.11568500
C	-1.01405300	-2.64451300	2.13760300
H	-8.25623200	1.20854000	0.34852300
H	-0.50845200	-3.43620100	2.67940400
H	-1.34578300	1.74739400	0.19388800
C	-6.96678200	3.34379900	-0.76698300
C	-7.42575700	-1.19064200	1.33617100
C	-0.00018900	-1.00640700	3.71536400
C	-2.02780300	-4.33998800	0.57970800
F	-1.08495400	-5.17133300	1.04247300
F	-2.00717900	-4.41297300	-0.76741700
F	-3.21521300	-4.82069100	0.96977000

F	0.34992700	0.28033300	3.76779100
F	1.11022800	-1.75101100	3.72344600
F	-0.66275900	-1.28682800	4.85267000
F	-6.24108700	4.41093900	-0.41239600
F	-7.01326500	3.33212600	-2.10948900
F	-8.21743500	3.52918800	-0.32761600
F	-7.02129200	-2.40604700	0.93550500
F	-8.71965000	-1.06538100	1.01554100
F	-7.33883900	-1.17044900	2.67229800
C	1.48562200	-3.09197100	-0.68450600
C	1.99094600	-3.44496300	0.71548100
C	1.17102600	-4.37851400	-1.46795400
H	0.55511800	-2.51970100	-0.56103100
H	2.17639500	-2.55431200	1.31690900
H	1.23870600	-4.06993800	1.20577100
H	2.91063300	-4.03764100	0.67070100
H	0.75509400	-4.16070300	-2.45419100
H	2.09076400	-4.95809700	-1.60225000
H	0.45916300	-4.99447600	-0.91363100
C	2.39067600	2.99920900	-1.10795900
C	1.57686300	1.88788900	-1.72220300
H	1.76429300	3.90393000	-1.08402300
C	0.58608300	1.20905200	-1.11303100
H	1.83856500	1.59677200	-2.73191900
C	3.60838000	3.26973200	-2.00956300
C	3.24697100	4.06720200	-3.26130200
H	4.05016000	2.30644900	-2.30092200
H	4.38541200	3.80723400	-1.45345300
C	4.42829600	4.23405500	-4.21230700
H	2.41605800	3.57687000	-3.78548600
H	2.87024800	5.05346300	-2.95899800
H	4.15835200	4.82358000	-5.09219100
H	5.26149500	4.73707500	-3.71224000
H	4.79070900	3.26034600	-4.55757400
O	0.09576000	1.40189400	0.09172800
H	1.14831100	0.52466200	0.97667500
C	5.17732100	-0.40313800	0.71090400
C	3.53350400	1.40405500	0.52052300
C	3.06815600	0.18757600	0.96535600
N	3.99896000	-0.80870900	1.08123000
O	1.81110800	-0.14665100	1.29617600
S	5.23703000	1.25922400	0.20621400
C	2.77236600	2.69398800	0.36805800
H	1.82127500	2.53303800	0.88703300

C	6. 34348400	-1. 29683500	0. 65179500
C	6. 22701900	-2. 59070600	1. 17574400
C	7. 54700600	-0. 90579900	0. 05706000
C	7. 29719500	-3. 47334700	1. 10189200
H	5. 28703500	-2. 87750300	1. 63748300
C	8. 61601400	-1. 79239100	-0. 01267900
H	7. 64675600	0. 09205800	-0. 36218300
C	8. 49469900	-3. 07880800	0. 50730100
H	7. 19822100	-4. 47287100	1. 51326900
H	9. 54525000	-1. 47795100	-0. 47691300
H	9. 32941900	-3. 76981300	0. 45052600
C	3. 44644700	3. 86239800	1. 09191200
C	4. 01823500	3. 63896600	2. 35056100
C	3. 45317400	5. 16780200	0. 59335900
C	4. 58122100	4. 67841200	3. 08074600
H	4. 01623000	2. 63192600	2. 75852100
C	4. 02117400	6. 21195700	1. 32126200
H	3. 01639400	5. 38864100	-0. 37547400
C	4. 58926900	5. 97280700	2. 56654700
H	5. 01639600	4. 47635300	4. 05451600
H	4. 01736900	7. 21555100	0. 90726200
H	5. 03366600	6. 78560800	3. 13197600

### M3(SS)

O	1. 61592900	0. 71515300	1. 51481100
N	-0. 45910100	-3. 69139600	1. 19158900
N	0. 60580100	-4. 55035500	1. 18914700
N	1. 25917600	-2. 43981700	1. 33870100
C	-2. 49418900	-4. 71563600	2. 02100100
H	-2. 07118000	-4. 64068200	3. 01791700
C	-3. 73902300	-5. 29066400	1. 80393600
H	-4. 31456000	-5. 67455200	2. 63880000
C	-4. 22957600	-5. 37313100	0. 50267000
H	-5. 19823000	-5. 82641400	0. 31723500
C	-3. 48569800	-4. 88638000	-0. 56606600
H	-3. 88819400	-4. 96577600	-1. 57003700
C	-2. 22158400	-4. 31393200	-0. 38403800
C	-1. 77170400	-4. 22960000	0. 93662700
C	-0. 09268000	-2. 40435200	1. 30857300
C	1. 62824800	-3. 75903000	1. 28695600
C	3. 09973700	-3. 93907500	1. 43300500
H	3. 50398700	-4. 63619900	0. 69819400
H	3. 31815600	-4. 33382800	2. 42963100
C	3. 61469900	-2. 49414500	1. 25565600

H	3.96899000	-2.34401100	0.23412000
H	4.45166400	-2.26551900	1.91560400
C	2.42815500	-1.53736500	1.55311100
H	2.41605700	-1.26063900	2.61204100
C	2.43072800	-0.16599200	0.80460400
C	3.86270500	0.37434400	0.93552600
C	4.83142400	0.18723800	-0.04770300
C	4.20741400	1.05328400	2.10590900
C	6.12890400	0.65502900	0.14794300
H	4.58096200	-0.30951400	-0.98127600
C	5.50634200	1.51317400	2.28880700
H	3.44373700	1.24270200	2.85259100
C	6.48115500	1.31743100	1.31561200
C	2.00775600	-0.22733200	-0.66856400
C	1.99299800	-1.37776700	-1.45252500
C	1.58964400	0.97942400	-1.23824500
C	1.55406400	-1.31620400	-2.77601500
H	2.29016400	-2.34384600	-1.06037600
C	1.13818100	1.02427700	-2.54669000
H	1.56272700	1.87304300	-0.62415900
C	1.11507700	-0.12432100	-3.33228500
H	7.49034300	1.68522300	1.46033300
H	0.73880200	-0.09014900	-4.34930300
H	0.66826100	0.48399700	1.24328100
C	5.86989300	2.18595500	3.58389600
C	7.13405400	0.46376600	-0.95378500
C	0.67727300	2.32658700	-3.14977000
C	1.59362200	-2.55206700	-3.62673600
F	0.57308900	-2.58928500	-4.49846100
F	1.52460400	-3.67394700	-2.88363600
F	2.72248000	-2.63258400	-4.34284800
F	0.41424100	3.24643200	-2.22336000
F	-0.40667800	2.15828000	-3.90956400
F	1.63943600	2.82904000	-3.95042600
F	4.86319900	2.93220600	4.05206300
F	6.16284900	1.28156900	4.53261400
F	6.94182400	2.97659200	3.44748700
F	7.08997700	-0.78963600	-1.43386200
F	8.38378600	0.69504300	-0.53419700
F	6.89565700	1.28349700	-1.98496300
C	-1.39707700	-3.82047300	-1.55984300
C	-1.72125800	-2.35387300	-1.88977100
C	-1.58299400	-4.69868700	-2.80065900
H	-0.33898500	-3.88191400	-1.27596800

H	-1.32601400	-1.66277600	-1.14053100
H	-1.27554900	-2.08199600	-2.85101800
H	-2.80462900	-2.20543800	-1.96369500
H	-1.45751800	-5.75967500	-2.56807600
H	-2.57265600	-4.55530300	-3.24543900
H	-0.84519300	-4.41739400	-3.55404700
C	-3.01674800	-0.01758800	1.93579200
C	-2.13783800	-1.23598900	2.01516800
H	-2.34764300	0.84591100	2.04663900
C	-0.97347300	-1.21106700	1.32686800
H	-2.44222700	-2.10978200	2.58308800
C	-4.06698200	0.05338500	3.04359900
C	-3.44851400	0.25908500	4.42517500
H	-4.67801900	-0.85871700	3.04206600
H	-4.75870800	0.88005600	2.82873200
C	-4.49717800	0.30701100	5.53227900
H	-2.73119800	-0.54720700	4.62734000
H	-2.86693800	1.18916100	4.42181900
H	-4.04088400	0.46021600	6.51370500
H	-5.20682200	1.12224700	5.36068500
H	-5.06975400	-0.62526800	5.56868300
O	-0.52903700	-0.20443800	0.61631000
H	-1.17473600	0.56648000	-0.71854000
C	-3.32575100	3.94434000	-0.47193100
C	-3.46535200	1.53890100	-0.01537400
C	-2.46583600	1.95681300	-0.86033500
N	-2.41500700	3.29568300	-1.13188500
O	-1.54321700	1.15449600	-1.42693300
S	-4.32732900	2.93652900	0.55041600
C	-3.60932800	0.13162900	0.47557200
H	-2.93329000	-0.43072300	-0.17687200
C	-3.50796900	5.40099200	-0.56649600
C	-2.61144000	6.13654800	-1.35093400
C	-4.54175100	6.06382200	0.10083400
C	-2.75412200	7.51326400	-1.46243200
H	-1.81339500	5.60507200	-1.85884800
C	-4.67863300	7.44240900	-0.01273900
H	-5.24642300	5.50074200	0.70740200
C	-3.78624700	8.17093400	-0.79479600
H	-2.05628800	8.07800100	-2.07243000
H	-5.48541400	7.94787900	0.50809100
H	-3.89485300	9.24712500	-0.88434100
C	-4.97132500	-0.52933400	0.30997300
C	-6.10745500	0.14074000	-0.14258600



C	-5.08408400	-1.89636700	0.60100000
C	-7.32659900	-0.52435100	-0.27413500
H	-6.04643200	1.18790700	-0.41508200
C	-6.29827600	-2.55918900	0.47524500
H	-4.20367600	-2.44589900	0.93118100
C	-7.43097500	-1.87307000	0.04064400
H	-8.19593300	0.02132900	-0.62790000
H	-6.35819900	-3.61592100	0.71715200
H	-8.38117400	-2.38820200	-0.05820000

**TS4(RR)**

O	-0.40959200	0.59905800	-1.33801600
N	2.73398600	2.08267100	1.24650400
N	2.01781600	2.89093400	2.08144500
N	0.74392900	1.36171700	1.11684700
C	4.82479300	1.47912500	2.25727500
H	4.22273100	1.02144600	3.03855000
C	6.21103300	1.42810700	2.24698800
H	6.74265100	0.93056300	3.05063300
C	6.90992900	2.01172000	1.18933100
H	7.99429600	1.96694000	1.16875300
C	6.23077900	2.64585400	0.15628800
H	6.79308200	3.09628300	-0.65665100
C	4.83198800	2.72453500	0.13570900
C	4.17171100	2.11971300	1.20480500
C	1.98588700	1.14454800	0.68001600
C	0.81353300	2.41580900	1.98883200
C	-0.49882500	2.65443500	2.64755700
H	-1.00081000	3.52649200	2.21743400
H	-0.37665200	2.81536300	3.71886900
C	-1.24036000	1.33051100	2.32637900
H	-2.30824900	1.49676500	2.18469400
H	-1.10998000	0.63257300	3.15850200
C	-0.57447200	0.70455900	1.06386400
H	-0.42052600	-0.37503200	1.17274300
C	-1.27027300	0.97981400	-0.30249900
C	-2.60819800	0.24895400	-0.40777900
C	-3.27127500	0.32986100	-1.63899000
C	-3.19664100	-0.47184300	0.62404200
C	-4.51294700	-0.26045900	-1.80404100
H	-2.79936200	0.85511900	-2.46341400
C	-4.46641500	-1.03052600	0.45711800
H	-2.69815400	-0.62105300	1.57636200
C	-5.13644600	-0.92722400	-0.74775400

C	-1.44463700	2.49021400	-0.45427100
C	-2.57893400	3.15999200	-0.00364100
C	-0.37348500	3.22971800	-0.96452400
C	-2.62062500	4.55281700	-0.01992200
H	-3.43940300	2.60488700	0.36089400
C	-0.42762600	4.61782700	-0.96709200
H	0.49339900	2.70582400	-1.35917600
C	-1.54562400	5.29547400	-0.48943600
H	-6.12067700	-1.36631900	-0.87251000
H	-1.58259400	6.37911300	-0.49331300
H	-0.34526000	-0.36953600	-1.44461400
C	-5.11421400	-1.66778100	1.65492600
C	-5.24803600	-0.16487100	-3.11236300
C	0.78797200	5.39471000	-1.38929400
C	-3.81046900	5.24339300	0.58454700
F	-3.71259600	5.26075900	1.92523100
F	-4.95312200	4.61352500	0.28493100
F	-3.91652600	6.51215600	0.17585500
F	1.48733000	4.75579800	-2.33913500
F	1.61887200	5.56957100	-0.34713500
F	0.47281100	6.60807700	-1.85449000
F	-4.28686400	-2.51808300	2.27105800
F	-5.44640300	-0.73002200	2.56047500
F	-6.23587300	-2.32376800	1.33629100
F	-6.34671800	0.59489100	-2.99188000
F	-5.65573900	-1.37426800	-3.52461500
F	-4.49206900	0.36578200	-4.07831300
C	4.10780600	3.44469500	-0.98466000
C	4.36603000	2.77481900	-2.33819300
C	4.50659200	4.92468200	-1.01671300
H	3.03201000	3.39786900	-0.78287000
H	4.06927200	1.72402100	-2.32129300
H	3.78985700	3.28412600	-3.11597500
H	5.42567000	2.83854000	-2.60778800
H	4.30635800	5.41190400	-0.05931500
H	5.57207700	5.03481500	-1.24349200
H	3.94005700	5.44454800	-1.79306800
C	3.49956500	-2.24849800	-0.38155700
C	2.90461800	-1.13477500	0.46981200
H	3.35636800	-2.00668800	-1.44463200
C	2.49784500	0.04253100	-0.22782700
H	3.48317000	-0.87959400	1.36660900
C	5.01940200	-2.32848800	-0.17672000
C	5.73680700	-1.04900500	-0.60804200

H	5.42575700	-3.17587000	-0.74168600
H	5.22660200	-2.52850700	0.88584500
C	7.24431600	-1.12067600	-0.38667200
H	5.52228100	-0.86148800	-1.66816600
H	5.33399600	-0.18997200	-0.05728700
H	7.73740500	-0.20483600	-0.72482000
H	7.47444700	-1.24975200	0.67653600
H	7.68537800	-1.96335200	-0.92860900
O	2.40956200	0.23927100	-1.43992200
H	1.59113300	-1.43150100	-1.83754200
C	-1.11155600	-3.88641700	0.13983000
C	1.29736100	-3.53730200	-0.19759600
C	0.44244700	-2.76990200	-0.94540600
N	-0.89501800	-2.94929700	-0.74128300
O	0.71951800	-1.85590900	-1.91633100
S	0.33427400	-4.58452600	0.79108400
C	2.80550900	-3.61276100	-0.11728700
H	3.05516500	-3.89034100	0.91678100
C	-2.45567600	-4.36962900	0.48694500
C	-3.51732600	-4.06459000	-0.37285200
C	-2.69201500	-5.14638000	1.62381700
C	-4.79358700	-4.53724100	-0.09729700
H	-3.31564200	-3.46369100	-1.25429700
C	-3.97166300	-5.61785000	1.89436500
H	-1.87523500	-5.37372700	2.30401900
C	-5.02498300	-5.31491300	1.03578600
H	-5.61233500	-4.29838200	-0.76942700
H	-4.14833400	-6.21687800	2.78176800
H	-6.02416600	-5.67999800	1.25019400
C	3.34053200	-4.69785800	-1.03840200
C	3.00516800	-4.69150000	-2.39552500
C	4.19171200	-5.69191200	-0.55808200
C	3.51948800	-5.65700900	-3.25336700
H	2.32445500	-3.93157900	-2.77438600
C	4.70548800	-6.66314100	-1.41513000
H	4.45653400	-5.70247500	0.49655500
C	4.37192800	-6.64608200	-2.76527300
H	3.24988600	-5.64238800	-4.30473500
H	5.36570900	-7.43184100	-1.02592500
H	4.76956200	-7.40120700	-3.43561400
H	1.85256300	-1.43538900	1.23409900
C	1.30262200	-1.01614000	3.25636000
O	1.00294500	-1.69605100	2.19708700
O	2.01266600	-0.00348700	3.27134000

C	0.70273100	-1.55819100	4.54288300
H	1.18971100	-2.50597100	4.78751100
H	0.84683500	-0.85165200	5.35963900
H	-0.35883900	-1.77350500	4.39832900

**TS4(RS)**

O	-0.19066800	-0.07177000	-0.42027800
N	1.24518800	3.59798300	1.05054500
N	0.16715200	4.10835600	1.72185300
N	-0.02718000	1.94054400	1.36229400
C	3.47639100	4.35390300	1.56749000
H	3.42568500	3.72463800	2.45126600
C	4.60292800	5.10740600	1.26930000
H	5.46738000	5.07550000	1.92277000
C	4.60696300	5.90353200	0.12486900
H	5.48262300	6.49670700	-0.11796200
C	3.49867500	5.94265300	-0.71224400
H	3.52181600	6.56560000	-1.60157600
C	2.34865300	5.19244000	-0.44387700
C	2.37977800	4.41276600	0.71136800
C	1.14950500	2.28747700	0.83911800
C	-0.58763100	3.06430800	1.90254500
C	-1.86068200	2.73320300	2.61116400
H	-2.72640500	3.00608300	2.00022200
H	-1.93365100	3.25434800	3.56581600
C	-1.70708300	1.19645500	2.78201400
H	-2.66020000	0.66711600	2.76918000
H	-1.21751700	0.99737000	3.73789300
C	-0.74442700	0.70247900	1.67638100
H	-0.00340900	0.01429600	2.06414200
C	-1.33159400	0.06091900	0.39268000
C	-1.86788800	-1.33500000	0.73089900
C	-3.04817800	-1.85336700	0.20137300
C	-1.06022700	-2.17595300	1.50809700
C	-3.44115600	-3.15689500	0.50145100
H	-3.66410700	-1.26471100	-0.47112800
C	-1.48461400	-3.45880000	1.82517400
H	-0.07235300	-1.86293800	1.84275300
C	-2.68319100	-3.96454300	1.33618500
C	-2.33358000	1.01821700	-0.24968300
C	-3.63160100	1.17644900	0.23894900
C	-1.90072600	1.84503200	-1.29063100
C	-4.47294500	2.14803900	-0.29343700
H	-4.00608100	0.54087700	1.03599300

C	-2.76189600	2.79808700	-1.82653700
H	-0.89083800	1.73151600	-1.67720500
C	-4.05116500	2.96556700	-1.33348300
H	-2.99138100	-4.97910700	1.55898000
H	-4.71717300	3.70898900	-1.75728200
H	1.83747100	0.59308400	-2.57958700
C	-0.61707700	-4.27649300	2.74237600
C	-4.70960400	-3.67555300	-0.11463700
C	-2.27445100	3.71050000	-2.91810000
C	-5.81621200	2.35985700	0.34552300
F	-5.68952300	3.08406200	1.47162900
F	-6.38730300	1.19941500	0.69080500
F	-6.65884200	3.01405100	-0.45910900
F	-1.73504400	4.83137900	-2.39956100
F	-3.27223000	4.09638400	-3.72191500
F	-1.33236200	3.13493900	-3.66935800
F	0.67661500	-4.19824300	2.40436300
F	-0.70920000	-3.83280600	4.00940200
F	-0.96615700	-5.56927400	2.75141300
F	-5.79373800	-3.11349900	0.44126200
F	-4.83048700	-5.00160500	0.02043700
F	-4.76004100	-3.39375900	-1.42716200
C	1.14956100	5.24755500	-1.36854800
C	1.52730800	4.80610700	-2.78594500
C	0.54018700	6.65429100	-1.35614500
H	0.39017700	4.55032900	-0.99717000
H	1.95661900	3.80147200	-2.77200100
H	0.63812900	4.79772300	-3.42043700
H	2.25511900	5.49208200	-3.23140700
H	0.23762200	6.94112100	-0.34529000
H	1.26321800	7.39283900	-1.71764900
H	-0.33551600	6.69144300	-2.00745000
C	4.19728800	-0.09171700	0.16886400
C	2.99708300	0.63241200	0.77220300
H	5.00579200	0.64146600	0.02252200
C	2.15591300	1.48465200	0.00949500
H	3.22571700	1.12905100	1.72164300
C	4.72887700	-1.15056600	1.14831500
C	5.18496700	-0.58756200	2.49484000
H	5.57576600	-1.66813700	0.68166500
H	3.95195600	-1.90052700	1.34259200
C	5.76505600	-1.67764700	3.39229700
H	5.93502900	0.19716000	2.32838400
H	4.34536500	-0.10873200	3.01299100

H	6.06987800	-1.28147700	4.36483100
H	5.02459500	-2.46611000	3.56365400
H	6.63978800	-2.14362700	2.92801100
O	2.05991300	1.71436400	-1.20027400
H	-0.36125800	-0.69466800	-1.14909200
C	0.80483100	-3.10676600	-1.36134100
C	2.67325600	-1.50826400	-1.36669000
C	1.63288600	-1.25339400	-2.22729500
N	0.59475600	-2.14409800	-2.22043000
O	1.51098700	-0.19530700	-3.05208000
S	2.27728100	-2.93705900	-0.46119500
C	3.92235000	-0.67667800	-1.25073500
H	3.72195100	0.19051900	-1.88654800
C	-0.12654000	-4.23308600	-1.18558400
C	-1.33073500	-4.22944800	-1.90071600
C	0.17021500	-5.31647700	-0.35167100
C	-2.22096400	-5.28931300	-1.77717300
H	-1.54758100	-3.39017300	-2.55326900
C	-0.72972500	-6.36859400	-0.22122300
H	1.10360600	-5.33698400	0.20319700
C	-1.92763300	-6.35830200	-0.93242400
H	-3.15495800	-5.27323300	-2.32909800
H	-0.49290400	-7.19624100	0.43917100
H	-2.63080900	-7.17881600	-0.83052600
C	5.18520500	-1.31373800	-1.82785300
C	5.33780800	-2.68078100	-2.05736000
C	6.25750000	-0.46823300	-2.13714100
C	6.53266600	-3.19003700	-2.56447200
H	4.51888500	-3.36124000	-1.85308400
C	7.44989400	-0.97190000	-2.64234800
H	6.14837000	0.60381200	-1.98882500
C	7.59408400	-2.34116500	-2.85501300
H	6.62747200	-4.25785500	-2.73567400
H	8.26460000	-0.29434800	-2.87860400
H	8.52260600	-2.73917700	-3.25144000
C	1.77670700	-0.38672700	3.50679800
O	1.59836400	0.83399300	3.57217200
O	1.83372700	-1.05203400	2.38934800
H	2.23110700	-0.24588000	1.45522000
C	1.94212300	-1.23441800	4.75156600
H	1.29674600	-2.11367600	4.68968200
H	2.97536600	-1.59192000	4.79673700
H	1.71768300	-0.65121100	5.64377000

**TS4(SR)**

N	-0.71421200	-1.04255300	1.97756100
N	0.16046100	-1.56212200	2.87951500
N	1.13207700	-0.07483800	1.57014200
C	-2.87923600	-0.86715800	3.00471600
H	-2.41937000	-0.14073900	3.67052600
C	-4.20956600	-1.25668800	3.10222700
H	-4.84434200	-0.83359400	3.87300000
C	-4.71658100	-2.19175700	2.20237200
H	-5.75735800	-2.49773200	2.26152500
C	-3.90894000	-2.72999100	1.20423700
H	-4.33873500	-3.43550800	0.50138100
C	-2.56444600	-2.37278300	1.07700500
C	-2.09886400	-1.43359000	2.00252600
C	-0.15316000	-0.12479400	1.20224700
C	1.26913000	-0.93765600	2.61944300
C	2.62563300	-0.86912100	3.22227300
H	3.13545200	-1.83344800	3.15395300
H	2.54464700	-0.60652900	4.27859700
C	3.30227800	0.25820700	2.39198700
H	4.28068000	-0.04917400	2.02215600
H	3.45946600	1.13691300	3.01960800
C	2.35530200	0.66768600	1.21623500
C	2.84561300	0.39716700	-0.26464700
C	4.34097000	0.71767200	-0.33652100
C	5.33152900	-0.23779000	-0.53521100
C	4.71277100	2.05937800	-0.19836300
C	6.67362400	0.14169000	-0.57437200
H	5.07985500	-1.28198500	-0.68877500
C	6.05151000	2.42226700	-0.23788400
H	3.94673600	2.82095000	-0.09300800
C	7.04826100	1.46714900	-0.42289700
C	2.50576600	-1.02646800	-0.70232100
C	2.82001900	-2.12511000	0.10025100
C	1.80284700	-1.24972700	-1.88252500
C	2.41917300	-3.40582700	-0.25671400
H	3.38849100	-1.99450300	1.01694100
C	1.40571300	-2.53844700	-2.23308800
H	1.54986700	-0.41486600	-2.52584100
C	1.70704900	-3.62900700	-1.42986700
H	8.09176300	1.75691500	-0.46895900
H	1.38712800	-4.62734400	-1.70461600
H	1.28958200	1.20790400	-1.13640200
C	6.43024200	3.86513000	-0.03898500

C	7.71225700	-0.93058800	-0.75848700
C	0.59969200	-2.70579700	-3.49239600
C	2.76242900	-4.53183200	0.67678400
F	2.37540800	-4.24126300	1.93328000
F	4.08451000	-4.74458000	0.72412800
F	2.17439800	-5.67772600	0.32286900
F	-0.51497300	-1.96590400	-3.44135500
F	0.23537800	-3.98096600	-3.68463700
F	1.28811000	-2.31020200	-4.57034500
F	6.55762000	4.15835500	1.26367300
F	7.59932200	4.15103500	-0.62589200
F	5.50316900	4.68926000	-0.54046400
F	7.86830700	-1.64935200	0.36379100
F	8.90617900	-0.42029600	-1.07829000
F	7.35808100	-1.78888100	-1.72421200
C	-1.63670000	-3.04584400	0.07680200
C	-2.36361900	-3.62432800	-1.13748800
C	-0.85545200	-4.15241600	0.80608300
H	-0.92361900	-2.29606900	-0.29892600
H	-3.00828100	-2.88381200	-1.61695900
H	-1.62602000	-3.96714200	-1.86876600
H	-2.96576500	-4.49446700	-0.85357600
H	-0.19065500	-3.75570100	1.57834900
H	-1.55868300	-4.84027400	1.28667400
H	-0.25596300	-4.73184200	0.09875100
C	-2.22312500	2.91751100	-0.07709700
C	-1.60246000	1.82641600	0.78399600
H	-1.40000400	3.56120000	-0.41919900
C	-0.81424400	0.79222300	0.18887700
H	-2.20881800	1.45354600	1.61618000
C	-3.14161200	3.79756800	0.78116600
C	-2.47463100	4.32848100	2.05336400
H	-4.04154500	3.23433000	1.06580600
H	-3.48294100	4.64160800	0.17041200
C	-3.33463200	5.38298200	2.74441500
H	-2.28568200	3.50112200	2.74884100
H	-1.48890100	4.74303500	1.80822200
H	-2.86445000	5.74297700	3.66333500
H	-3.49970000	6.24457400	2.09008100
H	-4.31619100	4.97563900	3.00819600
O	-0.41986200	0.68597600	-0.98037900
H	-1.80389000	-0.00629200	-2.23575400
C	-5.52982800	-0.46862100	-0.64625800
C	-3.80247600	1.20333300	-1.15099100



C	-3.63605500	-0.05247900	-1.68283800
N	-4.61028100	-0.97113100	-1.41634400
O	-2.61901700	-0.48039000	-2.46002800
S	-5.24415000	1.18265700	-0.17727700
C	-2.90437000	2.38410600	-1.37593100
H	-2.08634900	1.99144200	-1.98846200
C	-6.68637100	-1.23942500	-0.16843400
C	-6.85860800	-2.54785000	-0.63588300
C	-7.58518600	-0.72137800	0.76868700
C	-7.90621100	-3.32612100	-0.16078300
H	-6.15565400	-2.93361200	-1.36730500
C	-8.63424700	-1.50327800	1.23929600
H	-7.45940200	0.29085800	1.14411800
C	-8.79570900	-2.80859200	0.78028500
H	-8.03204300	-4.33966900	-0.52770900
H	-9.32564800	-1.09350600	1.96832500
H	-9.61340000	-3.41848500	1.15022800
C	-3.49415200	3.53208300	-2.19316400
C	-4.85397700	3.68970300	-2.45715600
C	-2.60553300	4.48501400	-2.70792300
C	-5.31482000	4.77822600	-3.19691200
H	-5.56707400	2.95571000	-2.10113100
C	-3.06161000	5.57107200	-3.44396900
H	-1.53804000	4.36633800	-2.53707500
C	-4.42474500	5.72516200	-3.68852900
H	-6.37814300	4.87885500	-3.39081500
H	-2.35164400	6.29335200	-3.83452500
H	-4.78501600	6.57099700	-4.26507800
H	-0.67053300	2.30526700	1.42936000
C	0.15551400	2.32889800	3.45214900
O	0.43504500	2.79963700	2.29000700
O	-0.49540200	1.28995000	3.65749700
C	0.64445600	3.15817100	4.63100200
H	0.01354300	4.04914800	4.70835700
H	0.57815500	2.59071100	5.55899600
H	1.66606100	3.50304000	4.45734900
H	2.11196600	1.73294100	1.27261000
O	2.25264500	1.34565400	-1.11538700

**TS4(SS)**

O	-1.23184100	1.52764700	-0.46880400
N	-0.37449700	-3.15598800	-1.07020600
N	-1.57899300	-3.67398500	-1.43447200
N	-1.58592200	-1.46573300	-1.48448800

C	1. 42149100	-4. 58649500	-1. 79139500
H	1. 12465200	-4. 33315400	-2. 80559800
C	2. 46375600	-5. 45545200	-1. 49644600
H	3. 01891900	-5. 92794000	-2. 29936600
C	2. 79422600	-5. 70352900	-0. 16497100
H	3. 60792100	-6. 38215600	0. 07249000
C	2. 10056900	-5. 08426100	0. 87084300
H	2. 38285700	-5. 29151600	1. 89766800
C	1. 03603600	-4. 21298900	0. 61574500
C	0. 73298700	-4. 00416700	-0. 73300000
C	-0. 35216600	-1. 83447700	-1. 12944100
C	-2. 29047800	-2. 61809000	-1. 69417400
C	-3. 66459100	-2. 34108700	-2. 19268200
H	-4. 41493600	-2. 75622200	-1. 51489300
H	-3. 80746000	-2. 80386100	-3. 17088100
C	-3. 69037800	-0. 78679700	-2. 27265000
H	-4. 54166200	-0. 37480800	-1. 72955800
H	-3. 79491300	-0. 46701600	-3. 31016700
C	-2. 34123900	-0. 22254600	-1. 71708400
H	-1. 80577400	0. 34042300	-2. 48622200
C	-2. 38483400	0. 72086900	-0. 45251600
C	-3. 54166500	1. 70292100	-0. 65301100
C	-4. 73898800	1. 63258100	0. 04857000
C	-3. 37661000	2. 70188500	-1. 62038400
C	-5. 76450700	2. 54005200	-0. 22279200
H	-4. 89333800	0. 87954400	0. 81527500
C	-4. 40463900	3. 59581900	-1. 87910100
H	-2. 43609000	2. 78420800	-2. 15514900
C	-5. 61186200	3. 52315000	-1. 18615900
C	-2. 48131400	-0. 06984000	0. 85201900
C	-3. 32747900	-1. 17192000	0. 97512300
C	-1. 66970400	0. 26306800	1. 93504900
C	-3. 33846900	-1. 93936400	2. 13391900
H	-3. 99363000	-1. 45267900	0. 16584400
C	-1. 68353200	-0. 51350500	3. 09049100
H	-1. 00031200	1. 11494100	1. 87459600
C	-2. 51443400	-1. 62040100	3. 20668500
H	-6. 41607200	4. 21843000	-1. 39981700
H	-2. 51218100	-2. 22515100	4. 10640600
H	-0. 46238900	1. 01459500	-0. 17263000
C	-4. 21310000	4. 69678800	-2. 88732200
C	-7. 03442100	2. 43688700	0. 57603000
C	-0. 74701600	-0. 12912500	4. 20480900
C	-4. 26503900	-3. 12092500	2. 17788400

F	-4.02515300	-3.91253100	3.22774000
F	-4.13848400	-3.86560200	1.06315400
F	-5.54714200	-2.73853100	2.23951500
F	-1.07455300	1.05621300	4.72931100
F	0.50996700	-0.03555300	3.75782200
F	-0.76281100	-1.03293200	5.19738900
F	-3.89713100	5.85290300	-2.29075800
F	-3.23619400	4.41004800	-3.75459400
F	-5.33655500	4.90943200	-3.58815700
F	-7.48296300	1.17198700	0.60387100
F	-8.00698100	3.20370800	0.07088500
F	-6.84245900	2.80887800	1.84799700
C	0.19013200	-3.62458600	1.73333600
C	1.00406800	-3.26131800	2.97508700
C	-0.93089500	-4.61788400	2.07239400
H	-0.27193400	-2.69447400	1.37618000
H	1.81592300	-2.56923800	2.73458000
H	0.35590100	-2.77874200	3.71127100
H	1.42959400	-4.14811600	3.45452000
H	-1.58712700	-4.78837800	1.21355200
H	-0.50318800	-5.58058900	2.37112700
H	-1.53788400	-4.24794600	2.90308100
C	2.84394800	0.31584400	-1.46044800
C	1.75939300	-0.68009600	-1.83745000
H	2.34627700	1.13642200	-0.92506900
C	0.81279300	-0.92791600	-0.80064900
H	2.06033400	-1.58446800	-2.38068200
C	3.53284000	0.94098800	-2.67427500
C	2.62669800	1.87539800	-3.47647500
H	3.92369800	0.15211600	-3.32997500
H	4.39930500	1.51671400	-2.31944500
C	3.37221200	2.52589800	-4.63909200
H	1.75877100	1.32632500	-3.85656400
H	2.23759100	2.65307100	-2.80681200
H	2.72234100	3.19915800	-5.20379700
H	4.22932700	3.10625600	-4.28248700
H	3.75075500	1.76778800	-5.33227700
O	0.71426700	-0.34901000	0.29425000
H	2.04315100	0.70707000	1.15808800
C	5.75643900	2.41778900	1.68803100
C	4.47057200	0.75440900	0.42905900
C	3.78726400	1.51012300	1.35116000
N	4.50550700	2.43584700	2.04673600
O	2.47392200	1.42960700	1.64439600

S	6.13717300	1.23616400	0.46495800
C	3.83471600	-0.31629400	-0.42269900
H	3.20614800	-0.89583400	0.27008300
C	6.77773800	3.30278500	2.27022800
C	6.41991400	4.12402400	3.34568000
C	8.08582300	3.34685000	1.77941100
C	7.35981800	4.97087100	3.91833200
H	5.40073700	4.07903100	3.71372900
C	9.02336800	4.19494200	2.35711100
H	8.37359900	2.72260400	0.93750400
C	8.66361000	5.00963700	3.42756500
H	7.07456200	5.60290600	4.75321200
H	10.03574400	4.22264000	1.96736300
H	9.39597000	5.67318200	3.87603100
C	4.78524900	-1.32552100	-1.04155300
C	5.88899000	-0.95048300	-1.81874200
C	4.54298400	-2.68955000	-0.85849100
C	6.73272100	-1.90761900	-2.37270000
H	6.09467500	0.09866200	-2.00289100
C	5.38823900	-3.64927800	-1.41026800
H	3.68415600	-3.00473000	-0.26747200
C	6.48901200	-3.26228500	-2.16632200
H	7.58401200	-1.59160500	-2.96715300
H	5.18682900	-4.70174800	-1.23977100
H	7.15246200	-4.00855400	-2.59138200
H	0.91837100	-0.31381600	-2.72129600
C	-0.19165000	-1.34727600	-4.31356000
O	-0.03199700	-0.19085500	-3.76740900
O	0.06551100	-2.42887600	-3.76426500
C	-0.73801700	-1.32192900	-5.73210600
H	-1.61959600	-0.67794500	-5.78115000
H	0.01377000	-0.88378500	-6.39364200
H	-0.97988200	-2.32935000	-6.06911900

**M4(RR)**

O	-0.58501900	-0.40054100	1.25843400
N	1.66598300	-2.40216000	-1.88690300
N	0.67569100	-2.68991100	-2.77893600
N	0.11383600	-1.02998000	-1.42108600
C	3.81405200	-2.57401300	-2.95698200
H	3.47040400	-1.79637200	-3.63177700
C	5.09744600	-3.09013600	-3.04208700
H	5.78172700	-2.72696100	-3.80048500
C	5.49709600	-4.06784700	-2.13166300

H	6.50294600	-4.47219400	-2.17877100
C	4.61333900	-4.53681800	-1.16821500
H	4.93840800	-5.31145500	-0.48061600
C	3.30490500	-4.04577500	-1.06066900
C	2.95201500	-3.04705400	-1.96925000
C	1.35054600	-1.40038600	-1.05667000
C	-0.25745300	-1.84261800	-2.46315500
C	-1.61168600	-1.49984000	-2.97735800
H	-2.34562700	-2.22962000	-2.62111600
H	-1.63911300	-1.48704700	-4.06729400
C	-1.82563500	-0.10201900	-2.34749100
H	-2.87132700	0.06773300	-2.09187000
H	-1.52775000	0.67312600	-3.05915800
C	-0.90290100	0.00215800	-1.10125800
H	-0.39836400	0.96898500	-1.04885100
C	-1.56314400	-0.28416000	0.27830800
C	-2.53049400	0.84667100	0.65680700
C	-3.13734500	0.72921200	1.91388000
C	-2.80150100	1.96981600	-0.11702600
C	-4.01963500	1.69615000	2.36271100
H	-2.90053100	-0.12745900	2.53675400
C	-3.70097900	2.93643800	0.34434400
H	-2.32799400	2.12668300	-1.08122700
C	-4.32040600	2.80764700	1.57573000
C	-2.29305700	-1.62781200	0.22347600
C	-3.60327900	-1.74730100	-0.23208800
C	-1.59405400	-2.77894500	0.60450400
C	-4.19165300	-3.00487400	-0.35720400
H	-4.18456500	-0.86303800	-0.47974800
C	-2.20489500	-4.02204400	0.49866300
H	-0.59046700	-2.67180100	1.00911000
C	-3.50150800	-4.15171100	0.00474600
H	-5.02977700	3.55359700	1.91953200
H	-3.97095600	-5.12655800	-0.07721100
H	0.14596200	0.26683100	1.07341300
C	-3.98646500	4.15039300	-0.49497600
C	-4.67984700	1.58015200	3.70879000
C	-1.48450000	-5.27387600	0.91346400
C	-5.56090800	-3.10244000	-0.96700200
F	-5.48826400	-3.00960700	-2.30654900
F	-6.35842200	-2.11068700	-0.55141600
F	-6.15911900	-4.26346200	-0.67958000
F	-0.30418500	-5.00888100	1.49082200
F	-1.24546000	-6.06792500	-0.14368600

F	-2.20890900	-5.99208200	1.78063400
F	-3.17018900	5.17181300	-0.19271400
F	-3.81953000	3.89620500	-1.80413800
F	-5.24067900	4.58519300	-0.32162500
F	-6.01491600	1.65013600	3.59589700
F	-4.30721300	2.58040700	4.51925400
F	-4.38220900	0.42826300	4.31930500
C	2.33224000	-4.64959000	-0.06624600
C	2.90730500	-4.71871200	1.35047200
C	1.91785700	-6.04154000	-0.56456600
H	1.43720900	-4.01975500	-0.02570300
H	3.20133000	-3.72806500	1.70285400
H	2.14703400	-5.11236400	2.02937300
H	3.77227300	-5.38855500	1.39861400
H	1.44130700	-5.98596700	-1.54758700
H	2.79432600	-6.69297600	-0.64608900
H	1.21438600	-6.49761500	0.13416400
C	4.15193100	0.46019000	0.89944700
C	3.60416100	-0.37853600	-0.27252500
H	3.41584300	0.40832100	1.70830100
C	2.30658800	-1.05293600	0.10072300
H	3.44772500	0.23426600	-1.16655900
C	5.47375700	-0.10920300	1.42445400
C	5.34294200	-1.53064900	1.97228400
H	5.85438100	0.54314700	2.21947000
H	6.22568700	-0.09062300	0.61997800
C	6.65913300	-2.05907100	2.53558700
H	4.56626600	-1.54436000	2.74635800
H	4.98873600	-2.20863400	1.18391400
H	6.54910900	-3.07565600	2.92273600
H	7.43658500	-2.07480000	1.76454000
H	7.01711400	-1.42560400	3.35301500
O	2.10295600	-1.65671500	1.13084900
H	4.30912500	-1.17352400	-0.54813600
C	1.41957400	3.75497300	-1.48784600
C	3.06780100	2.47685200	-0.20215600
C	1.77756200	1.97779700	-0.18467600
N	0.86460000	2.71849200	-0.93177600
O	1.39194100	0.88224200	0.41217900
S	3.11700800	3.92815400	-1.15075100
C	4.29833600	1.95199000	0.49423800
H	5.14382900	2.01137800	-0.20991700
C	0.69037000	4.72904400	-2.31442700
C	-0.68710500	4.88059700	-2.12674800

C	1. 34049800	5. 50200800	-3. 28062700
C	-1. 40347200	5. 78946600	-2. 89493400
H	-1. 17024800	4. 30021300	-1. 34898400
C	0. 62164200	6. 41267000	-4. 04669500
H	2. 40781400	5. 37664000	-3. 44188100
C	-0. 75090900	6. 55677000	-3. 85806800
H	-2. 46969800	5. 90213700	-2. 73095500
H	1. 13356700	7. 00611600	-4. 79739900
H	-1. 31005600	7. 26836400	-4. 45709300
C	4. 64831400	2. 80595200	1. 70375100
C	3. 69119200	3. 01431600	2. 70156200
C	5. 91170200	3. 37638000	1. 84964900
C	3. 99807300	3. 77168500	3. 82550600
H	2. 70015400	2. 58241000	2. 57878500
C	6. 22034800	4. 14146600	2. 97353600
H	6. 66060500	3. 21880400	1. 07694200
C	5. 26474800	4. 33903400	3. 96424800
H	3. 24667900	3. 92561900	4. 59363500
H	7. 20720700	4. 58296500	3. 07276400
H	5. 50283000	4. 93436700	4. 83995200

#### M4(RS)

O	-1. 01685500	-0. 10781900	1. 56403000
N	1. 67319100	-1. 94593900	-1. 67556000
N	0. 84992500	-2. 00882300	-2. 76052600
N	0. 04994000	-0. 66458900	-1. 19227700
C	3. 96523000	-1. 94628200	-2. 40156800
H	3. 73018900	-1. 03336900	-2. 93975200
C	5. 25091300	-2. 46816000	-2. 38727200
H	6. 04779600	-1. 96930800	-2. 92692600
C	5. 50111000	-3. 62292900	-1. 65147700
H	6. 50422400	-4. 03525900	-1. 61639900
C	4. 47671900	-4. 25877800	-0. 95579000
H	4. 70285300	-5. 15792200	-0. 39487800
C	3. 16671300	-3. 76718900	-0. 95607900
C	2. 96209700	-2. 59090400	-1. 68572600
C	1. 21531100	-1. 13076500	-0. 71788800
C	-0. 13392400	-1. 22703600	-2. 42919600
C	-1. 38596900	-0. 76084300	-3. 08554100
H	-2. 11740700	-1. 57271600	-3. 11466800
H	-1. 19643200	-0. 44174800	-4. 11146100
C	-1. 80485500	0. 41192900	-2. 16238200
H	-2. 88149000	0. 45102600	-1. 99504900
H	-1. 52166000	1. 35992000	-2. 62521700

C	-1.02639900	0.28650900	-0.82194200
H	-0.54775300	1.23218800	-0.57072100
C	-1.81971500	-0.19766600	0.43531400
C	-3.00862900	0.76374300	0.61692600
C	-4.33106300	0.36128700	0.75630100
C	-2.70192700	2.12732700	0.74916600
C	-5.33670200	1.30360700	0.98763300
H	-4.60263200	-0.68835200	0.71906300
C	-3.71122000	3.05011100	0.97645200
H	-1.66863900	2.47285200	0.70254900
C	-5.04193300	2.65124100	1.09349100
C	-2.20741600	-1.66859800	0.25037500
C	-3.11503800	-2.11168800	-0.71074900
C	-1.54884500	-2.62201800	1.03296800
C	-3.33257800	-3.47461000	-0.90866100
H	-3.67550100	-1.40748200	-1.31959700
C	-1.80356900	-3.97615700	0.84980100
H	-0.83346300	-2.27970700	1.77307000
C	-2.68499800	-4.42290000	-0.13091100
H	-5.82395500	3.37722000	1.28521300
H	-2.86394900	-5.48151600	-0.28329500
H	-0.21470900	0.49058600	1.39810700
C	-3.38646600	4.51578700	1.06302300
C	-6.75752900	0.82345200	1.08508000
C	-1.16931100	-4.97115400	1.78072200
C	-4.25174200	-3.88178500	-2.02335100
F	-3.70390900	-3.59207400	-3.22145700
F	-5.41546900	-3.22112700	-1.96858300
F	-4.51696500	-5.19078600	-2.01192800
F	-0.00654600	-4.52302300	2.26965100
F	-0.92333100	-6.14285900	1.16104500
F	-1.96323100	-5.24591100	2.82224900
F	-2.11555300	4.72854400	1.40870600
F	-3.58993100	5.12092800	-0.12345700
F	-4.17014500	5.14095300	1.95256300
F	-6.85875600	-0.25455400	1.87417200
F	-7.23166000	0.46789700	-0.12000200
F	-7.57206700	1.76707300	1.57264700
C	2.02129100	-4.49182100	-0.26754500
C	2.49675500	-5.50850300	0.76890500
C	1.14052800	-5.18144500	-1.32212200
H	1.41162700	-3.74760400	0.26149100
H	3.13254300	-5.04334200	1.52793700
H	1.63291700	-5.94471900	1.27082500



H	3. 05082200	-6. 32728300	0. 29807200
H	0. 74086000	-4. 47268200	-2. 05213600
H	1. 72246600	-5. 93323600	-1. 86536300
H	0. 30322500	-5. 68477200	-0. 83253900
C	3. 69307900	0. 50853100	1. 75937200
C	3. 33238400	-0. 30163700	0. 49855400
H	2. 80063500	0. 54492400	2. 39085200
C	1. 99047900	-0. 98303500	0. 60905100
H	3. 31151700	0. 33971900	-0. 38716300
C	4. 80928000	-0. 16504900	2. 56199400
C	4. 41503500	-1. 54195800	3. 09753300
H	5. 07835700	0. 48028400	3. 41035700
H	5. 71394800	-0. 25928100	1. 94613500
C	5. 52540900	-2. 17297400	3. 93263000
H	3. 49655900	-1. 45293300	3. 68853100
H	4. 16029100	-2. 20749400	2. 26196800
H	5. 23434000	-3. 15782800	4. 30723500
H	6. 43965200	-2. 29392500	3. 34223300
H	5. 77149700	-1. 54659500	4. 79594400
O	1. 59416700	-1. 63220200	1. 54609500
H	4. 08421300	-1. 07889400	0. 30599700
C	1. 26294000	4. 25756300	-0. 26055500
C	2. 83425900	2. 66743100	0. 76225200
C	1. 53884900	2. 20752200	0. 58866500
N	0. 67575700	3. 12464200	-0. 00730500
O	1. 08428000	1. 02633100	0. 89792600
S	2. 94485200	4. 30323600	0. 18426100
C	4. 02637200	1. 98496900	1. 38878800
H	4. 25530600	2. 48504700	2. 34175600
C	0. 59436700	5. 40279800	-0. 90039800
C	-0. 74329400	5. 28191600	-1. 29116700
C	1. 26247700	6. 61091300	-1. 12537500
C	-1. 39785800	6. 34852000	-1. 89363900
H	-1. 25873700	4. 34513400	-1. 10706800
C	0. 60691000	7. 67451700	-1. 73322400
H	2. 29942200	6. 72371000	-0. 82050500
C	-0. 72495600	7. 54684600	-2. 12014500
H	-2. 44002800	6. 24504000	-2. 17659900
H	1. 13603100	8. 60684100	-1. 90158500
H	-1. 23722400	8. 37949000	-2. 59130800
C	5. 28801700	2. 08534000	0. 53528000
C	5. 24597000	2. 05185900	-0. 86238400
C	6. 53886900	2. 18244400	1. 15294000
C	6. 41651700	2. 08143300	-1. 61568800

H	4. 28223500	2. 03601900	-1. 36432000
C	7. 71164400	2. 21561800	0. 40472800
H	6. 59043900	2. 23463200	2. 23786700
C	7. 65465700	2. 15816600	-0. 98519200
H	6. 35883100	2. 06097700	-2. 69989900
H	8. 67021000	2. 29507600	0. 90800100
H	8. 56715900	2. 18946500	-1. 57197200

**M4(SR)**

O	1. 48089500	1. 14719600	-0. 73336000
N	-0. 64343300	-1. 01679500	2. 72584600
N	0. 39654400	-1. 56127100	3. 43279900
N	1. 07445200	0. 04699500	2. 08629900
C	-2. 55204100	-0. 90011300	4. 17499700
H	-1. 95994100	-0. 22327800	4. 78348600
C	-3. 86019800	-1. 21574100	4. 51292500
H	-4. 31218200	-0. 79012400	5. 40200900
C	-4. 57767800	-2. 07436700	3. 68540100
H	-5. 60680600	-2. 32306200	3. 92372000
C	-3. 98448700	-2. 62881300	2. 55589600
H	-4. 56497800	-3. 30307400	1. 93790200
C	-2. 66299800	-2. 34291200	2. 18948900
C	-1. 98957600	-1. 44196000	3. 02340000
C	-0. 25491100	-0. 02156900	1. 91864200
C	1. 42861900	-0. 89604000	3. 00906700
C	2. 88575200	-0. 85655100	3. 31842600
H	3. 37346600	-1. 77145700	2. 97480400
H	3. 05243700	-0. 77403100	4. 39376700
C	3. 33738700	0. 41882000	2. 55260800
H	4. 29131500	0. 28544000	2. 04137700
H	3. 47311800	1. 23632500	3. 26331500
C	2. 21209900	0. 82103000	1. 55339300
H	1. 95152200	1. 87688000	1. 63194500
C	2. 45462100	0. 52767500	0. 02465400
C	3. 79821500	1. 18434400	-0. 35024200
C	4. 92459800	0. 51797000	-0. 81360100
C	3. 84183500	2. 58444800	-0. 26456600
C	6. 08450900	1. 22873700	-1. 14066400
H	4. 92332300	-0. 55637400	-0. 95986900
C	4. 99702600	3. 27651400	-0. 58220000
H	2. 94673500	3. 13049500	0. 01510400
C	6. 14005800	2. 60400000	-1. 01901400
C	2. 41433100	-0. 98989700	-0. 21167900
C	3. 34007800	-1. 87802100	0. 33496000

C	1. 35986100	-1. 51302900	-0. 96564200
C	3. 21180500	-3. 25224200	0. 14554900
H	4. 18973400	-1. 51889800	0. 90814100
C	1. 26090600	-2. 88498700	-1. 17349100
H	0. 62810500	-0. 82651100	-1. 37875500
C	2. 17729200	-3. 77292500	-0. 61603800
H	7. 04217700	3. 14848700	-1. 27580700
H	2. 08448000	-4. 84210200	-0. 77046800
H	0. 70923800	1. 54342500	-0. 14330400
C	5. 05449800	4. 77518200	-0. 47815900
C	7. 28083900	0. 44568800	-1. 60355900
C	0. 18537200	-3. 41381100	-2. 08168600
C	4. 22856500	-4. 14049800	0. 80058900
F	4. 05655800	-5. 42814300	0. 49287800
F	4. 16755100	-4. 03302000	2. 14384500
F	5. 47489400	-3. 79344500	0. 45010100
F	-0. 91926500	-2. 66067600	-2. 03313300
F	-0. 16558300	-4. 67248600	-1. 75266600
F	0. 59266700	-3. 44795900	-3. 35680300
F	3. 88440100	5. 30155200	-0. 10048700
F	5. 97933900	5. 16057700	0. 41573000
F	5. 39418800	5. 33146300	-1. 64894900
F	6. 96349400	-0. 37952000	-2. 61044900
F	7. 76641000	-0. 32089800	-0. 61378900
F	8. 27297100	1. 24052300	-2. 02126200
C	-1. 99313200	-3. 01594800	1. 00124100
C	-2. 98388300	-3. 76197700	0. 10867800
C	-0. 91399100	-3. 99861800	1. 48792100
H	-1. 52349800	-2. 23304600	0. 39115100
H	-3. 79055400	-3. 11158100	-0. 23647800
H	-2. 45903700	-4. 13492400	-0. 77257100
H	-3. 41154100	-4. 62671800	0. 62908800
H	-0. 10920900	-3. 50806700	2. 04034900
H	-1. 36068900	-4. 75436400	2. 14265700
H	-0. 47576500	-4. 51222200	0. 62823800
C	-2. 96880400	2. 73662200	1. 31910400
C	-2. 32860800	1. 44014200	1. 84546600
H	-2. 33741800	3. 57762300	1. 63245200
C	-1. 06975100	1. 00567300	1. 07179700
H	-3. 07086900	0. 63378600	1. 84541800
C	-4. 36000300	2. 89728500	1. 94158400
C	-4. 38787300	2. 78593300	3. 46746900
H	-5. 03192900	2. 13521800	1. 51583500
H	-4. 77048400	3. 87251800	1. 65791100

C	-5.76522600	3.11408300	4.03748900
H	-4.10339800	1.77233700	3.77597200
H	-3.63806500	3.46613900	3.89370200
H	-5.78403000	3.02130900	5.12666900
H	-6.06137500	4.13603200	3.78178400
H	-6.52325800	2.43779500	3.62964500
O	-0.27586600	2.00445900	0.76060600
H	-2.03427500	1.60176100	2.88819800
C	-4.24025100	-0.59246200	-1.89301600
C	-3.37419000	1.42815700	-0.80254800
C	-2.62528100	0.28472300	-0.69370100
N	-3.10814500	-0.83815700	-1.29752200
O	-1.42769600	0.14363900	-0.07052300
S	-4.78312600	1.05352000	-1.74139300
C	-2.96556200	2.76502500	-0.23920600
H	-1.90521200	2.85748200	-0.49761100
C	-4.99093700	-1.60293400	-2.65318300
C	-4.32244000	-2.75411600	-3.08738200
C	-6.34801100	-1.44259500	-2.94748100
C	-5.00887200	-3.72810300	-3.80143800
H	-3.26597000	-2.85747700	-2.86217900
C	-7.02783000	-2.41770200	-3.66824800
H	-6.87771500	-0.55936300	-2.60007800
C	-6.36144400	-3.56367100	-4.09475800
H	-4.48405200	-4.61693400	-4.13692100
H	-8.08162600	-2.28502700	-3.89062800
H	-6.89385000	-4.32594100	-4.65433700
C	-3.66087800	3.97751500	-0.82702200
C	-5.05250500	4.10766900	-0.90722800
C	-2.87413100	5.03756900	-1.28499700
C	-5.63416100	5.25366800	-1.44159100
H	-5.69538600	3.31294100	-0.53997600
C	-3.45140800	6.18834700	-1.81371600
H	-1.79215000	4.95234400	-1.22802600
C	-4.83576100	6.29862900	-1.89759400
H	-6.71552600	5.32982200	-1.49815200
H	-2.81719700	6.99588200	-2.16562300
H	-5.28951800	7.19171600	-2.31501000

**M4(SS)**

O	1.04648200	-0.96444300	0.24695000
N	-1.35393800	0.34855800	-3.25906600
N	-0.59404000	1.42514900	-3.62867400
N	0.58248200	-0.04871900	-2.47938000

C	-3.01353200	-0.68210700	-4.67782300
H	-2.20659200	-1.25331900	-5.12760200
C	-4.33011800	-0.85114600	-5.08452400
H	-4.57192800	-1.56672300	-5.86237300
C	-5.32739000	-0.08755000	-4.48331600
H	-6.36076700	-0.20985200	-4.79112800
C	-5.01273700	0.83121500	-3.48755500
H	-5.80752400	1.40861800	-3.02755800
C	-3.69901300	1.02230300	-3.04699400
C	-2.72627500	0.23862800	-3.67492000
C	-0.65907000	-0.54751500	-2.55976300
C	0.57847800	1.14933000	-3.13900300
C	1.95155700	1.72718000	-3.20978400
H	2.06644300	2.54231300	-2.48935000
H	2.17269200	2.11027800	-4.20642000
C	2.80992500	0.48925300	-2.83360200
H	3.71770400	0.78160000	-2.30646400
H	3.10178800	-0.04212000	-3.74393600
C	1.91242600	-0.44669400	-1.97109900
H	2.03998000	-1.50755900	-2.19036200
C	2.03572100	-0.26513000	-0.41475000
C	3.34615600	-0.91068600	0.06302900
C	4.35386000	-1.40223600	-0.75410900
C	3.49220100	-1.03024400	1.45309500
C	5.49570000	-1.98917700	-0.19596200
H	4.28839300	-1.35884000	-1.83684700
C	4.62569200	-1.60903400	1.99335700
H	2.69143700	-0.68190300	2.09615300
C	5.64629600	-2.09565400	1.17262000
C	2.04396900	1.24545900	-0.09998200
C	0.83691200	1.95774900	0.00223200
C	3.24477900	1.94813300	-0.02090700
C	0.86869500	3.34428500	0.11150900
H	-0.12315900	1.43887000	-0.00975000
C	3.25658900	3.33728300	0.09881400
H	4.19365400	1.42003500	-0.06088400
C	2.07110300	4.04974300	0.15015800
H	6.53256000	-2.55315300	1.59833900
H	2.07688700	5.13183100	0.22628400
H	0.08099600	-0.63539200	0.11149700
C	4.80288800	-1.70889400	3.48346700
C	6.54795200	-2.50741400	-1.13436100
C	4.58735200	4.03438000	0.12992700
C	-0.39491400	4.15813900	0.17796100

F	-1.49279200	3.41890200	0.02229700
F	-0.40384700	5.10498200	-0.77693100
F	-0.49617100	4.80130200	1.35426100
F	5.34748400	3.59493000	1.14040500
F	4.45951100	5.35936100	0.25787700
F	5.27405500	3.80023600	-1.00187900
F	3.68068800	-1.40967000	4.14472100
F	5.17663500	-2.94538000	3.84457900
F	5.76221700	-0.87430800	3.91196600
F	6.06907400	-3.49190800	-1.90958700
F	7.61475200	-2.98342600	-0.48468700
F	6.97281300	-1.53923900	-1.96322400
C	-3.34876700	2.04036900	-1.97934600
C	-4.41999600	2.14267200	-0.89253800
C	-3.11595200	3.40907500	-2.63897400
H	-2.42092100	1.71450000	-1.49137400
H	-4.65347200	1.15982700	-0.46936200
H	-4.05277400	2.78000900	-0.08447700
H	-5.34221800	2.59038700	-1.27799300
H	-2.32368200	3.36155700	-3.38981700
H	-4.03483100	3.74828900	-3.12980600
H	-2.83675700	4.14638100	-1.88326900
C	-2.48602200	-3.13490400	-0.45032500
C	-2.46050100	-2.28582900	-1.74656500
H	-1.49578200	-3.06792700	0.01690800
C	-1.03802700	-1.93562800	-2.08889300
H	-3.05181300	-1.37551300	-1.63586800
C	-2.78068000	-4.60968300	-0.75928500
C	-1.78035700	-5.28904400	-1.69309500
H	-3.79246600	-4.68469200	-1.18913100
H	-2.80684700	-5.17157900	0.18021600
C	-2.12911600	-6.75825700	-1.91764000
H	-1.74101100	-4.77134100	-2.65971000
H	-0.77459000	-5.19821300	-1.26965200
H	-1.41221900	-7.24257100	-2.58578000
H	-2.13030100	-7.30795900	-0.97143600
H	-3.12496900	-6.86291700	-2.36078300
O	-0.10968800	-2.70880900	-2.04207200
H	-2.87814400	-2.85478400	-2.58875800
C	-3.40684700	1.04537700	2.07628900
C	-3.29075800	-1.12320700	0.93153800
C	-2.28146800	-0.22354500	0.62489400
N	-2.37679200	0.99275200	1.28942700
O	-1.30176500	-0.38024400	-0.23222600

S	-4.37238500	-0.40149600	2.09122200
C	-3.51945200	-2.57153100	0.55717800
H	-4.50959300	-2.66151000	0.08112000
C	-3.76164500	2.23515500	2.86653100
C	-2.82713000	3.27066200	2.97734000
C	-5.00698400	2.36782200	3.48794800
C	-3.13651300	4.41956600	3.69320000
H	-1.86382300	3.15174800	2.49773500
C	-5.30994800	3.51610100	4.21088400
H	-5.74622100	1.57651800	3.39622500
C	-4.37795600	4.54606900	4.31420500
H	-2.40347100	5.21694800	3.76618400
H	-6.27975300	3.61010200	4.68896800
H	-4.61938400	5.44294800	4.87559000
C	-3.54703700	-3.43049600	1.81612600
C	-2.45237800	-3.42177500	2.68564300
C	-4.64032900	-4.24084600	2.11654500
C	-2.44891300	-4.21801500	3.82427800
H	-1.60831800	-2.77092300	2.46786600
C	-4.64245900	-5.03625200	3.26181600
H	-5.49690800	-4.25035600	1.44660700
C	-3.54563300	-5.02860700	4.11623900
H	-1.59205500	-4.20216200	4.49041200
H	-5.50308300	-5.65902900	3.48551500
H	-3.54498100	-5.64580200	5.00893400

#### TS5(RR)

O	-0.40959200	0.59905800	-1.33801600
N	2.73398600	2.08267100	1.24650400
N	2.01781600	2.89093400	2.08144500
N	0.74392900	1.36171700	1.11684700
C	4.82479300	1.47912500	2.25727500
H	4.22273100	1.02144600	3.03855000
C	6.21103300	1.42810700	2.24698800
H	6.74265100	0.93056300	3.05063300
C	6.90992900	2.01172000	1.18933100
H	7.99429600	1.96694000	1.16875300
C	6.23077900	2.64585400	0.15628800
H	6.79308200	3.09628300	-0.65665100
C	4.83198800	2.72453500	0.13570900
C	4.17171100	2.11971300	1.20480500
C	1.98588700	1.14454800	0.68001600
C	0.81353300	2.41580900	1.98883200
C	-0.49882500	2.65443500	2.64755700

H	-1.00081000	3.52649200	2.21743400
H	-0.37665200	2.81536300	3.71886900
C	-1.24036000	1.33051100	2.32637900
H	-2.30824900	1.49676500	2.18469400
H	-1.10998000	0.63257300	3.15850200
C	-0.57447200	0.70455900	1.06386400
H	-0.42052600	-0.37503200	1.17274300
C	-1.27027300	0.97981400	-0.30249900
C	-2.60819800	0.24895400	-0.40777900
C	-3.27127500	0.32986100	-1.63899000
C	-3.19664100	-0.47184300	0.62404200
C	-4.51294700	-0.26045900	-1.80404100
H	-2.79936200	0.85511900	-2.46341400
C	-4.46641500	-1.03052600	0.45711800
H	-2.69815400	-0.62105300	1.57636200
C	-5.13644600	-0.92722400	-0.74775400
C	-1.44463700	2.49021400	-0.45427100
C	-2.57893400	3.15999200	-0.00364100
C	-0.37348500	3.22971800	-0.96452400
C	-2.62062500	4.55281700	-0.01992200
H	-3.43940300	2.60488700	0.36089400
C	-0.42762600	4.61782700	-0.96709200
H	0.49339900	2.70582400	-1.35917600
C	-1.54562400	5.29547400	-0.48943600
H	-6.12067700	-1.36631900	-0.87251000
H	-1.58259400	6.37911300	-0.49331300
H	-0.34526000	-0.36953600	-1.44461400
C	-5.11421400	-1.66778100	1.65492600
C	-5.24803600	-0.16487100	-3.11236300
C	0.78797200	5.39471000	-1.38929400
C	-3.81046900	5.24339300	0.58454700
F	-3.71259600	5.26075900	1.92523100
F	-4.95312200	4.61352500	0.28493100
F	-3.91652600	6.51215600	0.17585500
F	1.48733000	4.75579800	-2.33913500
F	1.61887200	5.56957100	-0.34713500
F	0.47281100	6.60807700	-1.85449000
F	-4.28686400	-2.51808300	2.27105800
F	-5.44640300	-0.73002200	2.56047500
F	-6.23587300	-2.32376800	1.33629100
F	-6.34671800	0.59489100	-2.99188000
F	-5.65573900	-1.37426800	-3.52461500
F	-4.49206900	0.36578200	-4.07831300
C	4.10780600	3.44469500	-0.98466000



C	4. 36603000	2. 77481900	-2. 33819300
C	4. 50659200	4. 92468200	-1. 01671300
H	3. 03201000	3. 39786900	-0. 78287000
H	4. 06927200	1. 72402100	-2. 32129300
H	3. 78985700	3. 28412600	-3. 11597500
H	5. 42567000	2. 83854000	-2. 60778800
H	4. 30635800	5. 41190400	-0. 05931500
H	5. 57207700	5. 03481500	-1. 24349200
H	3. 94005700	5. 44454800	-1. 79306800
C	3. 49956500	-2. 24849800	-0. 38155700
C	2. 90461800	-1. 13477500	0. 46981200
H	3. 35636800	-2. 00668800	-1. 44463200
C	2. 49784500	0. 04253100	-0. 22782700
H	3. 48317000	-0. 87959400	1. 36660900
C	5. 01940200	-2. 32848800	-0. 17672000
C	5. 73680700	-1. 04900500	-0. 60804200
H	5. 42575700	-3. 17587000	-0. 74168600
H	5. 22660200	-2. 52850700	0. 88584500
C	7. 24431600	-1. 12067600	-0. 38667200
H	5. 52228100	-0. 86148800	-1. 66816600
H	5. 33399600	-0. 18997200	-0. 05728700
H	7. 73740500	-0. 20483600	-0. 72482000
H	7. 47444700	-1. 24975200	0. 67653600
H	7. 68537800	-1. 96335200	-0. 92860900
O	2. 40956200	0. 23927100	-1. 43992200
H	1. 59113300	-1. 43150100	-1. 83754200
C	-1. 11155600	-3. 88641700	0. 13983000
C	1. 29736100	-3. 53730200	-0. 19759600
C	0. 44244700	-2. 76990200	-0. 94540600
N	-0. 89501800	-2. 94929700	-0. 74128300
O	0. 71951800	-1. 85590900	-1. 91633100
S	0. 33427400	-4. 58452600	0. 79108400
C	2. 80550900	-3. 61276100	-0. 11728700
H	3. 05516500	-3. 89034100	0. 91678100
C	-2. 45567600	-4. 36962900	0. 48694500
C	-3. 51732600	-4. 06459000	-0. 37285200
C	-2. 69201500	-5. 14638000	1. 62381700
C	-4. 79358700	-4. 53724100	-0. 09729700
H	-3. 31564200	-3. 46369100	-1. 25429700
C	-3. 97166300	-5. 61785000	1. 89436500
H	-1. 87523500	-5. 37372700	2. 30401900
C	-5. 02498300	-5. 31491300	1. 03578600
H	-5. 61233500	-4. 29838200	-0. 76942700
H	-4. 14833400	-6. 21687800	2. 78176800

H	-6.02416600	-5.67999800	1.25019400
C	3.34053200	-4.69785800	-1.03840200
C	3.00516800	-4.69150000	-2.39552500
C	4.19171200	-5.69191200	-0.55808200
C	3.51948800	-5.65700900	-3.25336700
H	2.32445500	-3.93157900	-2.77438600
C	4.70548800	-6.66314100	-1.41513000
H	4.45653400	-5.70247500	0.49655500
C	4.37192800	-6.64608200	-2.76527300
H	3.24988600	-5.64238800	-4.30473500
H	5.36570900	-7.43184100	-1.02592500
H	4.76956200	-7.40120700	-3.43561400
H	1.85256300	-1.43538900	1.23409900
C	1.30262200	-1.01614000	3.25636000
O	1.00294500	-1.69605100	2.19708700
O	2.01266600	-0.00348700	3.27134000
C	0.70273100	-1.55819100	4.54288300
H	1.18971100	-2.50597100	4.78751100
H	0.84683500	-0.85165200	5.35963900
H	-0.35883900	-1.77350500	4.39832900

**TS5(RS)**

O	-0.19066800	-0.07177000	-0.42027800
N	1.24518800	3.59798300	1.05054500
N	0.16715200	4.10835600	1.72185300
N	-0.02718000	1.94054400	1.36229400
C	3.47639100	4.35390300	1.56749000
H	3.42568500	3.72463800	2.45126600
C	4.60292800	5.10740600	1.26930000
H	5.46738000	5.07550000	1.92277000
C	4.60696300	5.90353200	0.12486900
H	5.48262300	6.49670700	-0.11796200
C	3.49867500	5.94265300	-0.71224400
H	3.52181600	6.56560000	-1.60157600
C	2.34865300	5.19244000	-0.44387700
C	2.37977800	4.41276600	0.71136800
C	1.14950500	2.28747700	0.83911800
C	-0.58763100	3.06430800	1.90254500
C	-1.86068200	2.73320300	2.61116400
H	-2.72640500	3.00608300	2.00022200
H	-1.93365100	3.25434800	3.56581600
C	-1.70708300	1.19645500	2.78201400
H	-2.66020000	0.66711600	2.76918000
H	-1.21751700	0.99737000	3.73789300

C	-0.74442700	0.70247900	1.67638100
H	-0.00340900	0.01429600	2.06414200
C	-1.33159400	0.06091900	0.39268000
C	-1.86788800	-1.33500000	0.73089900
C	-3.04817800	-1.85336700	0.20137300
C	-1.06022700	-2.17595300	1.50809700
C	-3.44115600	-3.15689500	0.50145100
H	-3.66410700	-1.26471100	-0.47112800
C	-1.48461400	-3.45880000	1.82517400
H	-0.07235300	-1.86293800	1.84275300
C	-2.68319100	-3.96454300	1.33618500
C	-2.33358000	1.01821700	-0.24968300
C	-3.63160100	1.17644900	0.23894900
C	-1.90072600	1.84503200	-1.29063100
C	-4.47294500	2.14803900	-0.29343700
H	-4.00608100	0.54087700	1.03599300
C	-2.76189600	2.79808700	-1.82653700
H	-0.89083800	1.73151600	-1.67720500
C	-4.05116500	2.96556700	-1.33348300
H	-2.99138100	-4.97910700	1.55898000
H	-4.71717300	3.70898900	-1.75728200
H	1.83747100	0.59308400	-2.57958700
C	-0.61707700	-4.27649300	2.74237600
C	-4.70960400	-3.67555300	-0.11463700
C	-2.27445100	3.71050000	-2.91810000
C	-5.81621200	2.35985700	0.34552300
F	-5.68952300	3.08406200	1.47162900
F	-6.38730300	1.19941500	0.69080500
F	-6.65884200	3.01405100	-0.45910900
F	-1.73504400	4.83137900	-2.39956100
F	-3.27223000	4.09638400	-3.72191500
F	-1.33236200	3.13493900	-3.66935800
F	0.67661500	-4.19824300	2.40436300
F	-0.70920000	-3.83280600	4.00940200
F	-0.96615700	-5.56927400	2.75141300
F	-5.79373800	-3.11349900	0.44126200
F	-4.83048700	-5.00160500	0.02043700
F	-4.76004100	-3.39375900	-1.42716200
C	1.14956100	5.24755500	-1.36854800
C	1.52730800	4.80610700	-2.78594500
C	0.54018700	6.65429100	-1.35614500
H	0.39017700	4.55032900	-0.99717000
H	1.95661900	3.80147200	-2.77200100
H	0.63812900	4.79772300	-3.42043700

H	2. 25511900	5. 49208200	-3. 23140700
H	0. 23762200	6. 94112100	-0. 34529000
H	1. 26321800	7. 39283900	-1. 71764900
H	-0. 33551600	6. 69144300	-2. 00745000
C	4. 19728800	-0. 09171700	0. 16886400
C	2. 99708300	0. 63241200	0. 77220300
H	5. 00579200	0. 64146600	0. 02252200
C	2. 15591300	1. 48465200	0. 00949500
H	3. 22571700	1. 12905100	1. 72164300
C	4. 72887700	-1. 15056600	1. 14831500
C	5. 18496700	-0. 58756200	2. 49484000
H	5. 57576600	-1. 66813700	0. 68166500
H	3. 95195600	-1. 90052700	1. 34259200
C	5. 76505600	-1. 67764700	3. 39229700
H	5. 93502900	0. 19716000	2. 32838400
H	4. 34536500	-0. 10873200	3. 01299100
H	6. 06987800	-1. 28147700	4. 36483100
H	5. 02459500	-2. 46611000	3. 56365400
H	6. 63978800	-2. 14362700	2. 92801100
O	2. 05991300	1. 71436400	-1. 20027400
H	-0. 36125800	-0. 69466800	-1. 14909200
C	0. 80483100	-3. 10676600	-1. 36134100
C	2. 67325600	-1. 50826400	-1. 36669000
C	1. 63288600	-1. 25339400	-2. 22729500
N	0. 59475600	-2. 14409800	-2. 22043000
O	1. 51098700	-0. 19530700	-3. 05208000
S	2. 27728100	-2. 93705900	-0. 46119500
C	3. 92235000	-0. 67667800	-1. 25073500
H	3. 72195100	0. 19051900	-1. 88654800
C	-0. 12654000	-4. 23308600	-1. 18558400
C	-1. 33073500	-4. 22944800	-1. 90071600
C	0. 17021500	-5. 31647700	-0. 35167100
C	-2. 22096400	-5. 28931300	-1. 77717300
H	-1. 54758100	-3. 39017300	-2. 55326900
C	-0. 72972500	-6. 36859400	-0. 22122300
H	1. 10360600	-5. 33698400	0. 20319700
C	-1. 92763300	-6. 35830200	-0. 93242400
H	-3. 15495800	-5. 27323300	-2. 32909800
H	-0. 49290400	-7. 19624100	0. 43917100
H	-2. 63080900	-7. 17881600	-0. 83052600
C	5. 18520500	-1. 31373800	-1. 82785300
C	5. 33780800	-2. 68078100	-2. 05736000
C	6. 25750000	-0. 46823300	-2. 13714100
C	6. 53266600	-3. 19003700	-2. 56447200

H	4.51888500	-3.36124000	-1.85308400
C	7.44989400	-0.97190000	-2.64234800
H	6.14837000	0.60381200	-1.98882500
C	7.59408400	-2.34116500	-2.85501300
H	6.62747200	-4.25785500	-2.73567400
H	8.26460000	-0.29434800	-2.87860400
H	8.52260600	-2.73917700	-3.25144000
C	1.77670700	-0.38672700	3.50679800
O	1.59836400	0.83399300	3.57217200
O	1.83372700	-1.05203400	2.38934800
H	2.23110700	-0.24588000	1.45522000
C	1.94212300	-1.23441800	4.75156600
H	1.29674600	-2.11367600	4.68968200
H	2.97536600	-1.59192000	4.79673700
H	1.71768300	-0.65121100	5.64377000

**TS5(SR)**

N	-0.71421200	-1.04255300	1.97756100
N	0.16046100	-1.56212200	2.87951500
N	1.13207700	-0.07483800	1.57014200
C	-2.87923600	-0.86715800	3.00471600
H	-2.41937000	-0.14073900	3.67052600
C	-4.20956600	-1.25668800	3.10222700
H	-4.84434200	-0.83359400	3.87300000
C	-4.71658100	-2.19175700	2.20237200
H	-5.75735800	-2.49773200	2.26152500
C	-3.90894000	-2.72999100	1.20423700
H	-4.33873500	-3.43550800	0.50138100
C	-2.56444600	-2.37278300	1.07700500
C	-2.09886400	-1.43359000	2.00252600
C	-0.15316000	-0.12479400	1.20224700
C	1.26913000	-0.93765600	2.61944300
C	2.62563300	-0.86912100	3.22227300
H	3.13545200	-1.83344800	3.15395300
H	2.54464700	-0.60652900	4.27859700
C	3.30227800	0.25820700	2.39198700
H	4.28068000	-0.04917400	2.02215600
H	3.45946600	1.13691300	3.01960800
C	2.35530200	0.66768600	1.21623500
C	2.84561300	0.39716700	-0.26464700
C	4.34097000	0.71767200	-0.33652100
C	5.33152900	-0.23779000	-0.53521100
C	4.71277100	2.05937800	-0.19836300
C	6.67362400	0.14169000	-0.57437200

H	5.07985500	-1.28198500	-0.68877500
C	6.05151000	2.42226700	-0.23788400
H	3.94673600	2.82095000	-0.09300800
C	7.04826100	1.46714900	-0.42289700
C	2.50576600	-1.02646800	-0.70232100
C	2.82001900	-2.12511000	0.10025100
C	1.80284700	-1.24972700	-1.88252500
C	2.41917300	-3.40582700	-0.25671400
H	3.38849100	-1.99450300	1.01694100
C	1.40571300	-2.53844700	-2.23308800
H	1.54986700	-0.41486600	-2.52584100
C	1.70704900	-3.62900700	-1.42986700
H	8.09176300	1.75691500	-0.46895900
H	1.38712800	-4.62734400	-1.70461600
H	1.28958200	1.20790400	-1.13640200
C	6.43024200	3.86513000	-0.03898500
C	7.71225700	-0.93058800	-0.75848700
C	0.59969200	-2.70579700	-3.49239600
C	2.76242900	-4.53183200	0.67678400
F	2.37540800	-4.24126300	1.93328000
F	4.08451000	-4.74458000	0.72412800
F	2.17439800	-5.67772600	0.32286900
F	-0.51497300	-1.96590400	-3.44135500
F	0.23537800	-3.98096600	-3.68463700
F	1.28811000	-2.31020200	-4.57034500
F	6.55762000	4.15835500	1.26367300
F	7.59932200	4.15103500	-0.62589200
F	5.50316900	4.68926000	-0.54046400
F	7.86830700	-1.64935200	0.36379100
F	8.90617900	-0.42029600	-1.07829000
F	7.35808100	-1.78888100	-1.72421200
C	-1.63670000	-3.04584400	0.07680200
C	-2.36361900	-3.62432800	-1.13748800
C	-0.85545200	-4.15241600	0.80608300
H	-0.92361900	-2.29606900	-0.29892600
H	-3.00828100	-2.88381200	-1.61695900
H	-1.62602000	-3.96714200	-1.86876600
H	-2.96576500	-4.49446700	-0.85357600
H	-0.19065500	-3.75570100	1.57834900
H	-1.55868300	-4.84027400	1.28667400
H	-0.25596300	-4.73184200	0.09875100
C	-2.22312500	2.91751100	-0.07709700
C	-1.60246000	1.82641600	0.78399600
H	-1.40000400	3.56120000	-0.41919900

C	-0.81424400	0.79222300	0.18887700
H	-2.20881800	1.45354600	1.61618000
C	-3.14161200	3.79756800	0.78116600
C	-2.47463100	4.32848100	2.05336400
H	-4.04154500	3.23433000	1.06580600
H	-3.48294100	4.64160800	0.17041200
C	-3.33463200	5.38298200	2.74441500
H	-2.28568200	3.50112200	2.74884100
H	-1.48890100	4.74303500	1.80822200
H	-2.86445000	5.74297700	3.66333500
H	-3.49970000	6.24457400	2.09008100
H	-4.31619100	4.97563900	3.00819600
O	-0.41986200	0.68597600	-0.98037900
H	-1.80389000	-0.00629200	-2.23575400
C	-5.52982800	-0.46862100	-0.64625800
C	-3.80247600	1.20333300	-1.15099100
C	-3.63605500	-0.05247900	-1.68283800
N	-4.61028100	-0.97113100	-1.41634400
O	-2.61901700	-0.48039000	-2.46002800
S	-5.24415000	1.18265700	-0.17727700
C	-2.90437000	2.38410600	-1.37593100
H	-2.08634900	1.99144200	-1.98846200
C	-6.68637100	-1.23942500	-0.16843400
C	-6.85860800	-2.54785000	-0.63588300
C	-7.58518600	-0.72137800	0.76868700
C	-7.90621100	-3.32612100	-0.16078300
H	-6.15565400	-2.93361200	-1.36730500
C	-8.63424700	-1.50327800	1.23929600
H	-7.45940200	0.29085800	1.14411800
C	-8.79570900	-2.80859200	0.78028500
H	-8.03204300	-4.33966900	-0.52770900
H	-9.32564800	-1.09350600	1.96832500
H	-9.61340000	-3.41848500	1.15022800
C	-3.49415200	3.53208300	-2.19316400
C	-4.85397700	3.68970300	-2.45715600
C	-2.60553300	4.48501400	-2.70792300
C	-5.31482000	4.77822600	-3.19691200
H	-5.56707400	2.95571000	-2.10113100
C	-3.06161000	5.57107200	-3.44396900
H	-1.53804000	4.36633800	-2.53707500
C	-4.42474500	5.72516200	-3.68852900
H	-6.37814300	4.87885500	-3.39081500
H	-2.35164400	6.29335200	-3.83452500
H	-4.78501600	6.57099700	-4.26507800

H	-0.67053300	2.30526700	1.42936000
C	0.15551400	2.32889800	3.45214900
O	0.43504500	2.79963700	2.29000700
O	-0.49540200	1.28995000	3.65749700
C	0.64445600	3.15817100	4.63100200
H	0.01354300	4.04914800	4.70835700
H	0.57815500	2.59071100	5.55899600
H	1.66606100	3.50304000	4.45734900
H	2.11196600	1.73294100	1.27261000
O	2.25264500	1.34565400	-1.11538700

**TS5(SS)**

O	-1.23184100	1.52764700	-0.46880400
N	-0.37449700	-3.15598800	-1.07020600
N	-1.57899300	-3.67398500	-1.43447200
N	-1.58592200	-1.46573300	-1.48448800
C	1.42149100	-4.58649500	-1.79139500
H	1.12465200	-4.33315400	-2.80559800
C	2.46375600	-5.45545200	-1.49644600
H	3.01891900	-5.92794000	-2.29936600
C	2.79422600	-5.70352900	-0.16497100
H	3.60792100	-6.38215600	0.07249000
C	2.10056900	-5.08426100	0.87084300
H	2.38285700	-5.29151600	1.89766800
C	1.03603600	-4.21298900	0.61574500
C	0.73298700	-4.00416700	-0.73300000
C	-0.35216600	-1.83447700	-1.12944100
C	-2.29047800	-2.61809000	-1.69417400
C	-3.66459100	-2.34108700	-2.19268200
H	-4.41493600	-2.75622200	-1.51489300
H	-3.80746000	-2.80386100	-3.17088100
C	-3.69037800	-0.78679700	-2.27265000
H	-4.54166200	-0.37480800	-1.72955800
H	-3.79491300	-0.46701600	-3.31016700
C	-2.34123900	-0.22254600	-1.71708400
H	-1.80577400	0.34042300	-2.48622200
C	-2.38483400	0.72086900	-0.45251600
C	-3.54166500	1.70292100	-0.65301100
C	-4.73898800	1.63258100	0.04857000
C	-3.37661000	2.70188500	-1.62038400
C	-5.76450700	2.54005200	-0.22279200
H	-4.89333800	0.87954400	0.81527500
C	-4.40463900	3.59581900	-1.87910100
H	-2.43609000	2.78420800	-2.15514900



C	-5.61186200	3.52315000	-1.18615900
C	-2.48131400	-0.06984000	0.85201900
C	-3.32747900	-1.17192000	0.97512300
C	-1.66970400	0.26306800	1.93504900
C	-3.33846900	-1.93936400	2.13391900
H	-3.99363000	-1.45267900	0.16584400
C	-1.68353200	-0.51350500	3.09049100
H	-1.00031200	1.11494100	1.87459600
C	-2.51443400	-1.62040100	3.20668500
H	-6.41607200	4.21843000	-1.39981700
H	-2.51218100	-2.22515100	4.10640600
H	-0.46238900	1.01459500	-0.17263000
C	-4.21310000	4.69678800	-2.88732200
C	-7.03442100	2.43688700	0.57603000
C	-0.74701600	-0.12912500	4.20480900
C	-4.26503900	-3.12092500	2.17788400
F	-4.02515300	-3.91253100	3.22774000
F	-4.13848400	-3.86560200	1.06315400
F	-5.54714200	-2.73853100	2.23951500
F	-1.07455300	1.05621300	4.72931100
F	0.50996700	-0.03555300	3.75782200
F	-0.76281100	-1.03293200	5.19738900
F	-3.89713100	5.85290300	-2.29075800
F	-3.23619400	4.41004800	-3.75459400
F	-5.33655500	4.90943200	-3.58815700
F	-7.48296300	1.17198700	0.60387100
F	-8.00698100	3.20370800	0.07088500
F	-6.84245900	2.80887800	1.84799700
C	0.19013200	-3.62458600	1.73333600
C	1.00406800	-3.26131800	2.97508700
C	-0.93089500	-4.61788400	2.07239400
H	-0.27193400	-2.69447400	1.37618000
H	1.81592300	-2.56923800	2.73458000
H	0.35590100	-2.77874200	3.71127100
H	1.42959400	-4.14811600	3.45452000
H	-1.58712700	-4.78837800	1.21355200
H	-0.50318800	-5.58058900	2.37112700
H	-1.53788400	-4.24794600	2.90308100
C	2.84394800	0.31584400	-1.46044800
C	1.75939300	-0.68009600	-1.83745000
H	2.34627700	1.13642200	-0.92506900
C	0.81279300	-0.92791600	-0.80064900
H	2.06033400	-1.58446800	-2.38068200
C	3.53284000	0.94098800	-2.67427500

C	2. 62669800	1. 87539800	-3. 47647500
H	3. 92369800	0. 15211600	-3. 32997500
H	4. 39930500	1. 51671400	-2. 31944500
C	3. 37221200	2. 52589800	-4. 63909200
H	1. 75877100	1. 32632500	-3. 85656400
H	2. 23759100	2. 65307100	-2. 80681200
H	2. 72234100	3. 19915800	-5. 20379700
H	4. 22932700	3. 10625600	-4. 28248700
H	3. 75075500	1. 76778800	-5. 33227700
O	0. 71426700	-0. 34901000	0. 29425000
H	2. 04315100	0. 70707000	1. 15808800
C	5. 75643900	2. 41778900	1. 68803100
C	4. 47057200	0. 75440900	0. 42905900
C	3. 78726400	1. 51012300	1. 35116000
N	4. 50550700	2. 43584700	2. 04673600
O	2. 47392200	1. 42960700	1. 64439600
S	6. 13717300	1. 23616400	0. 46495800
C	3. 83471600	-0. 31629400	-0. 42269900
H	3. 20614800	-0. 89583400	0. 27008300
C	6. 77773800	3. 30278500	2. 27022800
C	6. 41991400	4. 12402400	3. 34568000
C	8. 08582300	3. 34685000	1. 77941100
C	7. 35981800	4. 97087100	3. 91833200
H	5. 40073700	4. 07903100	3. 71372900
C	9. 02336800	4. 19494200	2. 35711100
H	8. 37359900	2. 72260400	0. 93750400
C	8. 66361000	5. 00963700	3. 42756500
H	7. 07456200	5. 60290600	4. 75321200
H	10. 03574400	4. 22264000	1. 96736300
H	9. 39597000	5. 67318200	3. 87603100
C	4. 78524900	-1. 32552100	-1. 04155300
C	5. 88899000	-0. 95048300	-1. 81874200
C	4. 54298400	-2. 68955000	-0. 85849100
C	6. 73272100	-1. 90761900	-2. 37270000
H	6. 09467500	0. 09866200	-2. 00289100
C	5. 38823900	-3. 64927800	-1. 41026800
H	3. 68415600	-3. 00473000	-0. 26747200
C	6. 48901200	-3. 26228500	-2. 16632200
H	7. 58401200	-1. 59160500	-2. 96715300
H	5. 18682900	-4. 70174800	-1. 23977100
H	7. 15246200	-4. 00855400	-2. 59138200
H	0. 91837100	-0. 31381600	-2. 72129600
C	-0. 19165000	-1. 34727600	-4. 31356000
O	-0. 03199700	-0. 19085500	-3. 76740900

O	0.06551100	-2.42887600	-3.76426500
C	-0.73801700	-1.32192900	-5.73210600
H	-1.61959600	-0.67794500	-5.78115000
H	0.01377000	-0.88378500	-6.39364200
H	-0.97988200	-2.32935000	-6.06911900

**M5(RR)**

O	-0.94878100	0.37207700	0.50237900
N	2.30117000	-1.55858300	-2.35947200
N	1.60235200	-2.55671400	-2.98978300
N	0.26090300	-1.08601900	-2.03666400
C	4.44668800	-1.31257000	-3.44428400
H	3.90479000	-0.99308300	-4.32826700
C	5.83181700	-1.37582500	-3.42349900
H	6.40284200	-1.10442600	-4.30422100
C	6.47649000	-1.78753300	-2.25788700
H	7.56012700	-1.83520000	-2.22573000
C	5.74032200	-2.13980000	-1.13329200
H	6.26095900	-2.45923700	-0.23505600
C	4.34054900	-2.08638200	-1.11824300
C	3.73348800	-1.65439700	-2.29918100
C	1.50695100	-0.64195000	-1.80078500
C	0.36363200	-2.22531100	-2.78184000
C	-0.96831000	-2.72377600	-3.22414000
H	-1.13246700	-3.75131300	-2.89274400
H	-1.02388200	-2.72221700	-4.31460500
C	-1.93779900	-1.68215200	-2.59108100
H	-2.74951900	-2.16489500	-2.04623800
H	-2.40262500	-1.08664900	-3.37819000
C	-1.12239100	-0.72481200	-1.66089800
H	-1.28007500	0.32697100	-1.91179000
C	-1.38655900	-0.79539900	-0.09452500
C	-2.91184300	-0.79006300	0.08166800
C	-3.66224200	-1.90077700	0.45900800
C	-3.56620700	0.42373500	-0.15312300
C	-5.04682200	-1.80389400	0.58327500
H	-3.18246200	-2.84737000	0.68600700
C	-4.94879300	0.50202700	-0.02733500
H	-2.97854700	1.30515100	-0.40724900
C	-5.70422000	-0.60696800	0.33885900
C	-0.71959300	-2.02020700	0.54632200
C	-0.78515200	-3.29180100	-0.01393400
C	-0.00592500	-1.86256900	1.73955500
C	-0.12499000	-4.37285000	0.56656500

H	-1.37024800	-3.47406700	-0.90739300
C	0.60735800	-2.95630200	2.33824800
H	0.06670200	-0.87853200	2.18649700
C	0.57013400	-4.22125100	1.75402300
H	-6.77983100	-0.53210300	0.44619400
H	1.07618500	-5.06333100	2.21328700
H	0.08524500	0.42270700	0.44228300
C	-5.62567700	1.81438600	-0.31261100
C	-5.83032400	-3.03631600	0.93678900
C	1.28087500	-2.80714100	3.67420600
C	-0.19461900	-5.69185800	-0.14497000
F	0.16464100	-5.55254100	-1.43623500
F	-1.44068000	-6.18671900	-0.14942000
F	0.60807300	-6.60852800	0.40291200
F	1.63828000	-1.54379400	3.92316400
F	2.39188000	-3.56550200	3.74556000
F	0.48038000	-3.20382800	4.67285100
F	-5.07514100	2.81506500	0.37978900
F	-5.52988300	2.12753300	-1.61679900
F	-6.93198500	1.77822800	-0.01052400
F	-6.03137100	-3.81055600	-0.14243300
F	-7.03441300	-2.73641500	1.43857100
F	-5.18525400	-3.78929000	1.83865700
C	3.57560800	-2.46834700	0.13830300
C	3.95442800	-1.54842400	1.30493700
C	3.81881500	-3.94250500	0.48488300
H	2.50006900	-2.33663600	-0.03694400
H	3.64030400	-0.52109100	1.10414900
H	3.44777900	-1.87637500	2.21513000
H	5.03274200	-1.57173900	1.49604700
H	3.43152300	-4.60541600	-0.29488800
H	4.88674100	-4.14805900	0.60956100
H	3.32413800	-4.18262100	1.42936300
C	3.51074400	2.31133500	-0.15276700
C	3.17098500	1.27538300	-1.22839000
H	3.30256800	1.83261400	0.81015400
C	1.79355700	0.64663500	-0.98574600
H	3.21280400	1.70458000	-2.23757100
C	5.01143400	2.64385500	-0.23002300
C	5.92653300	1.53443600	0.28947500
H	5.21806100	3.55106300	0.34961800
H	5.27325700	2.87843200	-1.27291500
C	7.40337900	1.89172900	0.14403400
H	5.68976300	1.34654700	1.34432900

H	5.73603400	0.59225000	-0.23968600
H	8.04838300	1.09777900	0.53019300
H	7.66189600	2.05261500	-0.90769000
H	7.64053300	2.81129200	0.68804600
O	1.51706300	0.40896000	0.27498500
H	3.93525400	0.49891500	-1.17046700
C	-1.19334200	4.06908900	-0.67456800
C	1.19058200	3.51724600	-0.40348000
C	0.41319200	2.63014500	-1.09648800
N	-0.91350800	2.93361600	-1.24665900
O	0.80772900	1.48961200	-1.70153500
S	0.16104700	4.82866800	0.10221300
C	2.69034300	3.63013500	-0.19799300
H	3.07924300	4.21595700	-1.04691000
C	-2.52582200	4.69268600	-0.70362100
C	-3.39950100	4.37264500	-1.74720800
C	-2.92690800	5.60796600	0.27444200
C	-4.65123900	4.97142200	-1.81671700
H	-3.07766400	3.65525200	-2.49512400
C	-4.18227100	6.19959800	0.20341400
H	-2.26118200	5.84238500	1.10069300
C	-5.04574000	5.88555700	-0.84373000
H	-5.32473400	4.71366700	-2.62736600
H	-4.48996500	6.90251500	0.97079000
H	-6.02551000	6.34913000	-0.89818900
C	2.96347600	4.42707400	1.07129200
C	2.55135400	3.91282400	2.30551100
C	3.60582600	5.66323600	1.03495800
C	2.78669100	4.62000200	3.47791500
H	2.02636300	2.95978600	2.32987300
C	3.84219200	6.37504200	2.21041400
H	3.92418500	6.07085800	0.07846300
C	3.43516500	5.85394000	3.43340100
H	2.45895700	4.21195700	4.42884800
H	4.34351100	7.33687100	2.16655700
H	3.61785300	6.40651600	4.34948300

**M5(RS)**

O	1.28560400	-0.12434900	-1.82001800
N	-1.65134300	-1.43817600	1.63964100
N	-0.80521400	-1.46440600	2.72214900
N	0.04733000	-0.32330000	1.03862900
C	-3.85503500	-1.45460000	2.60753200
H	-3.56197200	-0.55399200	3.13835300

C	-5.12366100	-2.00108000	2.75034900
H	-5.84997600	-1.53189500	3.40442500
C	-5.44811900	-3.15108900	2.03825900
H	-6.43888800	-3.58384400	2.13075100
C	-4.50920700	-3.75831600	1.21004400
H	-4.78666900	-4.65739100	0.67190200
C	-3.21875000	-3.24294300	1.05193300
C	-2.93979200	-2.06951900	1.76062000
C	-1.16225600	-0.72412000	0.61866100
C	0.21634800	-0.77202700	2.31815400
C	1.47605300	-0.25282400	2.92261800
H	2.20355800	-1.05741500	3.05012100
H	1.28501800	0.18359600	3.90418400
C	1.89867800	0.81270600	1.87398100
H	2.97897300	0.86665700	1.73708400
H	1.56827700	1.79840900	2.21228100
C	1.15647700	0.50866000	0.53811000
H	0.71202000	1.41301800	0.12705400
C	1.98231300	-0.16429800	-0.62463400
C	3.18478700	0.76811000	-0.84842000
C	4.51594300	0.36889600	-0.86062100
C	2.89250300	2.11579200	-1.09665900
C	5.53256700	1.30625300	-1.06071300
H	4.78599100	-0.67404700	-0.73079400
C	3.91103600	3.04232100	-1.25867800
H	1.85821200	2.43822200	-1.18298600
C	5.24748100	2.64997100	-1.23883100
C	2.35994000	-1.59914300	-0.23385600
C	3.22976000	-1.89459900	0.81649300
C	1.77163700	-2.66389600	-0.92176800
C	3.47850100	-3.21256200	1.19185500
H	3.74531000	-1.10118400	1.34971600
C	2.05204700	-3.97639700	-0.55614800
H	1.08896000	-2.46473100	-1.73984800
C	2.89483400	-4.27062700	0.51046300
H	6.04295300	3.37248400	-1.37725000
H	3.09556900	-5.29631600	0.79791700
H	0.37077500	-0.57278300	-1.76210600
C	3.55174500	4.49637800	-1.37640700
C	6.95528700	0.82217200	-1.03587000
C	1.48324400	-5.09504600	-1.38321000
C	4.36675000	-3.44754200	2.37871500
F	3.75779700	-3.06060900	3.51791000
F	5.49846300	-2.73514300	2.29278100

F	4. 69754800	-4. 73389300	2. 52116400
F	0. 27249200	-4. 78213400	-1. 86711900
F	1. 35337600	-6. 22552500	-0. 66791600
F	2. 26578800	-5. 38209000	-2. 43056500
F	3. 31233900	5. 02652600	-0. 15760000
F	4. 53289700	5. 21778300	-1. 92928800
F	2. 44092000	4. 68203100	-2. 09662300
F	7. 13447900	-0. 21205600	-1. 86856900
F	7. 29878100	0. 39625300	0. 19024400
F	7. 81888400	1. 78358200	-1. 38432400
C	-2. 16126900	-3. 94406100	0. 21449700
C	-2. 75947500	-4. 91597100	-0. 80253700
C	-1. 19135800	-4. 67504900	1. 15679700
H	-1. 59932900	-3. 19070300	-0. 35429000
H	-3. 50945400	-4. 42664500	-1. 43263800
H	-1. 96706900	-5. 29468600	-1. 44902800
H	-3. 22706400	-5. 77689800	-0. 31267200
H	-0. 68752600	-3. 98196500	1. 83787800
H	-1. 73575500	-5. 40635600	1. 76380800
H	-0. 43261700	-5. 21110200	0. 58257500
C	-3. 77246900	0. 27226500	-2. 06964400
C	-3. 21396200	-0. 60719800	-0. 94249000
H	-2. 94760100	0. 52670000	-2. 74675000
C	-1. 68474600	-0. 49912800	-0. 83157600
H	-3. 71165500	-0. 35381900	-0. 00228400
C	-4. 82011400	-0. 48888000	-2. 88630100
C	-4. 17300700	-1. 53806800	-3. 79372500
H	-5. 39891100	0. 20903300	-3. 50639200
H	-5. 54017700	-0. 96582900	-2. 20705700
C	-5. 19282100	-2. 50399200	-4. 38891700
H	-3. 63338000	-1. 02198800	-4. 59668000
H	-3. 40560100	-2. 09131600	-3. 23739300
H	-4. 71912700	-3. 22523500	-5. 05964100
H	-5. 70471500	-3. 06400900	-3. 59930600
H	-5. 95757000	-1. 96707200	-4. 95972100
O	-0. 99667000	-1. 28278600	-1. 61721400
H	-3. 42748200	-1. 66280000	-1. 13014500
C	-1. 75576800	3. 91228600	0. 45096000
C	-3. 20617200	2. 32605700	-0. 74681500
C	-1. 89276400	1. 96827400	-0. 58643700
N	-1. 09040300	2. 85404600	0. 09045000
O	-1. 26373400	0. 89564400	-1. 10942900
S	-3. 44002400	3. 87534200	0. 00555700
C	-4. 30623800	1. 62006000	-1. 49803200

H	-4.57523600	2.24159500	-2.36357500
C	-1.14105400	5.06102700	1.13289800
C	0.23631800	5.26747300	0.99297300
C	-1.89821600	5.95315400	1.89664100
C	0.84411500	6.35344500	1.60923700
H	0.81511800	4.58350600	0.38177400
C	-1.28505900	7.03834000	2.51295900
H	-2.96561700	5.79004000	2.02068000
C	0.08563400	7.24070800	2.37109900
H	1.90952000	6.51094700	1.47817900
H	-1.87874600	7.72423800	3.10826900
H	0.56120700	8.09040000	2.85006600
C	-5.57134400	1.46001200	-0.66317300
C	-5.52713600	1.24120900	0.71719100
C	-6.82354500	1.51364200	-1.28250500
C	-6.69542600	1.05885800	1.45141100
H	-4.56669700	1.23415700	1.22660000
C	-7.99389700	1.33183000	-0.55269900
H	-6.88037700	1.70746900	-2.35048800
C	-7.93363700	1.09934500	0.81890600
H	-6.63518500	0.89656600	2.52345700
H	-8.95471300	1.38175000	-1.05518800
H	-8.84627000	0.96441800	1.39044200

### M5(SR)

O	-1.43757500	0.05834700	0.82956700
N	0.77435800	-1.98847200	-1.58453700
N	-0.20973600	-2.67590300	-2.25464800
N	-0.86329900	-0.65564200	-1.68096200
C	3.10133500	-2.32018400	-2.17411700
H	2.94115000	-1.63662100	-3.00169400
C	4.34321200	-2.90126200	-1.95113900
H	5.18134400	-2.65731200	-2.59429000
C	4.48917000	-3.80342400	-0.90319200
H	5.45466700	-4.25991300	-0.70896800
C	3.40192300	-4.12963700	-0.09922000
H	3.53811000	-4.85025500	0.70010000
C	2.14369000	-3.55080700	-0.28282000
C	2.04188700	-2.62899700	-1.32914800
C	0.39299700	-0.75524100	-1.23411800
C	-1.19578000	-1.82849000	-2.29407500
C	-2.58007100	-1.75346700	-2.85668200
H	-3.26347200	-2.39257100	-2.29084900
H	-2.60597000	-2.06764400	-3.90105600



C	-2.88992300	-0.23692600	-2.68522900
H	-3.94615400	-0.04438000	-2.50590200
H	-2.61108100	0.28763300	-3.60272400
C	-1.97621300	0.28416000	-1.54347900
H	-1.60326700	1.28589500	-1.74181200
C	-2.50891800	0.21653300	-0.03479500
C	-3.21278700	1.54765000	0.29805200
C	-4.44155500	1.64052700	0.94775600
C	-2.48673000	2.72939900	0.09594800
C	-4.96119900	2.88188600	1.31354700
H	-5.00642300	0.75329300	1.21125800
C	-3.01074600	3.95823100	0.47346300
H	-1.47246900	2.68931900	-0.29744000
C	-4.26257700	4.05421100	1.07235000
C	-3.38508800	-1.03047800	0.08612300
C	-4.70034200	-1.09428900	-0.38001500
C	-2.79467500	-2.20201800	0.56791500
C	-5.39448500	-2.29984100	-0.38900000
H	-5.20329100	-0.20566700	-0.74989500
C	-3.49799800	-3.40330100	0.54680900
H	-1.78175000	-2.15287500	0.95786500
C	-4.80070900	-3.47016400	0.06561700
H	-4.66777800	5.01424900	1.36888800
H	-5.34410100	-4.40775600	0.05708700
H	-0.66010000	0.69927500	0.52190000
C	-2.19488900	5.19239800	0.20447900
C	-6.31777600	2.91753700	1.95931800
C	-2.80707900	-4.66204100	0.99152500
C	-6.77794900	-2.31457500	-0.97515400
F	-6.72747200	-2.16324500	-2.31026900
F	-7.52210000	-1.30845800	-0.49974900
F	-7.42043300	-3.45975900	-0.72374300
F	-2.03428400	-4.44991000	2.06618200
F	-2.00681200	-5.14224800	0.02397700
F	-3.67896400	-5.62940600	1.29913700
F	-0.92477100	5.03825700	0.60429100
F	-2.15595100	5.47425400	-1.10751100
F	-2.69245500	6.26702500	0.82961200
F	-6.39966900	2.04523900	2.97398800
F	-7.27904400	2.58318800	1.08396200
F	-6.61576000	4.13131900	2.43723100
C	0.96713300	-3.88696900	0.61853700
C	0.84841100	-2.86868100	1.76382200
C	1.05032400	-5.30894800	1.17860600

H	0.05649900	-3.83655200	0.00976600
H	0.57748500	-1.87083900	1.41069000
H	0.09067300	-3.20564700	2.47748500
H	1.80676100	-2.77280000	2.28511800
H	1.22802300	-6.04562700	0.39009800
H	1.84811500	-5.39772500	1.92316500
H	0.11138100	-5.55592900	1.67712500
C	2.70931400	2.36893500	-1.42899900
C	2.13581100	0.97629500	-1.74005900
H	1.90113500	3.10149800	-1.54782700
C	1.18013900	0.45389300	-0.64658600
H	2.95362300	0.26625500	-1.89872400
C	3.83870600	2.70267000	-2.40779100
C	3.46204400	2.56968700	-3.88418400
H	4.70204000	2.05213600	-2.19555900
H	4.17249400	3.73051500	-2.22670000
C	4.56372000	3.09048000	-4.80360100
H	3.25446900	1.52113100	-4.12942100
H	2.53141200	3.12212000	-4.07132500
H	4.29676800	2.97736400	-5.85752400
H	4.75756000	4.15085500	-4.61636600
H	5.49956200	2.54852000	-4.63377100
O	0.32926600	1.37428400	-0.23821300
H	1.56035300	1.03017600	-2.67148000
C	5.23031400	-0.74105000	1.10969100
C	3.87877200	1.20344000	0.46921000
C	3.23219900	0.00472500	0.61722900
N	3.97848300	-1.07475100	0.98293200
O	1.90288200	-0.19204000	0.45066600
S	5.55900600	0.94423100	0.79370800
C	3.14318000	2.45433600	0.06636400
H	2.19865600	2.39433400	0.61989300
C	6.28549100	-1.68975300	1.49407600
C	5.91792600	-2.90937200	2.07548000
C	7.63847500	-1.41286900	1.28001600
C	6.89132700	-3.83442700	2.43011200
H	4.86341600	-3.10608600	2.23989900
C	8.60992100	-2.33928900	1.64228200
H	7.93307200	-0.47556500	0.81521200
C	8.24004900	-3.55303500	2.21541900
H	6.59870200	-4.77592000	2.88457600
H	9.65755200	-2.11511500	1.46992000
H	8.99913400	-4.27602000	2.49619000
C	3.76887900	3.78593200	0.42521500

C	5. 11343000	4. 09931200	0. 20098600
C	2. 94037000	4. 77576000	0. 96221500
C	5. 61813500	5. 35458300	0. 52887300
H	5. 77692000	3. 36744000	-0. 25125400
C	3. 43936400	6. 03391000	1. 28396800
H	1. 88854600	4. 55372100	1. 12477200
C	4. 78402500	6. 32576400	1. 07485300
H	6. 66635800	5. 57383800	0. 35145600
H	2. 77612600	6. 78397100	1. 70300500
H	5. 17874900	7. 30362700	1. 33145200

**M5(SS)**

O	-0. 81106900	1. 04209500	-0. 08269200
N	1. 04527400	-2. 67396600	-2. 02964100
N	-0. 04933800	-3. 28894200	-2. 57980500
N	-0. 43934800	-1. 16558400	-2. 12915900
C	2. 93158000	-3. 64045500	-3. 15473400
H	2. 49422300	-3. 25353700	-4. 06966500
C	4. 12510500	-4. 34389000	-3. 16784400
H	4. 64432800	-4. 51884100	-4. 10343800
C	4. 64222600	-4. 82133500	-1. 96432800
H	5. 57430100	-5. 37688500	-1. 95641800
C	3. 96756500	-4. 59475400	-0. 77266600
H	4. 38151800	-4. 98258800	0. 15280300
C	2. 76176700	-3. 88096600	-0. 72010200
C	2. 27868600	-3. 41424700	-1. 94374600
C	0. 83371300	-1. 37990900	-1. 76796800
C	-0. 93514200	-2. 33906800	-2. 62393400
C	-2. 31701800	-2. 17694400	-3. 16017100
H	-3. 03853600	-2. 71676200	-2. 54357600
H	-2. 38615100	-2. 57069800	-4. 17558400
C	-2. 48850300	-0. 63221900	-3. 11461100
H	-3. 48980000	-0. 32468900	-2. 81164700
H	-2. 32250900	-0. 22503300	-4. 11418400
C	-1. 40176200	-0. 04573100	-2. 16639600
H	-0. 88739100	0. 80400300	-2. 61500900
C	-1. 85132800	0. 40352100	-0. 72517900
C	-2. 97208100	1. 44683200	-0. 91781300
C	-2. 60015300	2. 63440700	-1. 56603400
C	-4. 27276700	1. 33641300	-0. 44311400
C	-3. 52195300	3. 64478300	-1. 77718300
H	-1. 56810200	2. 77850700	-1. 86994100
C	-5. 19319400	2. 36869900	-0. 65137800
H	-4. 59263500	0. 46979900	0. 12444200

C	-4.83733500	3.52086700	-1.32730400
C	-2.27717000	-0.82868100	0.08662800
C	-1.48358400	-1.21300200	1.17317400
C	-3.38492000	-1.61235400	-0.23671600
C	-1.80979800	-2.35705200	1.89751200
H	-0.62123600	-0.60524100	1.44534500
C	-3.68116400	-2.76781400	0.48225000
H	-4.04800200	-1.33435100	-1.05060300
C	-2.89851100	-3.15484100	1.55886500
H	-5.55852100	4.31525300	-1.48660500
H	-3.13147600	-4.05200100	2.12064500
H	0.07379000	1.03708800	-0.64556400
C	-6.59898600	2.17772400	-0.15555700
C	-3.12438400	4.92042500	-2.46580800
C	-4.86309400	-3.57917600	0.04137900
C	-1.00325400	-2.70190300	3.11679100
F	-1.44883800	-2.04877600	4.20302700
F	0.28647200	-2.37637600	2.96720900
F	-1.06215900	-4.01422700	3.40119200
F	-5.98780800	-2.85064700	0.04460000
F	-5.06339800	-4.65105500	0.81186500
F	-4.69861700	-4.01665500	-1.22498900
F	-7.26258300	1.28793400	-0.91157500
F	-6.61647600	1.70730400	1.09888600
F	-7.29700300	3.31981100	-0.17605100
F	-1.88110800	4.86272100	-2.95727500
F	-3.18306600	5.96622900	-1.63026200
F	-3.95250300	5.19412700	-3.48703700
C	2.05820000	-3.67931600	0.60898300
C	3.02843700	-3.12786500	1.66058500
C	1.41704600	-4.99383500	1.07012800
H	1.26559800	-2.93763500	0.48260500
H	3.54059000	-2.23711800	1.28694400
H	2.48230200	-2.84929200	2.56285500
H	3.78037900	-3.87282900	1.94082000
H	0.69696300	-5.36176500	0.33316600
H	2.17649700	-5.76904300	1.21773700
H	0.89567000	-4.84252700	2.01863700
C	4.03178100	0.86849900	-1.53616700
C	3.19044400	-0.38173000	-1.81099600
H	3.42050200	1.73159200	-1.82323300
C	1.77262800	-0.26281000	-1.22949300
H	3.69712000	-1.27846000	-1.43359700
C	5.31243000	0.84644200	-2.39082200

C	5. 10047000	0. 62874800	-3. 89019400
H	5. 99274800	0. 07050400	-2. 00693300
H	5. 83617500	1. 79902700	-2. 25616300
C	6. 36702000	0. 92849700	-4. 68893800
H	4. 79273900	-0. 40506500	-4. 08702000
H	4. 28086600	1. 27097200	-4. 23894600
H	6. 22202200	0. 74576900	-5. 75688600
H	6. 67000900	1. 97217400	-4. 56280200
H	7. 19742300	0. 30048600	-4. 35044600
O	1. 22356800	0. 90617800	-1. 45074300
H	3. 08087500	-0. 49543900	-2. 89518400
C	1. 89888900	1. 30205400	2. 97608000
C	3. 29065400	1. 06582100	0. 95978100
C	2. 18464200	0. 26773100	1. 06278900
N	1. 41058100	0. 39763100	2. 17593800
O	1. 80020400	-0. 68455700	0. 17985200
S	3. 35030800	2. 05765300	2. 38925300
C	4. 43112700	1. 02897800	-0. 03901500
H	5. 03876900	0. 14373900	0. 21143400
C	1. 28070900	1. 64570500	4. 26558500
C	0. 30347700	0. 78719300	4. 78128800
C	1. 63490800	2. 79306800	4. 98048600
C	-0. 30907600	1. 07511200	5. 99280700
H	0. 04422100	-0. 10403800	4. 22231600
C	1. 01988400	3. 07599100	6. 19517200
H	2. 38137200	3. 47460500	4. 58086400
C	0. 04617600	2. 22005700	6. 70409400
H	-1. 06420600	0. 39981900	6. 38265700
H	1. 29726700	3. 97104500	6. 74242900
H	-0. 43392600	2. 44459200	7. 65115100
C	5. 32129100	2. 24912100	0. 13668000
C	4. 81161000	3. 52798200	-0. 11291000
C	6. 65355800	2. 11938000	0. 52535900
C	5. 62170100	4. 64967600	0. 01976500
H	3. 76915800	3. 63693900	-0. 40298000
C	7. 46750100	3. 24228000	0. 65994500
H	7. 05701000	1. 12903700	0. 72088200
C	6. 95390500	4. 50940000	0. 40551000
H	5. 21249600	5. 63598500	-0. 17515000
H	8. 50268800	3. 12475100	0. 96458500
H	7. 58619900	5. 38541600	0. 50914000
<b>TS6(RR)</b>			
O	-0. 82508900	0. 94007700	0. 87947500

N	0.26839300	-2.73267000	-1.94241600
N	-0.59476000	-2.67401000	-3.02079900
N	-0.64433600	-0.87209600	-1.76025400
C	2.00885200	-4.16964000	-2.78416200
H	2.00925100	-3.54637200	-3.67243000
C	2.89252000	-5.22912000	-2.64169400
H	3.60445900	-5.45408900	-3.42838700
C	2.86200200	-5.98770800	-1.47241400
H	3.55956600	-6.80824000	-1.33733500
C	1.93753100	-5.69722100	-0.47657100
H	1.92181300	-6.30485000	0.42369200
C	1.01651100	-4.64761400	-0.59955300
C	1.10054900	-3.88151400	-1.76721500
C	0.28161700	-1.64683500	-1.14528800
C	-1.14070000	-1.50867900	-2.86365700
C	-2.16636900	-0.68422300	-3.56375600
H	-3.10648100	-1.23254800	-3.66738900
H	-1.82987200	-0.41625300	-4.56756500
C	-2.29283100	0.56041300	-2.63575100
H	-3.31118500	0.65510600	-2.25742100
H	-2.08389100	1.47903200	-3.18522300
C	-1.26640700	0.41506700	-1.46240000
H	-0.50118000	1.19587400	-1.50375200
C	-1.82656300	0.49744400	0.01011300
C	-2.85760100	1.63108000	0.03880300
C	-4.23440200	1.43185900	0.05841400
C	-2.36184300	2.93774800	0.00966100
C	-5.10177000	2.52301600	0.02720800
H	-4.64915700	0.42921100	0.11049900
C	-3.23957400	4.01430100	-0.02521700
H	-1.28604700	3.09503000	0.04102700
C	-4.61749800	3.82204400	-0.02015900
C	-2.40365500	-0.84125300	0.47989200
C	-3.14878800	-1.66994800	-0.36398200
C	-2.15859800	-1.26662200	1.78383300
C	-3.61542000	-2.90013700	0.07890400
H	-3.36689700	-1.37862300	-1.38457400
C	-2.66014000	-2.48881500	2.22887400
H	-1.56482400	-0.64355400	2.44336600
C	-3.38647100	-3.31869700	1.38529100
H	-5.29612000	4.66604700	-0.04115200
H	-3.75213300	-4.28004200	1.73237300
H	-0.04288400	0.34907200	0.92384200
C	-2.66311600	5.40081600	-0.07761300

C	-6.57995800	2.25231000	0.01499000
C	-2.45663500	-2.91027700	3.65801500
C	-4.36375600	-3.80872600	-0.85547000
F	-4.34557100	-3.35147500	-2.11681400
F	-5.64688600	-3.94095900	-0.49393400
F	-3.83038100	-5.03830200	-0.86036700
F	-1.37847100	-2.33546400	4.20172200
F	-2.29763000	-4.24276200	3.75257600
F	-3.51054800	-2.58930600	4.41992100
F	-1.80513800	5.61810900	0.92506800
F	-1.97474900	5.59568900	-1.22082700
F	-3.60939400	6.34557800	-0.02040500
F	-6.95084200	1.65736800	-1.13044000
F	-7.29862000	3.37424600	0.13697100
F	-6.93478200	1.42780600	1.00992000
C	-0.00498400	-4.39787100	0.49885400
C	0.66392000	-3.81288500	1.74919000
C	-0.77581400	-5.67838000	0.83980100
H	-0.73284800	-3.66488800	0.13224200
H	1.01642300	-2.79176000	1.57844100
H	-0.04369500	-3.78806400	2.58221800
H	1.51404300	-4.43254500	2.05796900
H	-1.28786400	-6.08284900	-0.03696300
H	-0.11398800	-6.45236500	1.24089600
H	-1.52038600	-5.45985000	1.61031400
C	4.35165900	-1.03439800	0.28160400
C	3.00999700	-1.54929500	-0.27164900
H	4.22294300	-0.87670100	1.36120100
C	1.89676100	-0.61399900	0.09080400
H	3.06266700	-1.67549200	-1.35842600
C	5.43857800	-2.10105100	0.05920700
C	5.06705800	-3.50831000	0.52871100
H	6.35177200	-1.78574700	0.57590300
H	5.69044300	-2.13388900	-1.01205300
C	6.26272300	-4.45600800	0.48879000
H	4.66400900	-3.45839100	1.54956300
H	4.27033600	-3.92068900	-0.10027700
H	5.97905300	-5.46603000	0.79646000
H	6.67449900	-4.51788500	-0.52380200
H	7.06272400	-4.11285500	1.15179700
O	1.47194000	-0.47719500	1.22123600
H	2.77609700	-2.51513800	0.17938400
C	2.73815100	3.67670700	-0.12652900
C	3.83653000	1.47724300	-0.20957000

C	2.49640000	1.53432200	-0.48003200
N	1.87778300	2.74362900	-0.43432100
O	1.74440000	0.44808000	-0.83381100
S	4.35907000	3.09544600	0.13226000
C	4.80103100	0.31241400	-0.36339900
H	4.88038800	0.11663700	-1.44436700
C	2.39796900	5.10311700	-0.00638500
C	1.13637700	5.54418400	-0.41955000
C	3.31334600	6.02816300	0.50687400
C	0.80211200	6.88928200	-0.32498200
H	0.43094900	4.82579800	-0.82210600
C	2.97524100	7.37227000	0.59899600
H	4.29140400	5.69759400	0.84631000
C	1.71934600	7.80673200	0.18211500
H	-0.17806500	7.21730200	-0.65165100
H	3.69244200	8.08064200	1.00046000
H	1.45588300	8.85699200	0.25411600
C	6.18626400	0.70022700	0.12684400
C	6.40446600	0.97984200	1.48048700
C	7.26314700	0.76696000	-0.75574200
C	7.67426300	1.31429700	1.93742900
H	5.57023300	0.94146900	2.17695700
C	8.53630100	1.10308000	-0.30069600
H	7.10187500	0.55223100	-1.80896700
C	8.74470600	1.37583900	1.04718300
H	7.82916400	1.52870900	2.99002500
H	9.36385100	1.15206700	-1.00117300
H	9.73544500	1.63801800	1.40388100

**TS6(RS)**

O	1.37619200	-0.02803700	-1.86442400
N	-1.56192000	-1.23694300	1.74724200
N	-0.72050700	-1.19757800	2.84191100
N	0.12675400	-0.21050400	1.06189000
C	-3.69902800	-1.24729300	2.85576400
H	-3.33224600	-0.40590400	3.43553400
C	-4.97760500	-1.75770300	3.04536800
H	-5.63414200	-1.32257200	3.79128200
C	-5.40299000	-2.82611600	2.26412500
H	-6.40450900	-3.22555800	2.38623400
C	-4.54235400	-3.40235000	1.33444900
H	-4.89061000	-4.24820600	0.75288600
C	-3.23838500	-2.93555000	1.14233000
C	-2.85928900	-1.82450700	1.90862600



C	-1.09859000	-0.61559300	0.64737500
C	0.30450000	-0.55612800	2.37771200
C	1.57660600	-0.01650800	2.93259500
H	2.28846700	-0.82213500	3.12551500
H	1.40304700	0.50541500	3.87496000
C	2.01995100	0.94773900	1.79892600
H	3.09942600	0.94137500	1.64294200
H	1.74351200	1.97053900	2.06834400
C	1.23519300	0.57611900	0.50140300
H	0.80314000	1.46687200	0.04362700
C	2.04106300	-0.14789700	-0.64344800
C	3.31616600	0.68040700	-0.85568800
C	4.61598100	0.19788500	-0.75499100
C	3.12968100	2.02513300	-1.19692300
C	5.70215600	1.05534800	-0.94070200
H	4.80953500	-0.84880700	-0.54502600
C	4.21635000	2.87255900	-1.35432300
H	2.12278600	2.40282100	-1.35721800
C	5.51926700	2.39981100	-1.22307200
C	2.28993800	-1.61068800	-0.27706100
C	3.05540000	-1.97885500	0.82980100
C	1.68403800	-2.62045500	-1.02653600
C	3.19305900	-3.31591300	1.19146200
H	3.57092400	-1.22656700	1.41984600
C	1.84649000	-3.95435800	-0.66716900
H	1.07760100	-2.36759400	-1.88907700
C	2.59172000	-4.32137200	0.44773900
H	6.36702300	3.06186600	-1.35150800
H	2.69809600	-5.36217900	0.73045400
H	0.47601400	-0.42964300	-1.86340700
C	3.94607900	4.32483600	-1.63046600
C	7.08477400	0.48371200	-0.79253700
C	1.24124800	-5.01238300	-1.54652100
C	4.01729800	-3.63096200	2.40653500
F	3.54115100	-2.98952900	3.49091300
F	5.28656300	-3.22854500	2.25326800
F	4.03254700	-4.93744600	2.68526700
F	2.01869700	-5.28221700	-2.60216100
F	0.04795700	-4.62682400	-2.02293000
F	1.05875800	-6.16610800	-0.88333100
F	3.35165000	4.91009600	-0.56924100
F	5.06715400	5.00956800	-1.88284700
F	3.11943400	4.48735500	-2.66817200
F	7.26114100	-0.58028000	-1.58726400

F	7.30219000	0.06838600	0.46518300
F	8.03374500	1.37896200	-1.09063100
C	-2.25619000	-3.65543500	0.23008400
C	-2.94013200	-4.59575300	-0.76238500
C	-1.25740800	-4.43110600	1.10405400
H	-1.69704700	-2.91706600	-0.35699400
H	-3.71418300	-4.08121000	-1.34207400
H	-2.19875700	-4.98888700	-1.45896900
H	-3.40430100	-5.44798600	-0.25438100
H	-0.66254400	-3.75894500	1.73099000
H	-1.79289300	-5.12303000	1.76271400
H	-0.57943600	-5.01708800	0.47908100
C	-3.99663000	0.38474400	-2.18598500
C	-3.25856600	-0.53707300	-1.19654100
H	-3.30339900	0.65430600	-2.99382800
C	-1.75641100	-0.38343600	-1.34846600
H	-3.58299100	-0.32902900	-0.17636500
C	-5.18876600	-0.33143000	-2.82715900
C	-4.75607900	-1.37589700	-3.85653800
H	-5.84030200	0.40085900	-3.32284400
H	-5.79808100	-0.80019800	-2.04234700
C	-5.93112800	-2.19732600	-4.37867700
H	-4.25816300	-0.86583400	-4.69008500
H	-4.00100100	-2.04386700	-3.42366400
H	-5.60963100	-2.92020600	-5.13247900
H	-6.41235700	-2.75000900	-3.56563400
H	-6.68936400	-1.55186400	-4.83358900
O	-1.07777400	-1.18760800	-1.98920000
H	-3.47461600	-1.58987100	-1.39260800
C	-1.63870000	3.79495800	0.40508100
C	-3.21086100	2.33808600	-0.80310500
C	-1.89119100	1.97304000	-0.80679200
N	-1.02060200	2.78484000	-0.13321300
O	-1.31274200	0.94563900	-1.47942600
S	-3.35643700	3.79998100	0.12556100
C	-4.39958600	1.72048400	-1.49556800
H	-4.70609300	2.40293200	-2.30044900
C	-0.94762900	4.84859500	1.16322300
C	0.42935800	5.01888800	0.97555800
C	-1.62941300	5.67762500	2.05756600
C	1.11152300	6.00526800	1.67584400
H	0.95007000	4.38485000	0.26594700
C	-0.94199500	6.66351400	2.75683700
H	-2.69563300	5.54252400	2.21985300

C	0.42797000	6.82896300	2.56872600
H	2.17593600	6.13610200	1.51060800
H	-1.47760100	7.30092900	3.45260600
H	0.96072600	7.60180600	3.11310900
C	-5.59920400	1.57888200	-0.56754900
C	-5.46634600	1.19395100	0.76994600
C	-6.88289700	1.82336500	-1.06426400
C	-6.58797700	1.04158800	1.57961900
H	-4.47667800	1.03440400	1.19143300
C	-8.00572200	1.66940300	-0.25826800
H	-7.00127900	2.14612500	-2.09558700
C	-7.86095400	1.27468700	1.06883500
H	-6.46200100	0.74793000	2.61658100
H	-8.99249400	1.86675200	-0.66493800
H	-8.73398900	1.16175300	1.70356700

**TS6(SR)**

O	1.75108700	1.68976700	-0.81955100
N	-0.44956000	-0.50415400	2.92169400
N	0.55433000	-0.76556700	3.83181700
N	1.20468000	0.51987300	2.16378900
C	-2.52766800	-0.39659900	4.14222000
H	-2.06746200	0.37943000	4.74685200
C	-3.85427000	-0.76844400	4.32650000
H	-4.45284800	-0.29016100	5.09502100
C	-4.40380900	-1.74209800	3.49821800
H	-5.44349100	-2.03063800	3.61583000
C	-3.62503400	-2.36385600	2.52514700
H	-4.07130700	-3.13210400	1.90342700
C	-2.28225200	-2.02515800	2.32924700
C	-1.77454900	-1.00549300	3.14513900
C	-0.10211100	0.28152500	1.88719900
C	1.55740400	-0.12417800	3.31922300
C	2.98815400	0.09208100	3.66896600
H	3.52010100	-0.86184800	3.72026700
H	3.08523600	0.57526300	4.64317200
C	3.48858100	0.99708600	2.50738400
H	4.33046100	0.53394100	1.99290600
H	3.85091100	1.95239600	2.88908300
C	2.30008900	1.25472000	1.52135400
H	2.03570600	2.31558100	1.50560000
C	2.52016400	0.86830300	0.00528600
C	3.97861700	1.19614000	-0.36659200
C	4.97996800	0.24669300	-0.55348100

C	4. 30358400	2. 54816800	-0. 51066400
C	6. 28150200	0. 64658300	-0. 85567400
H	4. 76827500	-0. 81420000	-0. 47366400
C	5. 60551100	2. 93423000	-0. 79995700
H	3. 51989900	3. 29328300	-0. 42367000
C	6. 61114900	1. 98813000	-0. 97529800
C	2. 18672400	-0. 60455200	-0. 23861900
C	2. 67752700	-1. 61556500	0. 58677300
C	1. 38141200	-0. 95561300	-1. 32108100
C	2. 38979000	-2. 95037000	0. 32626900
H	3. 30594900	-1. 38170600	1. 44169900
C	1. 10959400	-2. 29647600	-1. 57921200
H	0. 97058700	-0. 17131800	-1. 94605100
C	1. 60908700	-3. 30773200	-0. 76514100
H	7. 62518300	2. 29207200	-1. 20890600
H	1. 38719700	-4. 34953900	-0. 97052200
H	0. 92725100	2. 01214200	-0. 36452000
C	5. 94348500	4. 39771100	-0. 87054300
C	7. 32390500	-0. 40718300	-1. 10867400
C	0. 34533100	-2. 67199700	-2. 81727000
C	2. 99990000	-3. 98725600	1. 22450100
F	2. 89060000	-3. 63529300	2. 51720500
F	4. 30989700	-4. 13367500	0. 97624900
F	2. 42670400	-5. 18792000	1. 07623000
F	-0. 50800100	-1. 71829200	-3. 19770400
F	-0. 36011600	-3. 80675800	-2. 63801200
F	1. 17512100	-2. 89873500	-3. 84672800
F	4. 92303700	5. 12091400	-1. 34622500
F	6. 23894100	4. 88626100	0. 34503600
F	7. 00741700	4. 62182700	-1. 65295100
F	7. 27589600	-0. 85358300	-2. 37120000
F	7. 14846500	-1. 47016900	-0. 31004200
F	8. 56154700	0. 06032000	-0. 89826400
C	-1. 38715400	-2. 77763700	1. 35832500
C	-2. 16082300	-3. 65404200	0. 37769800
C	-0. 40948700	-3. 64875400	2. 16547300
H	-0. 81975400	-2. 03965800	0. 77379700
H	-2. 95012300	-3. 09708300	-0. 12830300
H	-1. 47926400	-4. 03108500	-0. 39010800
H	-2. 60455700	-4. 51920700	0. 88356100
H	0. 28296900	-3. 05596800	2. 76873000
H	-0. 97183000	-4. 30299600	2. 84031800
H	0. 17220200	-4. 28655200	1. 49507100
C	-3. 34725900	2. 89123400	0. 98047200

C	-2.35946100	1.82432900	1.50016300
H	-2.92396900	3.88429300	1.18131500
C	-1.13654200	1.66547000	0.62076600
H	-2.87355300	0.86384600	1.60548400
C	-4.67519500	2.75546300	1.72969500
C	-4.54287200	2.82598200	3.25156900
H	-5.14224900	1.79615800	1.45452000
H	-5.35831100	3.54704300	1.40250300
C	-5.90003700	2.75473800	3.94550000
H	-3.91749500	2.00139500	3.61095300
H	-4.02889300	3.75633700	3.52704400
H	-5.79814700	2.81054700	5.03266600
H	-6.55014500	3.57527700	3.62661200
H	-6.40742900	1.81498900	3.70314000
O	-0.28620500	2.55946600	0.54666500
H	-1.98960900	2.11724800	2.48514400
C	-3.94887200	-0.97854600	-1.69223700
C	-3.58254700	1.33536800	-0.98405000
C	-2.52278000	0.47302000	-0.90344000
N	-2.71496200	-0.81334800	-1.29996000
O	-1.27228300	0.85687800	-0.51035900
S	-4.93550000	0.45797600	-1.59606500
C	-3.47633200	2.78077900	-0.57035000
H	-2.49523300	3.09421400	-0.95299500
C	-4.49036100	-2.24122500	-2.21598500
C	-3.60585400	-3.18478100	-2.74993300
C	-5.86009200	-2.51967100	-2.18471800
C	-4.08848800	-4.39120900	-3.24031400
H	-2.54849900	-2.95147100	-2.77404000
C	-6.33864400	-3.72543600	-2.68486000
H	-6.55186300	-1.80074600	-1.75375300
C	-5.45484000	-4.66462600	-3.21118200
H	-3.39356600	-5.11657500	-3.65107400
H	-7.40274700	-3.93560400	-2.65508600
H	-5.83057600	-5.60685400	-3.59676000
C	-4.48934400	3.73002200	-1.17833500
C	-5.87012600	3.50577600	-1.13651100
C	-4.02813600	4.89812900	-1.78947100
C	-6.75763700	4.41696700	-1.70159800
H	-6.26498900	2.61868700	-0.64949500
C	-4.91263500	5.81490600	-2.35022100
H	-2.95857900	5.08699700	-1.83079900
C	-6.28232200	5.57454600	-2.31106900
H	-7.82435000	4.22081900	-1.66209800

H	-4.52881700	6.71370700	-2.82213500
H	-6.97574900	6.28381100	-2.75110700

**TS6(SS)**

O	-1.25356000	1.12827400	-1.10185800
N	0.45855100	-3.42514100	-0.93768800
N	-0.60804900	-4.22645700	-1.30625800
N	-0.96464900	-2.08176100	-1.64493900
C	2.20284500	-5.01229900	-1.38279500
H	1.66445800	-5.23808300	-2.29700200
C	3.39370600	-5.65025800	-1.07044300
H	3.80776000	-6.39007300	-1.74696500
C	4.04889900	-5.32348800	0.11426700
H	4.98400000	-5.80955100	0.37327000
C	3.49988900	-4.37980300	0.97335700
H	4.01347400	-4.15061600	1.90224600
C	2.29492500	-3.72208000	0.69229800
C	1.67080500	-4.05827900	-0.51585400
C	0.29631000	-2.10071500	-1.13473400
C	-1.46567400	-3.35401100	-1.72811200
C	-2.85256800	-3.37735300	-2.26889500
H	-3.53871000	-3.84102100	-1.55504800
H	-2.90401800	-3.95298400	-3.19527800
C	-3.15245300	-1.86793800	-2.49609300
H	-4.04806000	-1.56587400	-1.95308200
H	-3.34968500	-1.66796300	-3.55013000
C	-1.90870800	-1.03321700	-2.03760000
H	-1.48821900	-0.47804900	-2.88151200
C	-2.14007500	0.06157800	-0.91788800
C	-3.52663000	0.68903400	-1.13386800
C	-3.67632900	1.53578800	-2.23968900
C	-4.62854200	0.45357600	-0.32088600
C	-4.90894100	2.09668400	-2.53330900
H	-2.81172900	1.76685000	-2.85153500
C	-5.86444200	1.02960100	-0.62478600
H	-4.54644500	-0.16630000	0.56600800
C	-6.02176700	1.84587700	-1.73088300
C	-1.99128700	-0.54371900	0.47691200
C	-1.20854700	0.09457400	1.43407600
C	-2.61636500	-1.74949300	0.80549000
C	-1.07439000	-0.47279800	2.70343300
H	-0.69021700	1.01615200	1.17929100
C	-2.45653300	-2.31346400	2.06195200
H	-3.23725000	-2.26854000	0.08271800

C	-1.69213400	-1.67153000	3.03178700
H	-6.98566100	2.28597100	-1.96219600
H	-1.56693400	-2.11009900	4.01604800
H	-0.36374900	0.83593000	-1.38337800
C	-7.03508300	0.70271900	0.25960700
C	-5.06660200	3.02444800	-3.70608500
C	-3.13017800	-3.61385600	2.39472600
C	-0.27855900	0.25825700	3.74828800
F	-0.99930000	1.23542700	4.32122000
F	0.81455100	0.83694400	3.23387100
F	0.12546100	-0.56486500	4.73073200
F	-4.18153000	-3.43440600	3.20634400
F	-2.29316500	-4.45163100	3.02353300
F	-3.57860300	-4.23692200	1.29339100
F	-7.42937400	-0.56915300	0.08803900
F	-6.72104700	0.83853400	1.55504900
F	-8.08961100	1.48718400	0.00819100
F	-4.01904500	2.96533700	-4.53704200
F	-5.19743900	4.29781200	-3.31044800
F	-6.16660200	2.72353200	-4.41459900
C	1.70882100	-2.75539300	1.70954900
C	2.75183700	-1.77112500	2.24841100
C	1.08294000	-3.54656700	2.86644800
H	0.92740200	-2.16296700	1.22325000
H	3.26327800	-1.24949300	1.43549500
H	2.26162600	-1.01590200	2.86705100
H	3.50144700	-2.27376800	2.86866100
H	0.22871500	-4.14268100	2.53335700
H	1.82053200	-4.22349300	3.31116300
H	0.74382100	-2.85946200	3.64757100
C	4.23451800	-0.09989200	-1.82906700
C	2.99359100	-1.00604100	-1.68247600
H	4.02418000	0.63215500	-2.62124100
C	1.76123800	-0.20277700	-1.40033600
H	3.15180800	-1.74001200	-0.88642700
C	5.44167200	-0.95766800	-2.24740400
C	5.21820500	-1.86095100	-3.46095700
H	5.74814500	-1.57601700	-1.38991900
H	6.28512700	-0.29183300	-2.45946100
C	6.53115700	-2.45198000	-3.96906100
H	4.53507300	-2.67874900	-3.20522800
H	4.73532700	-1.28565700	-4.26207200
H	6.36709400	-3.12256900	-4.81621400
H	7.21785200	-1.66299900	-4.29019300

H	7.02931400	-3.02359400	-3.17955900
O	1.14025100	0.41263300	-2.23936400
H	2.81811700	-1.53605900	-2.62035700
C	2.13827000	3.31606100	1.11173400
C	3.50015200	1.59361200	0.00775000
C	2.18672100	1.30746500	0.25953800
N	1.42269000	2.25626700	0.85840900
O	1.59174600	0.11080900	-0.04479300
S	3.79815100	3.19811800	0.60041400
C	4.58736800	0.67646300	-0.52303300
H	4.75380600	-0.09205900	0.24749200
C	1.61302000	4.50799100	1.79320900
C	0.49456900	4.37399600	2.62326500
C	2.20975800	5.76168600	1.63221500
C	-0.01754200	5.48621000	3.27891000
H	0.05284900	3.39217400	2.75751000
C	1.69442000	6.87015300	2.29365600
H	3.06597500	5.87283600	0.97208200
C	0.57944800	6.73526600	3.11661200
H	-0.88266200	5.37758900	3.92495300
H	2.15866800	7.84162800	2.15922100
H	0.17567400	7.60176900	3.63027600
C	5.89369900	1.43682200	-0.68257200
C	6.00986600	2.45810900	-1.63200000
C	7.00036300	1.12156000	0.10458700
C	7.20926700	3.14360600	-1.79000600
H	5.15146000	2.72068200	-2.24588800
C	8.20259500	1.80784600	-0.05054700
H	6.91800800	0.33059000	0.84539800
C	8.31010100	2.81939300	-0.99904800
H	7.28570600	3.93320300	-2.53070000
H	9.05438400	1.55034500	0.57070800
H	9.24613100	3.35440700	-1.12197200

**P(RR)**

C	-2.41750400	-0.84247200	0.22535600
C	-1.92161500	-2.24259400	0.64837000
H	-2.53199400	-0.82197400	-0.86809200
C	-1.21147700	-2.91758600	-0.49514100
H	-1.26133600	-2.15997300	1.51957400
C	-3.78440100	-0.53546100	0.84671900
C	-4.93626400	-1.29746000	0.19284500
H	-3.98566100	0.53957500	0.76559500
H	-3.74383300	-0.76648100	1.92163500



C	-6.26941200	-1.03194700	0.88664300
H	-5.00019900	-0.99984400	-0.86077800
H	-4.73042200	-2.37463600	0.19249500
H	-7.08794600	-1.56278500	0.39480200
H	-6.23797000	-1.35675700	1.93129400
H	-6.50792200	0.03610400	0.87774800
O	-1.59137800	-3.91124800	-1.04246000
H	-2.75180300	-2.89908200	0.91047100
C	2.47590100	-0.31194200	0.09447000
C	0.02889400	-0.18589200	0.29186500
C	0.55120700	-1.26538600	-0.36866000
N	1.90967500	-1.33224000	-0.47689700
O	-0.10331600	-2.28945200	-0.99901900
S	1.35135300	0.81121200	0.81238600
C	-1.38258600	0.23452800	0.61180000
H	-1.44861900	0.35013500	1.70508800
C	3.93199900	-0.10638600	0.13603800
C	4.76120600	-1.03602500	-0.50139600
C	4.50044400	0.98878800	0.79213100
C	6.13927800	-0.86600600	-0.48018200
H	4.30383800	-1.88032000	-1.00558700
C	5.88012800	1.15431300	0.81014100
H	3.86694300	1.71686300	1.29245300
C	6.70256700	0.22803700	0.17413800
H	6.77735500	-1.58974900	-0.97674100
H	6.31354200	2.00775100	1.32095700
H	7.77972700	0.35853900	0.18856000
C	-1.70742600	1.58157800	-0.01462200
C	-1.56048000	1.76682100	-1.39207400
C	-2.16728200	2.64164500	0.76534400
C	-1.87809300	2.98651300	-1.97717300
H	-1.18138100	0.95020700	-2.00269200
C	-2.48384800	3.86684300	0.18129100
H	-2.28007600	2.50538800	1.83837100
C	-2.34152300	4.04043800	-1.19095400
H	-1.75862200	3.11871100	-3.04778300
H	-2.83866800	4.68413500	0.80099100
H	-2.58504900	4.99400800	-1.64811900

**P(RS)**

C	-2.35732900	-0.88539800	-0.46532100
C	-2.16733600	-1.42447200	0.96757000
H	-2.11887600	-1.69238300	-1.17317400
C	-1.29253400	-2.64757300	0.96859000

H	-1.73664100	-0.65218800	1.61334900
C	-3.81008800	-0.47467400	-0.72183400
C	-4.75849800	-1.66765200	-0.84046500
H	-3.86321800	0.10501200	-1.65319300
H	-4.14678800	0.19929800	0.07691600
C	-6.20855300	-1.23189200	-1.03169000
H	-4.44321600	-2.29003900	-1.68693400
H	-4.68232800	-2.30545600	0.04849800
H	-6.87395200	-2.09274400	-1.13139200
H	-6.55280000	-0.63762500	-0.17974400
H	-6.31689500	-0.61718900	-1.93090200
O	-1.62452500	-3.72528100	1.36908000
H	-3.11240600	-1.73410800	1.41460800
C	2.49754800	-0.33951700	-0.22072000
C	0.05436000	-0.20261000	-0.46312500
C	0.57015100	-1.36702900	0.04613700
N	1.92782400	-1.43642000	0.17748300
O	-0.05271300	-2.53420400	0.39774800
S	1.38065500	0.87515900	-0.77956500
C	-1.34970500	0.25122300	-0.76349500
H	-1.41658300	0.44795000	-1.84229700
C	3.95289400	-0.12447800	-0.19694500
C	4.77873200	-1.16166300	0.25057600
C	4.52367000	1.08323500	-0.60751300
C	6.15601700	-0.98698600	0.28379700
H	4.32041000	-2.09263200	0.56631800
C	5.90262800	1.25271700	-0.57237600
H	3.89236700	1.89706000	-0.95522600
C	6.72185400	0.21867300	-0.12668100
H	6.79143300	-1.79512400	0.63105600
H	6.33708000	2.19357100	-0.89382800
H	7.79839600	0.35234100	-0.09955900
C	-1.69738800	1.55671400	-0.05585400
C	-1.23218600	1.85084200	1.22935600
C	-2.52197300	2.48884600	-0.69248600
C	-1.60790000	3.02687300	1.87232100
H	-0.54326200	1.16868400	1.72063000
C	-2.89664400	3.66706800	-0.05449800
H	-2.86918400	2.29119900	-1.70353400
C	-2.44570000	3.93646900	1.23469500
H	-1.23435600	3.23576100	2.86965200
H	-3.53497000	4.37838400	-0.56882500
H	-2.73366500	4.85619700	1.73337400

**P(SR)**

C	2.31909900	-1.16850600	0.17796800
C	1.55831700	-2.51475500	0.13631700
H	3.32394800	-1.32933800	-0.23518700
C	1.07365400	-2.91352600	-1.24084100
H	0.70011500	-2.46228900	0.81590800
C	2.46215200	-0.69678300	1.62630500
C	3.09569500	-1.73000000	2.55923500
H	1.46931700	-0.41824500	2.01347000
H	3.07395400	0.21158700	1.64479200
C	3.36447200	-1.15407900	3.94692500
H	2.44287000	-2.60512800	2.65224600
H	4.03470500	-2.08839300	2.11730900
H	3.79912600	-1.90277700	4.61354300
H	4.05685600	-0.30862000	3.89219300
H	2.43721300	-0.79516900	4.40468100
O	1.61961700	-3.70478600	-1.95336400
H	2.21311200	-3.32163200	0.46689500
C	-2.29882700	-0.10155900	-0.25377900
C	0.12739300	-0.19235500	-0.59591100
C	-0.61643300	-1.25633500	-1.02185600
N	-1.95994900	-1.21589700	-0.83819700
O	-0.09394500	-2.33642800	-1.68116200
S	-0.95574600	0.96200100	0.09876200
C	1.62390400	-0.13716900	-0.76435700
H	1.79008200	-0.52641200	-1.77974500
C	-3.68620600	0.25088700	0.08325300
C	-4.71451700	-0.60905700	-0.31907200
C	-3.99972300	1.41426400	0.79189200
C	-6.03467100	-0.30337300	-0.01529000
H	-4.45623500	-1.50726900	-0.86914000
C	-5.32272500	1.71607600	1.09194200
H	-3.21056400	2.08766700	1.11641300
C	-6.34333600	0.85854600	0.68966900
H	-6.82708300	-0.97379200	-0.33176600
H	-5.55650700	2.62100500	1.64284600
H	-7.37602400	1.09468700	0.92500500
C	2.25229600	1.24195200	-0.74154400
C	2.03209000	2.16527900	0.28679400
C	3.11418300	1.60114200	-1.78014000
C	2.64877800	3.41262700	0.26704000
H	1.38516200	1.90942700	1.12106000
C	3.73646200	2.84556000	-1.80093900
H	3.29445000	0.89574000	-2.58719700

C	3. 50281300	3. 75750900	-0. 77686500
H	2. 46242300	4. 11568600	1. 07253400
H	4. 39811200	3. 10312500	-2. 62160200
H	3. 98192500	4. 73103400	-0. 79132600

**P(SS)**

C	2. 41754200	-0. 84252200	0. 22524600
C	1. 92161000	-2. 24268500	0. 64805600
H	2. 53218900	-0. 82190500	-0. 86818600
C	1. 21140600	-2. 91751500	-0. 49551700
H	1. 26141400	-2. 16017300	1. 51933700
C	3. 78433400	-0. 53557200	0. 84688100
C	4. 93635600	-1. 29743200	0. 19313600
H	3. 74356400	-0. 76673900	1. 92176400
H	3. 98559300	0. 53948500	0. 76594900
C	6. 26934600	-1. 03195800	0. 88725100
H	4. 73057400	-2. 37461900	0. 19260600
H	5. 00049800	-0. 99966600	-0. 86043600
H	7. 08800600	-1. 56269800	0. 39550800
H	6. 50781400	0. 03610700	0. 87855600
H	6. 23769400	-1. 35691500	1. 93185300
O	1. 59125100	-3. 91114100	-1. 04295500
H	2. 75178600	-2. 89925800	0. 91000400
C	-2. 47591800	-0. 31189800	0. 09449800
C	-0. 02890300	-0. 18591200	0. 29182900
C	-0. 55125600	-1. 26531100	-0. 36881800
N	-1. 90972800	-1. 33214200	-0. 47702100
O	0. 10325800	-2. 28929300	-0. 99932800
S	-1. 35132600	0. 81114600	0. 81252600
C	1. 38259700	0. 23446800	0. 61170600
H	1. 44867100	0. 35006900	1. 70499800
C	-3. 93201000	-0. 10632900	0. 13614600
C	-4. 76126400	-1. 03609000	-0. 50104800
C	-4. 50040400	0. 98898000	0. 79206800
C	-6. 13934100	-0. 86606500	-0. 47975800
H	-4. 30393000	-1. 88048300	-1. 00511400
C	-5. 88008500	1. 15450500	0. 81016100
H	-3. 86685200	1. 71717900	1. 29215900
C	-6. 70257800	0. 22809900	0. 17440000
H	-6. 77746000	-1. 58990700	-0. 97612700
H	-6. 31346100	2. 00805100	1. 32083500
H	-7. 77974100	0. 35860400	0. 18888400
C	1. 70743600	1. 58152200	-0. 01472000
C	1. 55997800	1. 76692200	-1. 39209300

C	2.16784400	2.64142200	0.76516100
C	1.87764400	2.98659700	-1.97721400
H	1.18041800	0.95045300	-2.00262900
C	2.48447400	3.86659200	0.18108900
H	2.28103000	2.50504000	1.83813700
C	2.34164300	4.04033900	-1.19109200
H	1.75776500	3.11891900	-3.04776700
H	2.83973600	4.68374600	0.80072400
H	2.58521300	4.99389500	-1.64827300

### Stereoselective TS optimized in solvent

#### TS3(RR)\_SMD

O	-1.06044100	1.02072500	1.26683500
N	-0.30150700	-3.26428700	-1.35527100
N	-1.27282600	-3.06705500	-2.31415500
N	-0.98107700	-1.23542100	-1.08151100
C	1.20639300	-4.82867800	-2.39440500
H	1.24742900	-4.14447600	-3.23669100
C	1.94490700	-6.00608200	-2.37930400
H	2.57872400	-6.26324300	-3.22135700
C	1.86864900	-6.83847200	-1.26770700
H	2.45066000	-7.75402800	-1.23479800
C	1.04172800	-6.51168800	-0.19526200
H	0.99174700	-7.18610700	0.65251200
C	0.27227700	-5.34536900	-0.18816500
C	0.39945400	-4.50940100	-1.30660800
C	-0.03568600	-2.13343500	-0.64111000
C	-1.65278100	-1.84999600	-2.11646900
C	-2.51099200	-0.89346300	-2.86328800
H	-3.55639400	-0.97824300	-2.55809200
H	-2.45644000	-1.07581500	-3.93695600
C	-1.87002000	0.45236100	-2.45487500
H	-2.60532400	1.25426600	-2.39473200
H	-1.13520500	0.74680800	-3.20784100
C	-1.12146600	0.24001900	-1.09877400
H	-0.11185300	0.66087900	-1.13349800
C	-1.87016300	0.89749100	0.12937100
C	-2.25141000	2.34342400	-0.24291900
C	-3.49127600	2.91775500	0.01039900
C	-1.21766600	3.16942900	-0.70947300
C	-3.70464600	4.27494700	-0.24425900
H	-4.30596900	2.33153900	0.42298500
C	-1.44064100	4.51631400	-0.94623500
H	-0.21564100	2.77173900	-0.85453000

C	-2.69358100	5.08701800	-0.72835400
C	-3.01879200	-0.02374800	0.51356200
C	-4.20807900	-0.09474500	-0.20771000
C	-2.80157800	-0.94047000	1.54637100
C	-5.16184600	-1.06383400	0.09918100
H	-4.40329900	0.59095900	-1.02857500
C	-3.76888800	-1.89180300	1.84769700
H	-1.85974500	-0.90752500	2.08624300
C	-4.95842600	-1.96991700	1.12998400
H	-2.86950300	6.13849400	-0.92565000
H	-5.70071200	-2.72546700	1.36055000
H	-0.18721700	1.36363400	1.00766100
C	-0.29544000	5.38872100	-1.37890900
C	-5.06832100	4.83601200	0.04208300
C	-3.52347200	-2.82638200	2.99821900
C	-6.41890400	-1.09410300	-0.72022500
F	-6.13736900	-1.05717100	-2.03751000
F	-7.20039800	-0.03390500	-0.46929900
F	-7.14593200	-2.19343800	-0.49635200
F	-3.77577300	-2.24214200	4.17687500
F	-2.24611600	-3.23949200	3.03446600
F	-4.29600200	-3.92265600	2.92832800
F	0.63289500	4.69633500	-2.05100200
F	-0.71166700	6.38743700	-2.17249000
F	0.31928000	5.95646400	-0.32913200
F	-6.02588800	4.12008800	-0.56948800
F	-5.19101400	6.10442200	-0.36816200
F	-5.34699300	4.80806700	1.35357900
C	-0.70273700	-5.01493600	0.92923400
C	-0.44832000	-5.80476000	2.21076300
C	-2.13944400	-5.24588800	0.43709000
H	-0.59063000	-3.95254400	1.17433300
H	0.58280200	-5.68860700	2.55838600
H	-1.11377200	-5.44249300	2.99769100
H	-0.65193800	-6.87217000	2.07338100
H	-2.37036600	-4.64750500	-0.44972100
H	-2.28356600	-6.30008800	0.17650200
H	-2.85601800	-4.99135600	1.22274100
C	3.31154900	-2.03704600	1.00401500
C	2.23589800	-2.54032500	0.29421700
H	3.10722600	-1.27693800	1.75391100
C	0.98432800	-1.90867100	0.30879100
H	2.41629200	-3.35467600	-0.40539700
C	4.59665500	-2.79690400	1.13959800

C	4.55704200	-3.80939400	2.29398200
H	5.42826500	-2.09910400	1.30902200
H	4.82187500	-3.32896000	0.20443900
C	5.88656000	-4.53473500	2.47067700
H	4.28760500	-3.29011900	3.22150700
H	3.75437300	-4.53178400	2.09949000
H	5.84291500	-5.26156500	3.28688100
H	6.16459400	-5.07172100	1.55764600
H	6.69147200	-3.82721800	2.69611800
O	0.74405900	-0.91621000	1.20176000
H	1.16306700	-0.06611400	0.87426300
C	4.24090800	3.20756500	0.80115700
C	3.86296500	0.93401000	-0.05609800
C	2.69662500	1.70564000	0.27658600
N	2.96572100	2.97963200	0.73107800
O	1.51008200	1.27645600	0.16258600
S	5.28915100	1.88833900	0.29612300
C	3.74885800	-0.31060700	-0.66280600
H	2.72865500	-0.51450700	-0.97826500
C	4.79624300	4.49350600	1.24037100
C	3.93936700	5.59933300	1.31797200
C	6.14613700	4.63669000	1.57756900
C	4.43425800	6.82990200	1.72758800
H	2.89728700	5.47500700	1.04245000
C	6.63434700	5.87103400	1.98790900
H	6.81456400	3.78074400	1.53555000
C	5.78005300	6.96862500	2.06389600
H	3.76949300	7.68589500	1.78284800
H	7.68127300	5.97534000	2.25322300
H	6.16291100	7.93217400	2.38520100
C	4.77650200	-1.06908400	-1.37462600
C	6.14978900	-0.97356400	-1.10855600
C	4.34982600	-1.98528700	-2.35144400
C	7.06199500	-1.75766400	-1.80755800
H	6.51505700	-0.31012600	-0.33130800
C	5.25999300	-2.76733700	-3.04662400
H	3.28487300	-2.07567900	-2.55259500
C	6.62426900	-2.65432000	-2.77795500
H	8.12096000	-1.67186400	-1.58561900
H	4.90774800	-3.46610800	-3.79925400
H	7.34034100	-3.26481100	-3.31876600

**TS3(RS)\_SMD**

O	-1.41595400	-0.15460200	-2.08460300
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N	1. 70060400	1. 38932900	0. 97156100
N	0. 89357300	1. 50158400	2. 08647000
N	0. 00439200	0. 14307300	0. 58284300
C	3. 92836300	1. 83494000	1. 78057700
H	3. 76975500	1. 03045700	2. 49031400
C	5. 13675400	2. 51479900	1. 71990500
H	5. 93972900	2. 25880700	2. 40327200
C	5. 30446200	3. 51874000	0. 76842300
H	6. 24922900	4. 04781500	0. 69462800
C	4. 25705800	3. 85944600	-0. 07781500
H	4. 39608200	4. 66277900	-0. 79585900
C	3. 01753100	3. 20932700	-0. 02540600
C	2. 89874600	2. 16552700	0. 89955800
C	1. 21533800	0. 49642200	0. 06306300
C	-0. 10994300	0. 73167300	1. 81764300
C	-1. 29113900	0. 20912500	2. 56458200
H	-2. 05897800	0. 97621900	2. 68290800
H	-0. 99066700	-0. 12205300	3. 56236200
C	-1. 72574900	-0. 97892300	1. 66675300
H	-2. 80760500	-1. 10696900	1. 61945000
H	-1. 30258700	-1. 90121500	2. 06848200
C	-1. 10022300	-0. 77473500	0. 26164200
H	-0. 66669600	-1. 71044400	-0. 09561100
C	-2. 06211100	-0. 21758100	-0. 84688700
C	-3. 21502600	-1. 22992100	-1. 01112800
C	-4. 56176500	-0. 88535000	-1. 00558900
C	-2. 87353200	-2. 56244700	-1. 28737300
C	-5. 54447500	-1. 85367700	-1. 22440700
H	-4. 87683500	0. 14138600	-0. 85393700
C	-3. 85885900	-3. 51398200	-1. 49803300
H	-1. 83316800	-2. 86437500	-1. 36686900
C	-5. 21066200	-3. 17418800	-1. 46225300
C	-2. 53884600	1. 19525600	-0. 48236400
C	-3. 40107800	1. 46146600	0. 58093800
C	-2. 07037000	2. 27530200	-1. 23591500
C	-3. 75491700	2. 77071800	0. 90194600
H	-3. 82259100	0. 65464800	1. 17271900
C	-2. 44852700	3. 57400200	-0. 91863200
H	-1. 42299700	2. 07847000	-2. 08207700
C	-3. 28528800	3. 84276900	0. 16025800
H	-5. 97661900	-3. 92189400	-1. 63667800
H	-3. 56893100	4. 85966200	0. 40947900
H	1. 20054200	-1. 89830100	-1. 58620300
C	-3. 48506400	-4. 95039500	-1. 73371000



C	-6.98077400	-1.41864000	-1.17646100
C	-2.01693200	4.71801200	-1.78928600
C	-4.63452500	2.98577200	2.09843200
F	-4.00099400	2.63370900	3.23338100
F	-5.74480100	2.23690300	2.03573700
F	-5.00976800	4.26192900	2.23171300
F	-0.95589900	4.40231900	-2.54815600
F	-1.68571900	5.79624200	-1.06047200
F	-2.99648000	5.10090200	-2.62065000
F	-2.23403600	-5.07921900	-2.18720700
F	-3.57444700	-5.67061100	-0.60339900
F	-4.30465000	-5.52887600	-2.62503600
F	-7.32002400	-1.00185400	0.05511000
F	-7.82159300	-2.40434400	-1.51083000
F	-7.21108800	-0.38913700	-2.00509200
C	1.89116500	3.67085900	-0.93342600
C	2.24170200	3.46155800	-2.41054000
C	1.56674500	5.14296400	-0.64968000
H	0.99415500	3.08181200	-0.70906500
H	2.44934300	2.40954500	-2.62576200
H	1.40990400	3.78323800	-3.04290800
H	3.12156800	4.05070600	-2.69122000
H	1.24900700	5.28544900	0.38735900
H	2.44143700	5.77747100	-0.82493100
H	0.76873000	5.49077400	-1.30753300
C	3.83137200	-0.79831500	-2.26798400
C	3.18547500	0.07855900	-1.41324200
H	3.20244000	-1.47225400	-2.84695400
C	1.83755100	-0.07700000	-1.08145800
H	3.79198000	0.79820900	-0.86944500
C	5.17891100	-0.48698300	-2.85387200
C	5.06886300	0.37239300	-4.12106600
H	5.70848500	-1.41658800	-3.10111700
H	5.79980400	0.03809200	-2.11649700
C	6.43087500	0.63638400	-4.75413400
H	4.41107900	-0.12640300	-4.84297500
H	4.58253700	1.32145000	-3.86357700
H	6.34383400	1.25930800	-5.64887300
H	7.09635000	1.14883400	-4.05158600
H	6.91631300	-0.30107200	-5.04474500
O	1.04325800	-0.88907300	-1.84121400
H	-0.47520200	-0.46071100	-2.02572500
C	1.82066800	-2.14752700	2.30286400
C	3.29746500	-2.38056500	0.35208400

C	1. 93313700	-2. 76790900	0. 16663700
N	1. 15089600	-2. 65460000	1. 31468200
O	1. 43473400	-3. 12826800	-0. 94170300
S	3. 50078800	-1. 77811500	1. 98404000
C	4. 25946200	-2. 43623100	-0. 65420400
H	4. 01182300	-3. 13128500	-1. 45328800
C	1. 22899400	-1. 89595700	3. 62513700
C	0. 19402100	-2. 72951300	4. 06891700
C	1. 64285700	-0. 82214600	4. 42037000
C	-0. 42140800	-2. 48544200	5. 28982500
H	-0. 10791200	-3. 56544800	3. 44547300
C	1. 02246200	-0. 58223600	5. 64294000
H	2. 42337900	-0. 15188100	4. 07104300
C	-0. 01010500	-1. 40967400	6. 07761600
H	-1. 21909000	-3. 13761000	5. 63074100
H	1. 33906600	0. 25904100	6. 25053800
H	-0. 49369600	-1. 21893500	7. 03033200
C	5. 69062900	-2. 18746600	-0. 42139000
C	6. 14089200	-1. 09122700	0. 32939600
C	6. 64246100	-3. 03843800	-0. 99731600
C	7. 49993800	-0. 87202500	0. 51954000
H	5. 42183400	-0. 37677200	0. 72376200
C	8. 00230400	-2. 82150300	-0. 80130400
H	6. 30660100	-3. 88068800	-1. 59622300
C	8. 43622700	-1. 73994900	-0. 03908100
H	7. 82999500	-0. 01229100	1. 09484200
H	8. 72483300	-3. 49735300	-1. 24802500
H	9. 49741000	-1. 56801900	0. 11017000

### TS3(SR)\_SMD

O	2. 24913700	1. 83843400	-0. 94415100
N	-0. 88297700	0. 03216900	2. 64997500
N	0. 03826300	-0. 54196600	3. 50549200
N	1. 05392100	0. 51516200	1. 83665300
C	-3. 23617800	0. 26666100	3. 25139800
H	-2. 99727000	1. 23380600	3. 67996500
C	-4. 52847400	-0. 23880300	3. 31056800
H	-5. 32239200	0. 34798200	3. 75917400
C	-4. 78280000	-1. 50667200	2. 79846100
H	-5. 78623900	-1. 91994100	2. 83380500
C	-3. 75293800	-2. 26713600	2. 25448500
H	-3. 97652800	-3. 26089400	1. 87716400
C	-2. 44063300	-1. 78898500	2. 18520900
C	-2. 22326200	-0. 49004900	2. 67159500

C	-0.28625300	0.73068300	1.64021300
C	1.17536900	-0.22980500	2.98494800
C	2.59368800	-0.40157200	3.39424300
H	2.91260400	-1.43515600	3.23217400
H	2.72180000	-0.17849400	4.45413700
C	3.32326300	0.61171600	2.47777200
H	4.21948200	0.17705200	2.03663500
H	3.64910900	1.47594300	3.05931100
C	2.32635800	1.10183800	1.37153500
H	2.22527700	2.19169000	1.40592700
C	2.72303400	0.80282100	-0.13770800
C	4.25061100	0.91155100	-0.26517900
C	5.10219500	-0.15770100	-0.51740800
C	4.80246100	2.19051400	-0.11761000
C	6.48214600	0.04585800	-0.59567000
H	4.71305500	-1.15982700	-0.66453000
C	6.17392700	2.37731000	-0.18712900
H	4.14490500	3.04143500	0.02277100
C	7.03199600	1.30510400	-0.42626600
C	2.18846100	-0.56031100	-0.56349300
C	2.43777100	-1.68888400	0.21451900
C	1.42441100	-0.69730400	-1.72154500
C	1.94036700	-2.93319900	-0.15524400
H	3.04269200	-1.61709800	1.11339100
C	0.93164100	-1.94595800	-2.08488000
H	1.21815500	0.16816400	-2.33970100
C	1.18784800	-3.07515700	-1.31338100
H	8.10389800	1.45567700	-0.48871700
H	0.80247000	-4.04525400	-1.61010200
H	1.26954700	1.91200200	-0.80273100
C	6.76569400	3.73985400	0.04614000
C	7.36264900	-1.13179900	-0.91139800
C	0.12600900	-2.13019100	-3.34465100
C	2.29533100	-4.11484600	0.69820400
F	1.43540800	-5.13039400	0.54549600
F	2.29994100	-3.78135000	2.00489300
F	3.51838600	-4.58297300	0.41817400
F	0.05844500	-1.02063500	-4.07664000
F	-1.11678700	-2.54336300	-3.07793800
F	0.68963700	-3.08660200	-4.11131800
F	5.87350500	4.71524700	-0.15893700
F	7.20758300	3.86299100	1.30835600
F	7.81419000	3.96306600	-0.75709000
F	7.00942900	-2.20651700	-0.19028800

F	8.65047000	-0.87250100	-0.65323800
F	7.27189500	-1.48033100	-2.20122200
C	-1.30630100	-2.70281500	1.74699000
C	-1.64048300	-3.56414900	0.52848300
C	-0.91858500	-3.60225700	2.93304700
H	-0.43687300	-2.08568900	1.48226600
H	-1.83102200	-2.95296700	-0.35735000
H	-0.79897900	-4.23275600	0.32862600
H	-2.51262200	-4.20009700	0.71163300
H	-0.64778800	-3.01238300	3.81132800
H	-1.76331900	-4.24812000	3.19633400
H	-0.07381800	-4.24042400	2.66100200
C	-2.32516000	3.54130600	0.26799500
C	-1.91296600	2.48107100	1.05039000
H	-1.66329100	3.84022800	-0.54098200
C	-0.89035000	1.59875900	0.69229800
H	-2.40723600	2.32233600	2.00437200
C	-3.21704900	4.60174900	0.85404800
C	-2.45425700	5.57934500	1.76011700
H	-4.02513700	4.13161200	1.43301200
H	-3.70588500	5.17564900	0.05842300
C	-3.36080100	6.66786500	2.32781900
H	-1.98077000	5.01921900	2.57576700
H	-1.63725200	6.03343500	1.18634000
H	-2.80822200	7.36047000	2.96822500
H	-3.82299200	7.24822200	1.52322200
H	-4.16830600	6.23041300	2.92389400
O	-0.26480500	1.74535900	-0.50931500
H	-0.77294400	1.14344500	-1.23268800
C	-4.29338000	-1.30404000	-0.96518100
C	-3.62249100	1.03442100	-1.24689500
C	-2.62860800	0.04325300	-1.57208000
N	-3.07956300	-1.25931100	-1.41144800
O	-1.47842600	0.29200800	-2.03405800
S	-5.05927100	0.24210200	-0.64544300
C	-3.43967900	2.38219500	-1.50604900
H	-2.53517500	2.56418200	-2.08273000
C	-5.02476900	-2.56269500	-0.76482200
C	-4.49018100	-3.74527000	-1.28932100
C	-6.22831700	-2.60579900	-0.05307500
C	-5.14025000	-4.95542700	-1.07589700
H	-3.56762100	-3.68971400	-1.85863100
C	-6.87366900	-3.81778000	0.15862300
H	-6.65106400	-1.69105200	0.35407100

C	-6.32715200	-4.99622300	-0.34674600
H	-4.72134800	-5.86990400	-1.48317400
H	-7.80296300	-3.84409300	0.71838700
H	-6.83060700	-5.94292900	-0.17964000
C	-4.48564000	3.40042800	-1.63547200
C	-5.65971900	3.40674300	-0.86830000
C	-4.28580500	4.44281800	-2.55290700
C	-6.60880400	4.40829200	-1.03305000
H	-5.81435900	2.65071000	-0.10508500
C	-5.23593900	5.44297400	-2.71791900
H	-3.37376500	4.45738200	-3.14344700
C	-6.40496000	5.42797300	-1.96017000
H	-7.50805700	4.39887300	-0.42550800
H	-5.06352500	6.23565000	-3.43889400
H	-7.14722800	6.20940000	-2.08501900

**TS3(SS)\_SMD**

O	1.96031800	-0.09741900	2.03402900
N	-0.73783800	-3.81321400	-0.10440100
N	0.27240700	-4.58446400	-0.64611300
N	1.08396800	-2.69159500	0.20203800
C	-2.84082500	-4.95756100	0.31171500
H	-2.43453300	-5.26864800	1.26931800
C	-4.09548300	-5.37778000	-0.10910600
H	-4.69584400	-6.01863000	0.52785100
C	-4.56156300	-4.98252900	-1.36247300
H	-5.53390800	-5.31659500	-1.71128400
C	-3.78524700	-4.16304900	-2.17281700
H	-4.16215400	-3.86707300	-3.14788100
C	-2.51711200	-3.72055400	-1.77398400
C	-2.07409100	-4.13712300	-0.51323200
C	-0.27011500	-2.65456700	0.45238100
C	1.33687900	-3.89318700	-0.42814700
C	2.79423300	-4.15624700	-0.57792700
H	3.06175700	-4.47110800	-1.58728400
H	3.08694600	-4.95081200	0.11481500
C	3.39809500	-2.80068100	-0.17982700
H	3.59027100	-2.20035200	-1.07274000
H	4.34490900	-2.90499100	0.34960600
C	2.35020000	-2.09236500	0.71876000
H	2.45991400	-2.43351200	1.75525700
C	2.51064800	-0.53771400	0.82218800
C	4.02167800	-0.28391900	0.95582000
C	4.83062100	0.01928800	-0.13853200

C	4.60741200	-0.40036000	2.21618500
C	6.20287300	0.17796400	0.02736500
H	4.39699700	0.14968400	-1.12593000
C	5.98102200	-0.23277600	2.36714300
H	3.98108800	-0.59657400	3.08013300
C	6.79515100	0.05155700	1.27818300
C	1.95028700	0.26935600	-0.35163400
C	1.65839400	-0.26322200	-1.60584800
C	1.77280700	1.63878200	-0.14756200
C	1.20343300	0.56578500	-2.62795700
H	1.77211400	-1.32129600	-1.80944400
C	1.31462800	2.45116700	-1.17657400
H	1.98685000	2.06186700	0.82956600
C	1.02334200	1.92708300	-2.42853300
H	7.86306600	0.19038200	1.40365200
H	0.65590100	2.56284200	-3.22628500
H	0.98180300	-0.14502100	1.91022200
C	6.58245300	-0.40823700	3.73287800
C	7.05559500	0.42868200	-1.18359500
C	1.20206500	3.92780200	-0.92995700
C	0.98108800	-0.00310200	-3.99753900
F	-0.07009100	0.55409000	-4.61378400
F	0.77141400	-1.33218900	-3.96274200
F	2.04489800	0.19559300	-4.79387700
F	0.63492700	4.20627300	0.24774900
F	0.49182600	4.54510000	-1.88776900
F	2.41696700	4.50784500	-0.91716600
F	5.83140100	0.16659500	4.68162500
F	6.68768800	-1.70814100	4.05772000
F	7.81168100	0.11787900	3.81157800
F	7.36039200	-0.72123200	-1.80976500
F	8.21407300	1.02198600	-0.86867600
F	6.43024600	1.20277400	-2.08037900
C	-1.66367400	-2.89737500	-2.72196200
C	-2.35511800	-1.59199900	-3.12535100
C	-1.29963500	-3.74437800	-3.94785700
H	-0.72993400	-2.63151100	-2.21385100
H	-2.43736300	-0.90751300	-2.27589800
H	-1.77476700	-1.08407200	-3.89941800
H	-3.35702500	-1.77534800	-3.52665600
H	-0.79208200	-4.66661000	-3.64894000
H	-2.19568100	-4.01782900	-4.51531800
H	-0.63967700	-3.18249700	-4.61348000
C	-2.96353600	-0.78724100	2.29210600

C	-2.24999000	-1.83121900	1.72411400
H	-2.44401300	0.16229900	2.38790800
C	-1.00623400	-1.64669100	1.10910900
H	-2.69483200	-2.82389000	1.71998800
C	-4.09513500	-1.02810000	3.24894200
C	-3.60817500	-1.26404200	4.68548100
H	-4.69012400	-1.89198200	2.92146800
H	-4.77516300	-0.16531100	3.24567400
C	-4.76284600	-1.45009000	5.66407600
H	-2.95696700	-2.14654000	4.69877300
H	-2.98565300	-0.41737900	4.99899800
H	-4.40250800	-1.63111100	6.68082400
H	-5.40230000	-0.56166200	5.68918000
H	-5.38969600	-2.29981000	5.37369800
O	-0.41932800	-0.41655700	1.16205500
H	-0.78828900	0.16845700	0.37679000
C	-3.12911400	3.72253900	0.07699300
C	-3.57846900	1.30837500	0.19935600
C	-2.29647700	1.69834300	-0.32239500
N	-2.11429500	3.07322100	-0.40009800
O	-1.39461200	0.88851500	-0.67440100
S	-4.47201100	2.73914100	0.65501800
C	-3.92842900	-0.03354400	0.30768500
H	-3.22575700	-0.67312600	-0.21973800
C	-3.20480100	5.18955100	0.14125200
C	-2.19183600	5.94671000	-0.45942400
C	-4.25684600	5.84230000	0.79347200
C	-2.23772500	7.33376200	-0.40808800
H	-1.38196200	5.43267100	-0.96216100
C	-4.29739100	7.23001800	0.84176000
H	-5.04525000	5.27037500	1.27522600
C	-3.28820200	7.97920400	0.24134600
H	-1.45015600	7.91407600	-0.87812900
H	-5.11658100	7.72623700	1.35179300
H	-3.32050700	9.06352100	0.27966800
C	-5.25659900	-0.62578700	0.49918800
C	-6.37024300	0.05789300	1.00482300
C	-5.39769200	-1.98812400	0.18936400
C	-7.58608000	-0.59764200	1.17658300
H	-6.30248100	1.10435500	1.28062500
C	-6.60965600	-2.64079000	0.36083700
H	-4.53183600	-2.53169400	-0.18148200
C	-7.71291300	-1.94545500	0.85542800
H	-8.43700400	-0.04920200	1.56828700

H	-6.69218400	-3.69454900	0.11239700
H	-8.66265500	-2.45214700	0.99459300

### Different substituents

#### 3(S1)

O	-0.83808400	-0.44272400	-1.49252700
N	1.01947200	2.34763100	1.87259800
N	0.00874600	2.41308600	2.79563100
N	-0.35237400	0.82986400	1.30008900
C	2.84793800	3.05083300	3.25683100
H	2.44951200	2.37270800	4.00415500
C	4.00181500	3.78480400	3.48800500
H	4.52567400	3.68952800	4.43252000
C	4.47824400	4.63263400	2.49051500
H	5.38601300	5.20502000	2.65107400
C	3.79319300	4.74985700	1.28784400
H	4.17369900	5.42176300	0.52420400
C	2.62070800	4.03108500	1.02209000
C	2.18429400	3.17742700	2.03812900
C	0.83410400	1.37076600	0.97222700
C	-0.80927500	1.47974100	2.41411800
C	-2.07503100	0.87960900	2.92104700
H	-2.91821400	1.54328700	2.71258100
H	-2.03041700	0.71858900	3.99887100
C	-2.12995700	-0.45123500	2.12321500
H	-3.14278600	-0.70740900	1.81082100
H	-1.77378400	-1.27316400	2.75037900
C	-1.17062100	-0.33267200	0.89946700
H	-0.50776100	-1.19868500	0.83785800
C	-1.80472900	-0.17118800	-0.53054900
C	-2.87819200	-1.25684500	-0.70276600
C	-4.14364500	-1.00870600	-1.22784300
C	-2.53222000	-2.57557200	-0.38599000
C	-5.05798200	-2.04897900	-1.39019200
H	-4.43816600	-0.00733500	-1.52186300
C	-3.45953300	-3.59902500	-0.53804800
H	-1.52631800	-2.81896000	-0.04443200
C	-4.73423700	-3.35007900	-1.03592600
C	-2.35259700	1.25279000	-0.66253400
C	-3.44855300	1.68461700	0.08408600
C	-1.70138300	2.17496100	-1.48475300
C	-3.86813600	3.01106800	0.03456900
H	-4.00583300	0.98606800	0.70283300
C	-2.14888600	3.49158800	-1.54557800



H	-0.83348000	1.86817800	-2.05952300
C	-3.22575600	3.93035500	-0.78158800
H	-5.45288000	-4.15283100	-1.15439200
H	-3.55523000	4.96223800	-0.82335900
H	0.15640900	-1.91512100	-1.95241500
C	-3.08007500	-4.98537200	-0.09887000
C	-6.39852000	-1.74738400	-2.00103200
C	-1.49815800	4.44584800	-2.50798500
C	-5.01435400	3.41335300	0.91722300
F	-4.67495700	3.30349800	2.21774700
F	-6.07524300	2.61744600	0.73362800
F	-5.40091400	4.67435900	0.70997700
F	-0.20603600	4.14513200	-2.70563100
F	-1.55761900	5.71091300	-2.06223300
F	-2.09646700	4.42122400	-3.70482200
F	-1.80692900	-5.26793100	-0.39945400
F	-3.20053500	-5.12014100	1.23743600
F	-3.85567500	-5.92052600	-0.65824000
F	-6.86107600	-0.55526100	-1.59620900
F	-7.31065000	-2.67210600	-1.67276400
F	-6.33286300	-1.70876900	-3.33843000
C	1.89803800	4.23475300	-0.29782400
C	2.80112900	3.89307300	-1.48785300
C	1.38288200	5.67739100	-0.38858200
H	1.03408700	3.56279600	-0.34694300
H	3.16204700	2.86454900	-1.41945300
H	2.23932100	3.99824900	-2.41837000
H	3.66247100	4.56790300	-1.53176700
H	0.70018100	5.90858300	0.43407000
H	2.21355900	6.38919000	-0.34672500
H	0.85542400	5.83045400	-1.33133100
C	4.09800200	0.14872200	-0.61735200
C	3.01730400	0.70539100	0.26792800
H	4.26353900	0.84225400	-1.45694800
C	1.74871300	0.94941100	-0.12733900
H	3.26108500	0.85808500	1.31557700
C	5.41469900	0.07966000	0.16701600
C	5.89191300	1.46747500	0.60195100
H	6.19076600	-0.39002900	-0.44628100
H	5.28811300	-0.55821800	1.05558500
C	7.18086800	1.41841200	1.41652800
H	6.04050000	2.08308200	-0.29542400
H	5.11199500	1.97343600	1.18543800
H	7.50451300	2.42042400	1.71217500

H	7.04194800	0.82901400	2.32864800
H	7.99191200	0.95673900	0.84499200
O	1.22353600	0.85281700	-1.31328100
H	0.04884200	0.14248500	-1.38899000
C	1.41415800	-2.99513000	1.37050000
C	2.79323100	-2.05542000	-0.43047000
C	1.52814900	-2.45773300	-0.76938100
N	0.76091600	-2.97902900	0.24050800
O	1.02966000	-2.35239300	-2.01157400
S	3.04545300	-2.40887800	1.24855000
C	3.65320900	-1.19515800	-1.30784800
H	2.95412400	-0.89033500	-2.09580200
C	0.78976400	-3.40942900	2.63563200
C	-0.40070400	-4.14658800	2.58798300
C	1.31450800	-3.03237400	3.87568500
C	-1.06072200	-4.48463400	3.76288300
H	-0.78092900	-4.46627500	1.62430100
C	0.65703100	-3.38480600	5.04939400
H	2.23023300	-2.44868300	3.92142200
C	-0.53476900	-4.10434100	4.99681400
H	-1.98225000	-5.05520500	3.70861000
H	1.07205800	-3.08859200	6.00742900
H	-1.04824500	-4.37274000	5.91438800
C	4.82579100	-1.88809000	-1.97457300
C	5.44191600	-3.02163900	-1.44582400
C	5.35739200	-1.33424300	-3.14253900
C	6.56039100	-3.57717600	-2.06197200
H	5.04304300	-3.48286800	-0.54672700
C	6.47480900	-1.88880800	-3.75430600
H	4.88482000	-0.45612000	-3.57698000
C	7.09624600	-3.02216500	-3.22401700
H	7.02401100	-4.46143500	-1.63158900
H	6.86860700	-1.44031200	-4.66305300
C	8.28493600	-3.64734100	-3.90847700
H	8.93137200	-4.15932800	-3.19120400
H	7.96521200	-4.38710500	-4.65009200
H	8.88237300	-2.89576900	-4.43084900

**TS4(S1)**

O	-0.41186800	0.07809600	-0.43728600
N	1.08646400	3.48335400	1.52596400
N	-0.01353800	3.98107000	2.17067800
N	-0.28682200	1.87840700	1.56186300
C	3.30561000	4.05150600	2.28063400

H	3. 15592100	3. 33641600	3. 08427700
C	4. 48750900	4. 76654200	2. 14794700
H	5. 29631800	4. 61646200	2. 85407900
C	4. 61909700	5. 67728300	1. 10067600
H	5. 53902800	6. 24164200	0. 98738500
C	3. 58207200	5. 86771300	0. 19574100
H	3. 70445100	6. 57853700	-0. 61621200
C	2. 37925600	5. 16043900	0. 29756200
C	2. 28262300	4. 26292300	1. 35990800
C	0. 94256900	2. 21034500	1. 16535900
C	-0. 83083700	2. 96902100	2. 18108900
C	-2. 16956900	2. 63864000	2. 75647400
H	-2. 97101900	3. 02376300	2. 11885700
H	-2. 29016200	3. 05938300	3. 75482600
C	-2. 10574400	1. 08618900	2. 76834400
H	-3. 08003900	0. 61679500	2. 62969600
H	-1. 70167600	0. 75944300	3. 72906400
C	-1. 08643500	0. 65734600	1. 68657600
H	-0. 41236200	-0. 10935800	2. 04830300
C	-1. 60401500	0. 18956100	0. 30183100
C	-2. 23307800	-1. 20114300	0. 44617000
C	-3. 39351300	-1. 59208300	-0. 21920600
C	-1. 52989500	-2. 16444800	1. 18180400
C	-3. 87233400	-2. 89526800	-0. 09227500
H	-3. 92620600	-0. 90136600	-0. 86518400
C	-2. 04029100	-3. 44708200	1. 32565800
H	-0. 55629700	-1. 94570300	1. 61785100
C	-3. 22144200	-3. 82870000	0. 70057600
C	-2. 50498100	1. 26523400	-0. 30166900
C	-3. 82735200	1. 44549000	0. 10755600
C	-1. 95278500	2. 17087300	-1. 21243800
C	-4. 57608600	2. 51446700	-0. 37409900
H	-4. 29312300	0. 75211400	0. 80164500
C	-2. 72187500	3. 22300600	-1. 70093000
H	-0. 92293700	2. 04081500	-1. 53605600
C	-4. 03547200	3. 41141200	-1. 28577100
H	-3. 59558400	-4. 84173600	0. 78850100
H	-4. 62923000	4. 23240000	-1. 67212500
H	1. 80623200	0. 84959900	-2. 36101300
C	-1. 28718800	-4. 40543500	2. 20705600
C	-5. 11397800	-3. 27225800	-0. 84968800
C	-2. 10711500	4. 21592900	-2. 64843400
C	-5. 95254500	2. 73443200	0. 18663500
F	-5. 87759200	3. 32620700	1. 39198000

F	-6.60563500	1.57882000	0.36000100
F	-6.69688200	3.51809800	-0.59905500
F	-1.55401800	5.24268200	-1.97308600
F	-3.01971000	4.74167600	-3.47392900
F	-1.13992200	3.66955100	-3.38947900
F	0.03085000	-4.36675400	1.97208200
F	-1.45388200	-4.09304500	3.50529800
F	-1.69978100	-5.66971600	2.05014800
F	-6.20837100	-2.71064500	-0.31372600
F	-5.31040700	-4.59600700	-0.86951800
F	-5.04982400	-2.85108900	-2.12372700
C	1.25925800	5.38126800	-0.69879400
C	1.72316000	5.07151400	-2.12546800
C	0.72030300	6.81121200	-0.57550700
H	0.44031800	4.69301000	-0.46142300
H	2.10051800	4.04825500	-2.19121600
H	0.88615300	5.18087800	-2.81883800
H	2.51574500	5.75829200	-2.43989500
H	0.35448900	7.00595400	0.43637800
H	1.50454600	7.54146700	-0.80049300
H	-0.09925500	6.96721900	-1.28007900
C	3.91167200	-0.25562200	0.45516200
C	2.70635900	0.46902300	1.04771800
H	4.76451800	0.44108800	0.44698100
C	1.96873500	1.44357800	0.32567300
H	2.88559300	0.84854400	2.05975700
C	4.31366400	-1.44010400	1.34869200
C	4.69228100	-1.04888500	2.77756600
H	5.16716700	-1.95321500	0.88933600
H	3.48814300	-2.16071400	1.40431900
C	5.14780600	-2.25861900	3.58954100
H	5.49043000	-0.29496900	2.75143100
H	3.83999400	-0.58022600	3.28420900
H	5.39702400	-1.98498300	4.61849200
H	4.35837900	-3.01698400	3.62143500
H	6.03115000	-2.72267500	3.13984100
O	1.97612300	1.80520300	-0.85534700
H	-0.55616000	-0.45371500	-1.24020400
C	0.50127700	-2.89293000	-1.63226000
C	2.44105800	-1.41227300	-1.32984700
C	1.48339800	-1.00872600	-2.22873100
N	0.40514100	-1.83420800	-2.39310600
O	1.47706900	0.13607100	-2.93888400
S	1.90735400	-2.90410900	-0.61753300

C	3. 71783300	-0. 67152200	-1. 03561400
H	3. 61033100	0. 26792700	-1. 58559800
C	-0. 49530300	-3. 97621800	-1. 64755400
C	-1. 63947700	-3. 82794500	-2. 44154800
C	-0. 31739800	-5. 15691800	-0. 91849400
C	-2. 58793400	-4. 84198500	-2. 49832300
H	-1. 76379100	-2. 91336400	-3. 01191400
C	-1. 27569900	-6. 16343300	-0. 96821400
H	0. 56854900	-5. 28950200	-0. 30446800
C	-2. 41358000	-6. 00928800	-1. 75711100
H	-3. 47489600	-4. 71403600	-3. 11001300
H	-1. 13148500	-7. 06841200	-0. 38732300
H	-3. 16227500	-6. 79417400	-1. 79581000
C	4. 98583300	-1. 31836700	-1. 58858700
C	5. 09130000	-2. 65931600	-1. 95075900
C	6. 12306600	-0. 51374000	-1. 73163800
C	6. 29504400	-3. 18003600	-2. 42428300
H	4. 23001500	-3. 31379400	-1. 87653100
C	7. 32024700	-1. 03385000	-2. 20269200
H	6. 06351200	0. 54202200	-1. 47608600
C	7. 42836900	-2. 38184800	-2. 55754700
H	6. 34822200	-4. 23067800	-2. 69822200
H	8. 18584100	-0. 38369400	-2. 30536800
C	1. 23020100	-0. 76072600	3. 56109200
O	1. 10776800	0. 45442600	3. 74708400
O	1. 33986200	-1. 30650500	2. 38436000
H	1. 84723200	-0. 43122800	1. 57492400
C	1. 25772000	-1. 74328400	4. 71401900
H	0. 57682500	-2. 57293200	4. 51031800
H	2. 26574000	-2. 16171300	4. 79314200
H	0. 99410400	-1. 24582300	5. 64652900
C	8. 72261100	-2. 93658400	-3. 09475800
H	8. 87841200	-2. 63156900	-4. 13477500
H	9. 57796400	-2. 57569600	-2. 51684600
H	8. 72810900	-4. 02856100	-3. 06439900

### 3(S2)

O	-0. 86398700	-0. 51681300	-1. 46259100
N	0. 56359200	2. 55828700	1. 86406400
N	-0. 48159400	2. 54363700	2. 75025100
N	-0. 61802900	0. 88562400	1. 29906200
C	2. 25555300	3. 49508200	3. 28313900
H	1. 90329400	2. 80230400	4. 04015400
C	3. 31678100	4. 35419400	3. 52662300

H	3.81270800	4.34470300	4.49077300
C	3.73795900	5.21606400	2.51638600
H	4.57423100	5.88618400	2.68677800
C	3.08888800	5.22232600	1.28833000
H	3.42454200	5.90657200	0.51468100
C	2.00882400	4.37527600	1.00914100
C	1.62751500	3.51225100	2.03934700
C	0.51581100	1.53990300	0.99234600
C	-1.18173900	1.51687500	2.37419100
C	-2.39441400	0.80030900	2.85932600
H	-3.29517800	1.36278500	2.60022200
H	-2.37250200	0.67835200	3.94296100
C	-2.27840000	-0.55273300	2.10666200
H	-3.24613100	-0.92582800	1.76999700
H	-1.86004300	-1.31182000	2.77336900
C	-1.29312000	-0.36965900	0.91189500
H	-0.54027400	-1.16105800	0.90195300
C	-1.88831400	-0.32098900	-0.54294700
C	-2.83375500	-1.52006700	-0.71319300
C	-4.09783600	-1.42498200	-1.28911700
C	-2.36230400	-2.78388200	-0.33957800
C	-4.89029500	-2.56156500	-1.44642100
H	-4.48541500	-0.47035500	-1.62737100
C	-3.16976600	-3.90485100	-0.48773600
H	-1.34977800	-2.90790400	0.04404500
C	-4.44415500	-3.80908600	-1.03680700
C	-2.57879000	1.03146100	-0.74178400
C	-3.74115700	1.36600100	-0.04755900
C	-1.99885800	1.99263300	-1.57272600
C	-4.29670200	2.63782800	-0.15642400
H	-4.24386200	0.63096500	0.57567400
C	-2.58069500	3.25131400	-1.69349700
H	-1.08264600	1.76320300	-2.10723700
C	-3.72547700	3.59534100	-0.98145500
H	-5.06886500	-4.68735100	-1.15190300
H	-4.16051000	4.58432600	-1.06942700
H	0.29518800	-1.88808600	-1.83691500
C	-2.66213800	-5.22857300	0.01108400
C	-6.23143200	-2.42375700	-2.11239400
C	-1.99969700	4.24027800	-2.66547600
C	-5.51094500	2.94176900	0.67298900
F	-5.21037500	2.90760000	1.98720500
F	-6.47442400	2.03219000	0.48059800
F	-6.02041800	4.14761000	0.41051100

F	-0.67700000	4.07244400	-2.81124500
F	-2.20736800	5.50450600	-2.26391000
F	-2.54925300	4.11719500	-3.87948100
F	-1.35604200	-5.38240700	-0.23709700
F	-2.81658200	-5.33468800	1.34649400
F	-3.31325900	-6.25802400	-0.54142900
F	-6.83301700	-1.27700400	-1.76296200
F	-7.05171600	-3.43123900	-1.78533100
F	-6.12010200	-2.41702500	-3.44728400
C	1.31769900	4.45992900	-0.34034000
C	2.29465900	4.17915600	-1.48716600
C	0.65780000	5.83628800	-0.49842900
H	0.53128900	3.69902200	-0.39461200
H	2.75920900	3.19759600	-1.37095600
H	1.75928800	4.19465700	-2.43883200
H	3.08113900	4.94016700	-1.52631000
H	-0.07553000	6.01919300	0.29218200
H	1.40711500	6.63311300	-0.45341100
H	0.15266600	5.90314200	-1.46319900
C	3.94629400	0.62225800	-0.44421100
C	2.78122800	1.08881800	0.38450000
H	4.06970700	1.30429900	-1.30043400
C	1.50939200	1.18451300	-0.06084900
H	2.96900500	1.29963400	1.43363300
C	5.23283700	0.71621000	0.38608800
C	5.54754800	2.15929600	0.78780300
H	6.07537100	0.31075600	-0.18378300
H	5.13969000	0.09705300	1.29189100
C	6.80211700	2.27094600	1.64856800
H	5.66669100	2.75814100	-0.12512000
H	4.69756700	2.59945000	1.32499600
H	7.00900300	3.31014400	1.91957200
H	6.68945700	1.69954500	2.57566100
H	7.67800900	1.87871300	1.12269000
O	1.04093200	0.99596300	-1.25956300
H	-0.04784200	0.16281000	-1.34976900
C	1.54032200	-2.72983900	1.56045800
C	2.87446400	-1.70044400	-0.22552900
C	1.67243500	-2.24663200	-0.59141200
N	0.92967200	-2.81729200	0.41017400
O	1.21058100	-2.23334900	-1.85199800
S	3.10329300	-1.97500800	1.47159300
C	3.67058500	-0.78107800	-1.10327900
H	2.97092000	-0.57596600	-1.92247400

C	0.91963000	-3.17219900	2.81788300
C	-0.18416600	-4.03286900	2.75629400
C	1.35871500	-2.70696300	4.06126700
C	-0.84492300	-4.40618300	3.92003300
H	-0.49531200	-4.41789900	1.79172800
C	0.70204600	-3.09436200	5.22435800
H	2.20563700	-2.02804800	4.11726500
C	-0.40476200	-3.93778200	5.15724100
H	-1.69886600	-5.07271500	3.85487700
H	1.05025900	-2.72890600	6.18509700
H	-0.91843000	-4.23344100	6.06628800
C	4.93052600	-1.36869100	-1.70844500
C	5.63106900	-2.42575300	-1.13904600
C	5.45307700	-0.78855200	-2.87252200
C	6.82261800	-2.89816300	-1.69427900
H	5.24382000	-2.91015100	-0.24714200
C	6.63345600	-1.23955100	-3.43617000
H	4.91499600	0.02947200	-3.34597500
C	7.32913300	-2.30071400	-2.84624700
H	7.33390000	-3.72844000	-1.22208400
H	7.03672300	-0.79788300	-4.34099800
O	8.47674300	-2.67861900	-3.47337100
C	9.19141500	-3.75819200	-2.91725600
H	9.52860700	-3.53367000	-1.89776500
H	8.58604600	-4.67283200	-2.89966600
H	10.05946900	-3.91274900	-3.55782800

**TS4(S2)**

O	-0.52885700	0.04663100	-0.41472500
N	0.57547300	3.58471500	1.58258100
N	-0.59079900	3.98681500	2.17556100
N	-0.65388100	1.86670800	1.56898200
C	2.69907700	4.34450700	2.43602800
H	2.57344300	3.62136800	3.23659400
C	3.81967700	5.15894000	2.35430000
H	4.60384100	5.08167900	3.09891800
C	3.92153200	6.07491900	1.30826500
H	4.79338400	6.71688200	1.23489000
C	2.91616700	6.17226100	0.35412400
H	3.01502200	6.88897500	-0.45587000
C	1.77557800	5.36349500	0.40388600
C	1.70656600	4.46401400	1.46668300
C	0.55842800	2.30308100	1.22428300
C	-1.31698000	2.90768500	2.15679400



C	-2.64651600	2.46437400	2.67464300
H	-3.44882500	2.77653700	1.99927700
H	-2.84775700	2.87637600	3.66359500
C	-2.44949900	0.92336300	2.70027300
H	-3.37232100	0.37113500	2.52058800
H	-2.06386600	0.63566100	3.68082300
C	-1.34829000	0.58068100	1.66918500
H	-0.62646800	-0.12186800	2.06753000
C	-1.75936500	0.06142400	0.26735100
C	-2.27384700	-1.37674200	0.39831100
C	-3.36858300	-1.86950000	-0.30939900
C	-1.52218600	-2.27137500	1.17170400
C	-3.73983500	-3.20782100	-0.18835600
H	-3.93052800	-1.23118000	-0.98383200
C	-1.92741100	-3.59181700	1.30816300
H	-0.58932800	-1.96703800	1.64419300
C	-3.04536000	-4.07684800	0.64008400
C	-2.71843100	1.05352500	-0.38759200
C	-4.06869300	1.12492000	-0.04090300
C	-2.20174800	1.99726800	-1.28045700
C	-4.88085500	2.12459200	-0.56683100
H	-4.50649400	0.39933300	0.63829200
C	-3.03225900	2.97851800	-1.81356000
H	-1.15050500	1.95268200	-1.55448500
C	-4.37509000	3.05832100	-1.46130900
H	-3.33567000	-5.11739700	0.72344900
H	-5.01660200	3.82433200	-1.88270800
H	1.69074600	0.99887400	-2.24884400
C	-1.13276900	-4.47634200	2.22938400
C	-4.91220600	-3.69498300	-0.99186900
C	-2.45967400	4.01483600	-2.74073500
C	-6.29551400	2.23161800	-0.07220200
F	-6.32691800	2.83736300	1.12809500
F	-6.85609700	1.02617600	0.08503000
F	-7.06608300	2.94282300	-0.90041200
F	-2.03878600	5.09361000	-2.05110600
F	-3.37053200	4.44832800	-3.62004300
F	-1.40874500	3.55242600	-3.42246700
F	0.18577100	-4.32823900	2.04641500
F	-1.37778000	-4.16858200	3.51629000
F	-1.43098900	-5.77208200	2.07061900
F	-6.07257300	-3.23091700	-0.50352600
F	-4.99023100	-5.03097200	-1.01109600
F	-4.83445200	-3.27339500	-2.26498000

C	0.68908100	5.48357400	-0.64543600
C	1.24539500	5.21196300	-2.04661900
C	0.02242900	6.86128900	-0.55695100
H	-0.07715400	4.72700000	-0.44254300
H	1.71083100	4.22431100	-2.08836000
H	0.43645400	5.24832300	-2.77976400
H	1.99093700	5.96317900	-2.32694700
H	-0.40604100	7.02586600	0.43550400
H	0.74970300	7.65671300	-0.75008900
H	-0.77364400	6.94298600	-1.29996800
C	3.76255600	0.10696700	0.66355300
C	2.47422100	0.72711600	1.19715800
H	4.55174400	0.87604700	0.67416200
C	1.68323500	1.62603100	0.43474300
H	2.57518500	1.12763700	2.21183200
C	4.23086300	-1.02505800	1.59199200
C	4.50311600	-0.58641500	3.03142500
H	5.14999600	-1.45943000	1.18116800
H	3.47482600	-1.82018800	1.61918900
C	5.03383200	-1.73944400	3.87943900
H	5.22592700	0.24045900	3.03129800
H	3.58748100	-0.19709100	3.49256300
H	5.20654500	-1.43418400	4.91514700
H	4.32015300	-2.57008400	3.88475800
H	5.97790100	-2.12029300	3.47747300
O	1.70635400	1.97807100	-0.74898400
H	-0.59085300	-0.49824200	-1.21944800
C	0.68404500	-2.83843100	-1.54381300
C	2.47445700	-1.19434700	-1.16835200
C	1.52808600	-0.88059300	-2.11417300
N	0.53353900	-1.79668200	-2.31911700
O	1.45665800	0.25550700	-2.83537800
S	2.03660200	-2.72103000	-0.46527200
C	3.66696800	-0.34028500	-0.82750800
H	3.49630900	0.58056100	-1.39169900
C	-0.21525400	-4.00274700	-1.59196700
C	-1.33413300	-3.95545600	-2.43302900
C	0.03126900	-5.16079600	-0.84668100
C	-2.19056800	-5.04630900	-2.52011500
H	-1.51158100	-3.05727100	-3.01526800
C	-0.83604800	-6.24487100	-0.92703800
H	0.89966800	-5.21558900	-0.19677200
C	-1.94938000	-6.19115700	-1.76276600
H	-3.05941000	-4.99649600	-3.16815400

H	-0.63983900	-7.13180400	-0.33367700
H	-2.62723000	-7.03653900	-1.82539300
C	5.00716800	-0.87297800	-1.32533000
C	5.30440900	-2.22916500	-1.49572600
C	6.01692600	0.04724900	-1.60182900
C	6.55880000	-2.64258400	-1.91704300
H	4.54614400	-2.98119500	-1.30642800
C	7.28487800	-0.34650300	-2.02590000
H	5.80964200	1.10959300	-1.49139700
C	7.55904200	-1.70470900	-2.18379500
H	6.78997600	-3.69354600	-2.05269700
H	8.03451400	0.40693200	-2.23577800
C	0.99971600	-0.61489000	3.65384800
O	0.76456500	0.58609600	3.82365700
O	1.20920300	-1.15480000	2.48818800
H	1.67516400	-0.24162100	1.69396700
C	1.05989800	-1.58551200	4.81565500
H	0.46516900	-2.47323900	4.58842600
H	2.09616000	-1.91245000	4.94490800
H	0.71035300	-1.10875000	5.73058700
O	8.75467400	-2.20940900	-2.59311600
C	9.78048800	-1.28911400	-2.88692800
H	9.49122000	-0.61256600	-3.70059300
H	10.05008600	-0.69347200	-2.00596700
H	10.64110900	-1.88036100	-3.19903000

### 3(S3)

O	-0.84544300	-0.43271200	-1.49317000
N	1.05061600	2.32408000	1.87832800
N	0.04359200	2.39510300	2.80478300
N	-0.33746300	0.82185200	1.30371900
C	2.89029400	3.00240500	3.26015800
H	2.48760600	2.32451800	4.00542100
C	4.05201100	3.72391400	3.49133400
H	4.57788500	3.61877400	4.43367300
C	4.53341000	4.57233000	2.49669800
H	5.44711500	5.13516200	2.65732200
C	3.84563000	4.70252600	1.29691900
H	4.23007800	5.37489800	0.53566800
C	2.66534200	3.99655700	1.03128100
C	2.22401000	3.14186600	2.04427900
C	0.85288500	1.35313900	0.97429500
C	-0.78454600	1.47121500	2.42204700
C	-2.05418100	0.88105500	2.93081200

H	-2.89159200	1.55400800	2.72898800
H	-2.00701000	0.71432700	4.00766100
C	-2.12515600	-0.44531300	2.12676600
H	-3.14150200	-0.68980500	1.81649300
H	-1.77525400	-1.27372700	2.74884000
C	-1.16875400	-0.33052300	0.90031600
H	-0.51488200	-1.20286000	0.83213500
C	-1.80633700	-0.15566400	-0.52660000
C	-2.89131100	-1.22949700	-0.70012700
C	-4.15680800	-0.96570900	-1.21744800
C	-2.55714300	-2.55333000	-0.39229900
C	-5.08235700	-1.99580700	-1.38084200
H	-4.44275200	0.04015700	-1.50449000
C	-3.49533300	-3.56663900	-0.54556100
H	-1.55222800	-2.80858400	-0.05675100
C	-4.76992700	-3.30209800	-1.03559000
C	-2.33971800	1.27450200	-0.65007600
C	-3.42805700	1.71427900	0.10305500
C	-1.68221600	2.19363300	-1.47064600
C	-3.83374300	3.04528700	0.06156400
H	-3.99027800	1.01873500	0.72071200
C	-2.11602300	3.51519800	-1.52344200
H	-0.82015500	1.88052800	-2.05075300
C	-3.18501000	3.96164100	-0.75289500
H	-5.49721200	-4.09690100	-1.15494800
H	-3.50369500	4.99714300	-0.78840200
H	0.13408400	-1.91067600	-1.96842100
C	-3.12721300	-4.95917900	-0.11638100
C	-6.42304600	-1.67706200	-1.98279000
C	-1.45909400	4.46700700	-2.48411300
C	-4.97204300	3.45534400	0.95098500
F	-4.62832800	3.33502100	2.24945700
F	-6.04199200	2.67167700	0.76765100
F	-5.34574200	4.72140100	0.75175300
F	-0.17045600	4.15446100	-2.68677700
F	-1.50483700	5.73068600	-2.03313800
F	-2.06109200	4.45276800	-3.67914400
F	-1.85916300	-5.25309900	-0.42809500
F	-3.23874200	-5.09947000	1.22009400
F	-3.91651500	-5.88324700	-0.67457100
F	-6.87175000	-0.48334900	-1.56731200
F	-7.34226700	-2.59517900	-1.65614300
F	-6.36349000	-1.62978800	-3.32011900
C	1.94032400	4.21423700	-0.28509000

C	2. 83618800	3. 87018900	-1. 47988500
C	1. 43889800	5. 66223400	-0. 36671100
H	1. 06967300	3. 55102300	-0. 33477500
H	3. 18703700	2. 83776000	-1. 41814700
H	2. 27260400	3. 98610900	-2. 40803400
H	3. 70410700	4. 53656300	-1. 52285400
H	0. 76125100	5. 89576700	0. 45942800
H	2. 27656200	6. 36572300	-0. 32407500
H	0. 90979800	5. 82518800	-1. 30687700
C	4. 10079200	0. 11186000	-0. 63272400
C	3. 02832000	0. 67159500	0. 26043700
H	4. 27010700	0. 81096900	-1. 46711000
C	1. 76057500	0. 92797100	-0. 12984700
H	3. 27772500	0. 81739800	1. 30761600
C	5. 41934500	0. 02445100	0. 14682700
C	5. 91125100	1. 40434400	0. 59072500
H	6. 19017700	-0. 44698700	-0. 47184900
H	5. 28981700	-0. 61897000	1. 03089600
C	7. 20337800	1. 33650200	1. 39887200
H	6. 06142800	2. 02577500	-0. 30235000
H	5. 13858700	1. 91256200	1. 18169700
H	7. 53717900	2. 33299900	1. 70151900
H	7. 06331200	0. 74061900	2. 30656900
H	8. 00783800	0. 87278700	0. 81975800
O	1. 23192000	0. 84019000	-1. 31453300
H	0. 04617400	0. 14282900	-1. 38988300
C	1. 39727000	-3. 02279200	1. 34068900
C	2. 77801300	-2. 08311000	-0. 45882800
C	1. 50760300	-2. 47014800	-0. 79539300
N	0. 73946000	-2. 99138900	0. 21380400
O	1. 00582000	-2. 35018800	-2. 03451500
S	3. 03376000	-2. 45077800	1. 21686500
C	3. 64038700	-1. 22192000	-1. 33278500
H	2. 93985100	-0. 90453600	-2. 11442500
C	0. 77573800	-3. 44269200	2. 60537100
C	-0. 42071100	-4. 16995800	2. 55733100
C	1. 31020300	-3. 08069900	3. 84574200
C	-1. 07700100	-4. 51333400	3. 73278100
H	-0. 80859900	-4. 47810500	1. 59294300
C	0. 65630800	-3. 43845100	5. 01978900
H	2. 23074800	-2. 50465700	3. 89182700
C	-0. 54134000	-4. 14821800	4. 96709600
H	-2. 00322200	-5. 07619700	3. 67860300
H	1. 07877000	-3. 15422000	5. 97817400

H	-1.05196000	-4.42088400	5.88499200
C	4.80489100	-1.91836600	-2.01051500
C	5.40956300	-3.06429900	-1.49249800
C	5.33715000	-1.35367500	-3.17412700
C	6.52579200	-3.62887300	-2.10499300
H	5.00198700	-3.53323300	-0.60190200
C	6.45194500	-1.89953700	-3.79949900
H	4.86647700	-0.47078800	-3.59952900
C	7.03239000	-3.03110400	-3.24666200
H	7.00218000	-4.52027600	-1.71307100
H	6.86958900	-1.47168900	-4.70374100
F	8.11344300	-3.56480900	-3.83942300

**TS4(S3)**

O	-0.40576400	0.08753400	-0.43825700
N	1.18185000	3.45293100	1.52330400
N	0.09642400	3.97620100	2.17225400
N	-0.22926900	1.88108500	1.56334400
C	3.41702200	3.96637700	2.26998800
H	3.25322000	3.25424800	3.07352100
C	4.61522900	4.65304000	2.13366900
H	5.42285400	4.48276900	2.83656900
C	4.76449200	5.56208900	1.08726600
H	5.69717800	6.10453100	0.97130200
C	3.72869000	5.77901300	0.18688600
H	3.86481800	6.48828900	-0.62422700
C	2.50956300	5.10078300	0.29247600
C	2.39580800	4.20382600	1.35360900
C	1.00612700	2.18398200	1.16262500
C	-0.74486300	2.98397900	2.18514900
C	-2.08897900	2.68520900	2.76522500
H	-2.88331300	3.09005600	2.13093200
H	-2.19572300	3.10781000	3.76436500
C	-2.06233700	1.13163700	2.77561600
H	-3.04812400	0.68593200	2.64011000
H	-1.66274000	0.79439700	3.73457200
C	-1.05761900	0.67948800	1.68968100
H	-0.40081600	-0.10362000	2.04803200
C	-1.59193600	0.22643000	0.30650600
C	-2.25336900	-1.14917400	0.45088000
C	-3.42306000	-1.51188200	-0.21429900
C	-1.57265500	-2.12971800	1.18488200
C	-3.93225300	-2.80367700	-0.08897200
H	-3.93998500	-0.80780600	-0.85868900

C	-2. 11275100	-3. 40031500	1. 32694600
H	-0. 59396600	-1. 93478700	1. 62075700
C	-3. 30282000	-3. 75333100	0. 70191700
C	-2. 46958800	1. 32409900	-0. 29168800
C	-3. 78617000	1. 53381800	0. 12222700
C	-1. 89969900	2. 21873800	-1. 20234600
C	-4. 51153600	2. 62086600	-0. 35466600
H	-4. 26564500	0. 84969700	0. 81617700
C	-2. 64584700	3. 28938400	-1. 68619200
H	-0. 87429300	2. 06577600	-1. 52988600
C	-3. 95335300	3. 50710200	-1. 26627900
H	-3. 70055500	-4. 75745200	0. 78864300
H	-4. 52931100	4. 34234200	-1. 64902100
H	1. 82262100	0. 80488400	-2. 36689000
C	-1. 38099900	-4. 37766700	2. 20552500
C	-5. 18303500	-3. 15003200	-0. 84615500
C	-2. 01121000	4. 26958400	-2. 63388600
C	-5. 88075100	2. 87148200	0. 21114700
F	-5. 78783300	3. 45967200	1. 41693900
F	-6. 55937000	1. 73084100	0. 38523300
F	-6. 60949400	3. 67305500	-0. 57095400
F	-1. 43086300	5. 28104500	-1. 95838400
F	-2. 91398100	4. 81885800	-3. 45460300
F	-1. 06017200	3. 70165800	-3. 37980900
F	-0. 06265800	-4. 36917600	1. 96816900
F	-1. 53805600	-4. 06400200	3. 50447800
F	-1. 82301900	-5. 63162600	2. 04655800
F	-6. 26278100	-2. 56079500	-0. 31043500
F	-5. 41234800	-4. 46843600	-0. 86523900
F	-5. 10816100	-2. 73126700	-2. 12042400
C	1. 39104700	5. 35048100	-0. 69871800
C	1. 84079700	5. 03043600	-2. 12766800
C	0. 88845500	6. 79331500	-0. 57212600
H	0. 55613600	4. 68281800	-0. 45819100
H	2. 19195900	3. 99803600	-2. 19602800
H	1. 00389100	5. 16154300	-2. 81736200
H	2. 64914000	5. 69722100	-2. 44494900
H	0. 53228300	6. 99643100	0. 44153500
H	1. 68946400	7. 50404800	-0. 80042900
H	0. 06974800	6. 97000400	-1. 27278400
C	3. 91148700	-0. 35419300	0. 44387800
C	2. 72608100	0. 39914600	1. 04083500
H	4. 78135600	0. 32149500	0. 43369800
C	2. 01108500	1. 39253000	0. 32065300

H	2.91850200	0.77404800	2.05212600
C	4.28654000	-1.54942200	1.33470000
C	4.67959800	-1.16949100	2.76275800
H	5.12556300	-2.08387700	0.87273900
H	3.44313900	-2.24878500	1.39243900
C	5.10670000	-2.39130600	3.57203000
H	5.49644400	-0.43596400	2.73492600
H	3.84080900	-0.68005000	3.27212300
H	5.36571500	-2.12489800	4.60038300
H	4.29838400	-3.12939400	3.60569200
H	5.97686300	-2.87710100	3.11962300
O	2.02638600	1.75349300	-0.86034500
H	-0.56781200	-0.43749400	-1.24208600
C	0.43046300	-2.90581600	-1.63720600
C	2.40590900	-1.47272900	-1.33700000
C	1.45732700	-1.04583800	-2.23452900
N	0.35939900	-1.84526200	-2.39781800
O	1.47833700	0.09847800	-2.94471500
S	1.83639800	-2.95057300	-0.62225000
C	3.70071900	-0.76258600	-1.04641600
H	3.61203000	0.17990400	-1.59411200
C	-0.59135500	-3.96530700	-1.65160400
C	-1.73226600	-3.78992300	-2.44470000
C	-0.44017500	-5.14997500	-0.92303600
C	-2.70405500	-4.78164600	-2.50103400
H	-1.83585600	-2.87252000	-3.01466800
C	-1.42156200	-6.13396900	-0.97242400
H	0.44279100	-5.30340300	-0.30955500
C	-2.55609400	-5.95297500	-1.76044700
H	-3.58825300	-4.63293900	-3.11195600
H	-1.29796900	-7.04231800	-0.39208900
H	-3.32274900	-6.72031800	-1.79898700
C	4.95002300	-1.43764200	-1.60912400
C	5.01852500	-2.78364900	-1.96961700
C	6.09987000	-0.65431400	-1.76743400
C	6.19795700	-3.34123000	-2.45929300
H	4.14184100	-3.41534500	-1.88425000
C	7.28597700	-1.18977200	-2.25332100
H	6.06240300	0.40279100	-1.51560800
C	7.31444600	-2.53471200	-2.58978700
H	6.25807400	-4.38552800	-2.74378800
H	8.17719900	-0.58691600	-2.38504800
C	1.22842100	-0.79655600	3.55653100
O	1.13753400	0.42145100	3.74244500



O	1. 32152500	-1. 34485200	2. 37956500
H	1. 84835300	-0. 47930400	1. 56826200
C	1. 23324600	-1. 77918000	4. 70969100
H	0. 53057800	-2. 59095300	4. 50789200
H	2. 23019200	-2. 22371000	4. 78671700
H	0. 98482300	-1. 27484100	5. 64266200
F	8. 45382400	-3. 06393200	-3. 06445100

**3(S4)**

O	-0. 86140300	-0. 50721600	-1. 45451500
N	0. 61202200	2. 53142300	1. 88744800
N	-0. 44239400	2. 54304000	2. 76230700
N	-0. 60462400	0. 88809400	1. 31023200
C	2. 31336100	3. 42258300	3. 32457900
H	1. 93581500	2. 73839200	4. 07721400
C	3. 39435500	4. 25327000	3. 57949700
H	3. 88050600	4. 22967100	4. 54835800
C	3. 84763000	5. 10514500	2. 57463200
H	4. 69947600	5. 75288700	2. 75411900
C	3. 21055600	5. 13040500	1. 34053800
H	3. 57113200	5. 80707400	0. 57145200
C	2. 11134800	4. 31235300	1. 04978300
C	1. 69803900	3. 45805800	2. 07482800
C	0. 54795800	1. 51447000	1. 01534700
C	-1. 16380000	1. 53369400	2. 37930900
C	-2. 39857300	0. 84769100	2. 85241200
H	-3. 28257500	1. 43191600	2. 58393200
H	-2. 39066300	0. 72613900	3. 93628200
C	-2. 30817200	-0. 50836500	2. 10171700
H	-3. 28131000	-0. 85822400	1. 75592200
H	-1. 91484300	-1. 27664400	2. 77300400
C	-1. 30734300	-0. 35013000	0. 91630700
H	-0. 57433100	-1. 16001700	0. 91302300
C	-1. 88886800	-0. 28629200	-0. 54333200
C	-2. 86222000	-1. 46121300	-0. 72374800
C	-4. 11518700	-1. 33395800	-1. 31769400
C	-2. 42917600	-2. 73637100	-0. 34278100
C	-4. 93437100	-2. 44971600	-1. 48576700
H	-4. 47309800	-0. 36987800	-1. 66183500
C	-3. 26284500	-3. 83645600	-0. 50263900
H	-1. 42614500	-2. 88668400	0. 05580400
C	-4. 52628100	-3. 70820000	-1. 06979600
C	-2. 54341800	1. 08299200	-0. 74739500
C	-3. 70474500	1. 44466300	-0. 06517500

C	-1.93117800	2.03088200	-1.57031500
C	-4.22748000	2.73000100	-0.17734900
H	-4.23222600	0.72099500	0.55085000
C	-2.48062000	3.30366700	-1.69500600
H	-1.01553100	1.77987600	-2.09603900
C	-3.62408000	3.67454500	-0.99441700
H	-5.17168400	-4.57014000	-1.19363800
H	-4.03377100	4.67405900	-1.08513000
H	0.26282700	-1.90799400	-1.82067600
C	-2.79466600	-5.17252700	0.00203300
C	-6.26225800	-2.27742100	-2.17031100
C	-1.86538900	4.27948200	-2.65925000
C	-5.44237700	3.06247900	0.64028200
F	-5.15541200	3.01944400	1.95728300
F	-6.42541000	2.17665100	0.43705900
F	-5.91953000	4.28056300	0.37433900
F	-0.54567200	4.07888600	-2.79163200
F	-2.04554500	5.54769500	-2.25744600
F	-2.40514900	4.17171900	-3.87892100
F	-1.49236800	-5.36322400	-0.24161600
F	-2.95572400	-5.26958000	1.33723700
F	-3.47246200	-6.18486200	-0.54934500
F	-6.83998000	-1.11691100	-1.82621800
F	-7.11138400	-3.26508700	-1.85730200
F	-6.13153400	-2.27028000	-3.50332200
C	1.43486800	4.41715400	-0.30565100
C	2.41467000	4.11405700	-1.44432900
C	0.81136900	5.81002900	-0.46676800
H	0.62987800	3.67662000	-0.36838000
H	2.85327800	3.12085300	-1.32590600
H	1.88853900	4.14508400	-2.40075800
H	3.22048000	4.85493100	-1.47472800
H	0.07624400	6.01004600	0.31797000
H	1.58019200	6.58752100	-0.41388100
H	0.31624100	5.89123200	-1.43562100
C	3.96718500	0.51582600	-0.39311300
C	2.80936500	1.01021900	0.42924500
H	4.11531200	1.19711300	-1.24606600
C	1.54390500	1.13455200	-0.02751700
H	2.99561300	1.21783600	1.47906900
C	5.25049500	0.56946000	0.44589400
C	5.60434800	2.00163200	0.85434900
H	6.08640300	0.14317600	-0.11890200
H	5.13377700	-0.04959100	1.34884600

C	6.85765700	2.07338900	1.72117200
H	5.74494700	2.59992200	-0.05586300
H	4.76466800	2.46390100	1.38900600
H	7.09296100	3.10512500	1.99704400
H	6.72431000	1.50202300	2.64546800
H	7.72440200	1.65825800	1.19778900
O	1.08428000	0.95377200	-1.23012900
H	-0.03141800	0.14970700	-1.33282800
C	1.46524800	-2.78927800	1.58274700
C	2.83405900	-1.78178400	-0.18852300
C	1.62271400	-2.29881300	-0.56549200
N	0.86027900	-2.85705400	0.42824700
O	1.17221400	-2.26949100	-1.82938100
S	3.04488600	-2.06743000	1.50916200
C	3.65347300	-0.87638900	-1.05882000
H	2.96211300	-0.64896300	-1.87914500
C	0.83010700	-3.22837900	2.83407500
C	-0.29047000	-4.06595800	2.76087000
C	1.27470000	-2.78312500	4.08277200
C	-0.96226900	-4.43631800	3.91919800
H	-0.60604400	-4.43615100	1.79195500
C	0.60670700	-3.16768500	5.24023200
H	2.13528000	-2.12243200	4.14785500
C	-0.51657300	-3.98806100	5.16181800
H	-1.82917000	-5.08492700	3.84564700
H	0.95931700	-2.81851800	6.20536100
H	-1.03895200	-4.28167200	6.06653200
C	4.90000200	-1.49071400	-1.66501800
C	5.57178400	-2.56887600	-1.08909900
C	5.43246900	-0.92077600	-2.82531500
C	6.74994400	-3.06224600	-1.64374100
H	5.16910300	-3.04308700	-0.19907900
C	6.60790800	-1.39778300	-3.39247600
H	4.91309300	-0.09059600	-3.29761200
C	7.26076400	-2.46779200	-2.78998400
H	7.26675400	-3.90268700	-1.19409500
H	7.01287700	-0.95494700	-4.29549200
Cl	8.73671200	-3.08064400	-3.49334000

**TS4(S4)**

O	-0.52979100	0.03563300	-0.41931900
N	0.35062800	3.65107900	1.54015700
N	-0.83694500	3.97982500	2.13556200
N	-0.75882400	1.85310700	1.55494100

C	2. 42600900	4. 56218200	2. 36467400
H	2. 35774200	3. 84094400	3. 17385800
C	3. 48788700	5. 44984500	2. 26337200
H	4. 28276800	5. 43359600	3. 00040600
C	3. 51686900	6. 36009300	1. 20780000
H	4. 34239500	7. 05881000	1. 11901400
C	2. 49742000	6. 37979500	0. 26388300
H	2. 53915300	7. 09363300	-0. 55355000
C	1. 41473900	5. 49639200	0. 33350000
C	1. 41802400	4. 60441400	1. 40486100
C	0. 41870200	2. 36689400	1. 19743300
C	-1. 48820100	2. 85360100	2. 13446200
C	-2. 78108600	2. 32667400	2. 66663000
H	-3. 60732300	2. 57637200	1. 99420200
H	-3. 00301700	2. 73478800	3. 65276400
C	-2. 47947900	0. 80290100	2. 70706400
H	-3. 36385700	0. 18721400	2. 54098500
H	-2. 06722800	0. 55310800	3. 68718900
C	-1. 36546400	0. 52471600	1. 67038200
H	-0. 59592900	-0. 12498700	2. 06883900
C	-1. 75213700	-0. 03109600	0. 27560500
C	-2. 16443600	-1. 50087300	0. 41836100
C	-3. 22069000	-2. 07321600	-0. 28803600
C	-1. 35373000	-2. 33656800	1. 19806300
C	-3. 49764200	-3. 43360700	-0. 16020700
H	-3. 82548700	-1. 47934100	-0. 96606400
C	-1. 66547100	-3. 68146400	1. 34082100
H	-0. 44539800	-1. 96598900	1. 67069800
C	-2. 74517800	-4. 24747800	0. 67343400
C	-2. 78491600	0. 88606300	-0. 37647700
C	-4. 13410200	0. 86166800	-0. 01893200
C	-2. 34540400	1. 85843300	-1. 27963000
C	-5. 02047900	1. 79681400	-0. 54340900
H	-4. 51306000	0. 11011300	0. 66739700
C	-3. 24901200	2. 77360500	-1. 81169700
H	-1. 29632200	1. 88748300	-1. 56364200
C	-4. 59089400	2. 75887100	-1. 44782100
H	-2. 96186600	-5. 30539000	0. 76204000
H	-5. 28957100	3. 47385200	-1. 86794000
H	1. 61951000	1. 11509200	-2. 26796100
C	-0. 81105200	-4. 50349900	2. 26650000
C	-4. 63256200	-4. 00516500	-0. 96216300
C	-2. 75951300	3. 84119100	-2. 75103200
C	-6. 43505700	1. 80507900	-0. 03673100

F	-6.49892700	2.41343500	1.16089100
F	-6.90655900	0.56357300	0.13111100
F	-7.26116700	2.45518200	-0.86139900
F	-2.39795400	4.94735400	-2.07147200
F	-3.70988800	4.21116900	-3.61705500
F	-1.69154300	3.44432200	-3.44779200
F	0.49396200	-4.26239400	2.08365000
F	-1.07818300	-4.20942300	3.55191200
F	-1.01565400	-5.81772600	2.11183700
F	-5.82215300	-3.61121300	-0.48301500
F	-4.62365900	-5.34343800	-0.96596900
F	-4.57653100	-3.59391700	-2.23984900
C	0.31203800	5.53250300	-0.70507700
C	0.87069000	5.28073200	-2.10906200
C	-0.44250700	6.86466900	-0.62542000
H	-0.40115400	4.73028100	-0.48486100
H	1.40076900	4.32592700	-2.14438800
H	0.05356700	5.25409000	-2.83352900
H	1.56167900	6.07614400	-2.40658500
H	-0.87081200	7.01325400	0.36961200
H	0.22892000	7.70355100	-0.83591100
H	-1.24972300	6.88495000	-1.36054700
C	3.75602200	0.37775000	0.64891300
C	2.43041700	0.91374300	1.18199800
H	4.49092700	1.19801000	0.66144200
C	1.58408300	1.75675500	0.41358600
H	2.50912700	1.32848600	2.19295200
C	4.29874300	-0.72112600	1.57687700
C	4.55440600	-0.26072500	3.01244900
H	5.23950900	-1.10207600	1.16094300
H	3.59194400	-1.55949700	1.61275400
C	5.15717600	-1.37698100	3.86144600
H	5.22747400	0.60702000	3.00429200
H	3.62010300	0.07601800	3.47739700
H	5.31882000	-1.05680500	4.89433500
H	4.49320000	-2.24771800	3.87572800
H	6.11926900	-1.70365700	3.45466800
O	1.58976800	2.10110700	-0.77232300
H	-0.56247000	-0.51839200	-1.21928500
C	0.87498800	-2.77515900	-1.52518800
C	2.55020200	-1.01102300	-1.17039500
C	1.58222500	-0.76948700	-2.11489900
N	0.65145400	-1.75306400	-2.30848000
O	1.43276500	0.35177600	-2.84580000

S	2. 21969400	-2. 55784600	-0. 45094100
C	3. 68545700	-0. 07987900	-0. 84061800
H	3. 45887300	0. 82546800	-1. 41106500
C	0. 05893500	-3. 99971500	-1. 56217500
C	-1. 05866700	-4. 03898000	-2. 40526600
C	0. 38579200	-5. 13043500	-0. 80606300
C	-1. 83540100	-5. 18859400	-2. 48359600
H	-1. 29823400	-3. 16101200	-2. 99602800
C	-0. 40201500	-6. 27408400	-0. 87807100
H	1. 25392800	-5. 11744700	-0. 15359800
C	-1. 51460900	-6. 30668100	-1. 71591500
H	-2. 70399600	-5. 20653800	-3. 13346500
H	-0. 14483000	-7. 13956100	-0. 27645600
H	-2. 13024500	-7. 19879800	-1. 77220300
C	5. 05759200	-0. 53208400	-1. 33495500
C	5. 37023500	-1. 84522000	-1. 68425600
C	6. 06635900	0. 43284600	-1. 43996100
C	6. 65081100	-2. 19468800	-2. 10776800
H	4. 61026700	-2. 61690400	-1. 64124800
C	7. 34858700	0. 10445400	-1. 86024400
H	5. 84146000	1. 46873700	-1. 19804300
C	7. 63178600	-1. 21705000	-2. 18805800
H	6. 88438700	-3. 21853000	-2. 37727100
H	8. 12124600	0. 86065700	-1. 94334400
C	1. 06209100	-0. 50268500	3. 65562500
O	0. 74925200	0. 68188600	3. 81495200
O	1. 30180300	-1. 03854600	2. 49375900
H	1. 70122800	-0. 10067700	1. 68838000
C	1. 19046900	-1. 45600500	4. 82608900
H	0. 65193300	-2. 38181900	4. 61092800
H	2. 24600000	-1. 71565300	4. 95210100
H	0. 81642300	-0. 99347000	5. 73858200
Cl	9. 23871900	-1. 64684100	-2. 71733800

### 3(S5)

O	-0. 89531000	-0. 53807400	-1. 43272300
N	0. 33886100	2. 61465700	1. 90165300
N	-0. 74127100	2. 59093600	2. 74391800
N	-0. 78298800	0. 90799000	1. 31579000
C	1. 95482000	3. 60197200	3. 37416200
H	1. 58620000	2. 91194000	4. 12590800
C	2. 98949700	4. 48413600	3. 64767400
H	3. 44729300	4. 49597600	4. 63045100
C	3. 43343700	5. 34201500	2. 64367400

H	4.24954600	6.03019100	2.83806400
C	2.83231600	5.32194700	1.39157200
H	3.18430200	6.00421800	0.62345700
C	1.77989800	4.45110300	1.08151800
C	1.37567400	3.59278500	2.10674000
C	0.34786200	1.58285600	1.04510200
C	-1.40371800	1.54345300	2.35671100
C	-2.61926300	0.80820100	2.80477100
H	-3.52087600	1.34617300	2.50059600
H	-2.63845000	0.70413800	3.89031500
C	-2.44362600	-0.55371900	2.08029900
H	-3.38861200	-0.95443000	1.71242500
H	-2.03514800	-1.29186300	2.77581900
C	-1.41652800	-0.36721800	0.92178700
H	-0.64735800	-1.14222400	0.95254700
C	-1.95826000	-0.35172000	-0.55422200
C	-2.87079400	-1.57280000	-0.74463800
C	-4.10661600	-1.51196100	-1.38349900
C	-2.39500900	-2.82065600	-0.32662700
C	-4.86860200	-2.66615100	-1.56002400
H	-4.49494800	-0.57064500	-1.75656300
C	-3.17217800	-3.96001900	-0.49631400
H	-1.40126000	-2.91954000	0.10923800
C	-4.41929700	-3.89819300	-1.10864100
C	-2.66856300	0.98262500	-0.79836700
C	-3.86601900	1.29821300	-0.15700300
C	-2.07576200	1.94725300	-1.61602100
C	-4.44377300	2.55626100	-0.30309800
H	-4.37838300	0.55853900	0.45275500
C	-2.67952600	3.19120400	-1.77568400
H	-1.13402400	1.73256900	-2.11090000
C	-3.85983300	3.51730300	-1.11506900
H	-5.02072200	-4.79033300	-1.23958200
H	-4.31236100	4.49535600	-1.23237900
H	0.29974800	-1.89130000	-1.74359900
C	-2.66036800	-5.26515000	0.04569800
C	-6.17835700	-2.56454600	-2.29233200
C	-2.08121800	4.18212100	-2.73528500
C	-5.69697400	2.84240200	0.47344100
F	-5.44751400	2.83010800	1.79872900
F	-6.63107900	1.90887600	0.25438400
F	-6.22155300	4.03316500	0.17580900
F	-0.75029400	4.04037400	-2.82659400
F	-2.33042400	5.44547300	-2.35620000

F	-2.57931500	4.03429100	-3.96819700
F	-1.34533000	-5.40364000	-0.16384000
F	-2.84868400	-5.34333800	1.37848100
F	-3.28060000	-6.31581700	-0.50096900
F	-6.82125000	-1.42888100	-1.98279600
F	-6.99041200	-3.58776800	-1.99631500
F	-6.00089900	-2.56554100	-3.61979800
C	1.13895200	4.50714900	-0.29389000
C	2.16390800	4.23376800	-1.39986900
C	0.45842500	5.86802800	-0.49311200
H	0.36996700	3.73030800	-0.36825800
H	2.64295400	3.26300600	-1.25479300
H	1.66502900	4.22871300	-2.37125500
H	2.93636700	5.00967900	-1.41796800
H	-0.30717900	6.04511100	0.26758800
H	1.18970700	6.68017700	-0.43022700
H	-0.01178700	5.91346400	-1.47660000
C	3.84877000	0.72678700	-0.25066800
C	2.64837200	1.17707100	0.53436000
H	3.98805500	1.40265500	-1.10930500
C	1.39238200	1.23365400	0.03911900
H	2.79640000	1.40923200	1.58490100
C	5.10621200	0.84776800	0.62008600
C	5.38478400	2.29933900	1.01853000
H	5.97651100	0.45467800	0.08335900
H	4.99410500	0.23453100	1.52743000
C	6.61293800	2.43777100	1.91281200
H	5.51929900	2.89285300	0.10432100
H	4.51250200	2.72844300	1.52778000
H	6.79398900	3.48217700	2.18137900
H	6.48445000	1.87111600	2.84063000
H	7.50998700	2.05781200	1.41440000
O	0.98035700	1.01050300	-1.17274000
H	-0.10224700	0.15631000	-1.29712500
C	1.44940300	-2.67379400	1.70315900
C	2.81602600	-1.62118500	-0.04230100
C	1.64127600	-2.19900900	-0.44554900
N	0.87939800	-2.78212500	0.53416100
O	1.22671000	-2.20509200	-1.72146800
S	2.99413200	-1.87647700	1.66392800
C	3.61210400	-0.68780200	-0.90369300
H	2.93269800	-0.50159400	-1.74439500
C	0.80638600	-3.13433400	2.94264000
C	-0.26935500	-4.02677500	2.84958900



C	1. 19994500	-2. 65998100	4. 19769700
C	-0. 94826700	-4. 42309500	3. 99508200
H	-0. 54384900	-4. 41814600	1. 87649600
C	0. 52552100	-3. 07031100	5. 34239400
H	2. 02538100	-1. 95742100	4. 27788400
C	-0. 55363800	-3. 94594600	5. 24414800
H	-1. 78004000	-5. 11437700	3. 90678100
H	0. 83838700	-2. 69880100	6. 31281600
H	-1. 08132000	-4. 25996500	6. 13885100
C	4. 90037100	-1. 24687500	-1. 47142700
C	5. 59983600	-2. 29425600	-0. 86660000
C	5. 43589100	-0. 65349900	-2. 62160700
C	6. 81427300	-2. 73337700	-1. 38079100
H	5. 18844300	-2. 78012600	0. 01224800
C	6. 64660700	-1. 07529900	-3. 15087200
H	4. 88899500	0. 14868400	-3. 10951600
C	7. 31898600	-2. 10989500	-2. 51244000
H	7. 36988500	-3. 54304900	-0. 92433700
H	7. 07242400	-0. 62897200	-4. 04077100
N	8. 60438500	-2. 56337200	-3. 05849600
O	9. 17554000	-3. 47058600	-2. 48045000
O	9. 02412000	-2. 00195900	-4. 05460300

**TS4(S5)**

O	-0. 61708800	0. 02021500	-0. 40730900
N	0. 04055600	3. 68609600	1. 54422900
N	-1. 17515000	3. 96100300	2. 10889500
N	-0. 98085500	1. 83639500	1. 54847200
C	2. 04945500	4. 69854200	2. 41351100
H	1. 99451100	3. 97981100	3. 22595500
C	3. 07063500	5. 63474000	2. 33283100
H	3. 84643500	5. 66029700	3. 08966800
C	3. 08302100	6. 53995500	1. 27257400
H	3. 87657100	7. 27653300	1. 19997800
C	2. 08737200	6. 50699500	0. 30391300
H	2. 11569600	7. 21822600	-0. 51635200
C	1. 04588600	5. 57393600	0. 35234700
C	1. 06488100	4. 68830500	1. 42875700
C	0. 17830900	2. 40421600	1. 21416600
C	-1. 77132700	2. 80460400	2. 10212000
C	-3. 04997700	2. 21970500	2. 60746100
H	-3. 87092900	2. 42600100	1. 91418200
H	-3. 31435600	2. 62258500	3. 58524500
C	-2. 67751000	0. 71220600	2. 66569600

H	-3.52740600	0.05435300	2.48224400
H	-2.27848500	0.48774500	3.65732800
C	-1.52621100	0.48122900	1.65853500
H	-0.73664600	-0.12873300	2.08015600
C	-1.85209400	-0.09979100	0.25866200
C	-2.19818000	-1.58651800	0.40089000
C	-3.20764100	-2.21179600	-0.32876100
C	-1.36949900	-2.37875100	1.20655600
C	-3.42315000	-3.58309700	-0.19955900
H	-3.82220400	-1.65064500	-1.02562000
C	-1.62051900	-3.73630800	1.34922300
H	-0.49240300	-1.96326800	1.70036400
C	-2.65462200	-4.35622400	0.65797000
C	-2.91030000	0.76427000	-0.42442500
C	-4.26530700	0.67779100	-0.09995800
C	-2.49500800	1.75172800	-1.32255900
C	-5.18154800	1.56716200	-0.65205600
H	-4.62523700	-0.08730400	0.58164200
C	-3.42723100	2.62023900	-1.88262100
H	-1.44190800	1.82937400	-1.58103600
C	-4.77556800	2.54368300	-1.55187000
H	-2.82335500	-5.42276700	0.74759300
H	-5.49659200	3.22238000	-1.99388100
H	1.52429100	1.19171000	-2.21104700
C	-0.75106000	-4.51250800	2.30024100
C	-4.50876700	-4.21204500	-1.02664400
C	-2.96557500	3.70472500	-2.81672200
C	-6.60719800	1.51093400	-0.18029100
F	-6.72912500	2.12244500	1.01109500
F	-7.02286100	0.24929900	-0.01546300
F	-7.44236000	2.11606900	-1.02948000
F	-2.67940400	4.83224300	-2.13640200
F	-3.90809200	4.02007500	-3.71209800
F	-1.85938900	3.35714800	-3.47965000
F	0.54537100	-4.21115300	2.14605900
F	-1.06195000	-4.22418200	3.57683300
F	-0.88998300	-5.83552400	2.14890400
F	-5.72748500	-3.87594400	-0.57817800
F	-4.43356400	-5.54819000	-1.02498600
F	-4.44145300	-3.80188200	-2.30412100
C	-0.03173400	5.55328700	-0.71266700
C	0.57212600	5.32062000	-2.10117000
C	-0.84925900	6.84911900	-0.65970300
H	-0.71210100	4.71985600	-0.50471900

H	1. 14566700	4. 39069700	-2. 11821400
H	-0. 22463600	5. 25360400	-2. 84537400
H	1. 23370100	6. 14500900	-2. 38628800
H	-1. 30801200	6. 98275700	0. 32378500
H	-0. 21290300	7. 71737800	-0. 85952400
H	-1. 63846500	6. 82741800	-1. 41408500
C	3. 61841500	0. 57217200	0. 77096400
C	2. 25480100	1. 04543100	1. 26563700
H	4. 31186200	1. 42724600	0. 79732300
C	1. 39174800	1. 84424200	0. 46758200
H	2. 28882600	1. 47071700	2. 27460900
C	4. 18886100	-0. 49596400	1. 71821900
C	4. 38559200	-0. 01724600	3. 15712400
H	5. 15752600	-0. 83465400	1. 32987800
H	3. 52147700	-1. 36638200	1. 74086800
C	5. 01567100	-1. 10092200	4. 02810000
H	5. 01833500	0. 88031200	3. 16135200
H	3. 42467900	0. 27857100	3. 59460400
H	5. 13462300	-0. 76856800	5. 06281200
H	4. 39192800	-2. 00097100	4. 02991800
H	6. 00245500	-1. 38507500	3. 64953600
O	1. 41816600	2. 18027300	-0. 72012300
H	-0. 60727800	-0. 53618300	-1. 20601500
C	0. 94399600	-2. 72415500	-1. 46023500
C	2. 52416300	-0. 88254200	-1. 07013100
C	1. 57511000	-0. 69180000	-2. 04477400
N	0. 69731800	-1. 71904700	-2. 25805500
O	1. 39790300	0. 41619900	-2. 78901300
S	2. 24336800	-2. 43734100	-0. 34614200
C	3. 60469800	0. 10288400	-0. 71710000
H	3. 35347700	0. 99402900	-1. 29970500
C	0. 18735100	-3. 98580600	-1. 51066200
C	-0. 90502200	-4. 08124200	-2. 38174900
C	0. 54782500	-5. 09613700	-0. 73979700
C	-1. 62444500	-5. 26662600	-2. 47310400
H	-1. 17066400	-3. 21837100	-2. 98349500
C	-0. 18301000	-6. 27605700	-0. 82533800
H	1. 39748200	-5. 03953700	-0. 06567700
C	-1. 27089600	-6. 36472200	-1. 69110700
H	-2. 47445800	-5. 32857400	-3. 14443600
H	0. 09933900	-7. 12580900	-0. 21275700
H	-1. 84215800	-7. 28515100	-1. 75800200
C	5. 00840700	-0. 28538900	-1. 17310600
C	5. 37940200	-1. 58439900	-1. 52675800

C	5.97630700	0.72753800	-1.23913700
C	6.68213300	-1.87671700	-1.91702000
H	4.64703600	-2.38250600	-1.51051100
C	7.28034500	0.45870800	-1.62505900
H	5.69676300	1.74842400	-0.99377700
C	7.61140900	-0.84956400	-1.95364600
H	6.98406200	-2.87953500	-2.19244600
H	8.03578500	1.23230500	-1.68440000
C	0.89526200	-0.42170300	3.71134800
O	0.52463600	0.74853500	3.85281300
O	1.19022500	-0.95328500	2.56032700
H	1.56456300	0.00217900	1.75723400
C	1.03577900	-1.35981000	4.89258600
H	0.54822400	-2.31176600	4.67019900
H	2.09845600	-1.56785400	5.05035100
H	0.61472200	-0.90940700	5.79053600
N	8.98949900	-1.15181700	-2.36250900
O	9.78844300	-0.23249100	-2.37399900
O	9.24935200	-2.30292400	-2.66235500

**3(S6)**

O	-0.68863300	-0.33933900	-1.51816900
N	1.54579500	2.10257000	1.89462700
N	0.57664000	2.21707200	2.85656200
N	0.02114900	0.74356500	1.30925100
C	3.46704700	2.58566200	3.24586800
H	3.02854000	1.91910200	3.98100000
C	4.68778400	3.20498400	3.46802500
H	5.22547600	3.02899800	4.39297300
C	5.21269300	4.04220000	2.48605700
H	6.17277000	4.52404200	2.63867600
C	4.50880800	4.26591100	1.30978400
H	4.92781400	4.92974400	0.55936300
C	3.26840000	3.66736400	1.05532600
C	2.78541500	2.81673300	2.05260000
C	1.24169000	1.18883900	0.96113900
C	-0.33613100	1.38033800	2.46651800
C	-1.63344000	0.87498800	2.99611000
H	-2.41803500	1.62223900	2.85190100
H	-1.56526100	0.65888600	4.06302700
C	-1.84034000	-0.40526800	2.14274600
H	-2.88299100	-0.55223700	1.85940200
H	-1.54070300	-1.28534900	2.71832900
C	-0.91818100	-0.31641000	0.88839600

H	-0.34385300	-1.23661900	0.75964500
C	-1.58721500	-0.02455100	-0.50473500
C	-2.76849000	-0.99087400	-0.68342100
C	-4.01747600	-0.59436100	-1.15438500
C	-2.54769100	-2.35077600	-0.43681000
C	-5.03584200	-1.53009600	-1.33202900
H	-4.21843600	0.44401500	-1.39384600
C	-3.57684600	-3.26933400	-0.60413600
H	-1.56226900	-2.70917700	-0.13969900
C	-4.83387600	-2.87230800	-1.04758700
C	-1.99748900	1.45016100	-0.54953900
C	-3.01948100	1.94785600	0.25824000
C	-1.28973400	2.34415700	-1.35591800
C	-3.31016000	3.30906400	0.28393200
H	-3.61987700	1.27626100	0.86648400
C	-1.61003500	3.69856700	-1.34150000
H	-0.47710000	1.98357900	-1.97827900
C	-2.61142600	4.20083700	-0.51632500
H	-5.63228300	-3.59366400	-1.17796200
H	-2.84108400	5.26012700	-0.49987200
H	0.12059500	-1.88027400	-2.08656200
C	-3.32441900	-4.70640600	-0.24340100
C	-6.35655800	-1.06848900	-1.88327100
C	-0.90631300	4.63085600	-2.28799500
C	-4.38056600	3.77573800	1.22798900
F	-4.00935700	3.56905600	2.50785100
F	-5.52009400	3.09598200	1.04911700
F	-4.64821800	5.07685400	1.09420800
F	0.34124700	4.21649400	-2.55481600
F	-0.82361600	5.87271100	-1.78464700
F	-1.55031300	4.72192500	-3.45759300
F	-2.09920500	-5.09985800	-0.61108300
F	-3.40643600	-4.89328700	1.08943900
F	-4.21218300	-5.53091300	-0.80999600
F	-6.68701300	0.14096800	-1.40678400
F	-7.34617700	-1.91528400	-1.56958300
F	-6.32499000	-0.96841400	-3.21867100
C	2.52862500	3.99229000	-0.23040200
C	3.36011800	3.62243600	-1.46336800
C	2.14715600	5.47866900	-0.24493400
H	1.60481000	3.40514700	-0.27752600
H	3.63668000	2.56607700	-1.44330900
H	2.77847000	3.80829200	-2.36874500
H	4.27278400	4.22549900	-1.51488900

H	1. 50924100	5. 73418700	0. 60601200
H	3. 04103700	6. 10875800	-0. 19653600
H	1. 61328500	5. 72158400	-1. 16483200
C	4. 30383900	-0. 27258100	-0. 81953300
C	3. 32904600	0. 35522000	0. 13891900
H	4. 51703400	0. 44174900	-1. 63076900
C	2. 07421900	0. 73472400	-0. 18948700
H	3. 63368600	0. 44359600	1. 17810700
C	5. 63518600	-0. 54049300	-0. 10499400
C	6. 28694400	0. 75345000	0. 38447700
H	6. 31892700	-1. 05349000	-0. 78709100
H	5. 47085600	-1. 21947100	0. 74409100
H	6. 46170500	1. 43214000	-0. 45768900
H	5. 66020000	1. 28837500	1. 10620500
O	1. 49690000	0. 73715300	-1. 35486100
H	0. 25523900	0. 14809300	-1. 41963600
C	1. 39112600	-3. 25388600	1. 12805200
C	2. 77808300	-2. 33565000	-0. 67793500
C	1. 47187500	-2. 61206900	-0. 98451800
N	0. 70017100	-3. 12086700	0. 02869900
O	0. 94098000	-2. 40144300	-2. 19973000
S	3. 06106200	-2. 79894200	0. 96909500
C	3. 68059600	-1. 51811200	-1. 55330900
H	2. 98086300	-1. 09737600	-2. 28525100
C	0. 78315600	-3. 68532200	2. 39549900
C	-0. 47127000	-4. 30819400	2. 36147000
C	1. 39167800	-3. 43428600	3. 62918200
C	-1. 11032000	-4. 65721800	3. 54465900
H	-0. 91921300	-4. 53209600	1. 39992800
C	0. 75383400	-3. 79793600	4. 81019900
H	2. 35895800	-2. 93997900	3. 66578600
C	-0. 50063200	-4. 40273500	4. 77234000
H	-2. 08236500	-5. 13775700	3. 50098800
H	1. 23417200	-3. 60030300	5. 76309700
H	-0. 99830400	-4. 67985400	5. 69600000
C	4. 73757400	-2. 29143600	-2. 31932500
C	5. 24232500	-3. 51755800	-1. 88560600
C	5. 26809200	-1. 72461600	-3. 48236200
C	6. 26084400	-4. 15630800	-2. 58998300
H	4. 83075300	-3. 98430200	-0. 99534200
C	6. 28593800	-2. 35812700	-4. 18651800
H	4. 87061600	-0. 77720000	-3. 83920800
C	6. 78934900	-3. 57786100	-3. 73941000
H	6. 63895000	-5. 11153800	-2. 23897400

H	6.68130300	-1.90399500	-5.08984300
H	7.58128200	-4.07678100	-4.28865400
H	7.25062100	0.55387400	0.86037300

**TS4(S6)**

O	-0.16656900	0.14127400	-0.43449000
N	3.18357800	1.76889400	1.52154500
N	2.66325500	2.84345800	2.19062100
N	1.10197000	1.41128500	1.57585500
C	5.25721500	0.77012800	2.24212600
H	4.69084800	0.30340900	3.04273400
C	6.62153300	0.56359300	2.09496900
H	7.15163600	-0.08199700	2.78600500
C	7.29803800	1.19631600	1.05306800
H	8.36491500	1.04181400	0.92859000
C	6.61703200	2.02276800	0.16779600
H	7.16017700	2.50379900	-0.64035100
C	5.24129200	2.24911600	0.28442000
C	4.60020600	1.60394100	1.34086600
C	2.25478300	0.88823100	1.15626100
C	1.38788300	2.58751600	2.21139200
C	0.15370400	3.17999800	2.80999200
H	-0.22113100	4.00097200	2.19139700
H	0.34033100	3.56160300	3.81391700
C	-0.79167500	1.94677000	2.80802600
H	-1.84161500	2.21297400	2.68316500
H	-0.68261700	1.41949900	3.75841500
C	-0.29349500	0.98386600	1.70460100
H	-0.26365100	-0.04307400	2.04723300
C	-1.00203900	0.98079200	0.32525000
C	-2.37804300	0.32015200	0.47076000
C	-3.52066700	0.77492600	-0.18517300
C	-2.45852000	-0.87476200	1.19800600
C	-4.72656700	0.08722500	-0.05660300
H	-3.48535100	1.65154100	-0.82437100
C	-3.67587900	-1.52475400	1.34631300
H	-1.57074400	-1.34099900	1.62261700
C	-4.82781200	-1.05008700	0.73076300
C	-1.00566200	2.39366900	-0.25525000
C	-1.89936700	3.37434200	0.17850500
C	-0.00944100	2.74762100	-1.16999600
C	-1.79074200	4.68233600	-0.28264100
H	-2.69544300	3.13035900	0.87582800
C	0.07226300	4.05574500	-1.63823100

H	0.69279600	1.99163700	-1.51280900
C	-0.80914900	5.03711700	-1.19832600
H	-5.76707800	-1.58256400	0.82142700
H	-0.74051200	6.05380600	-1.56915900
H	2.00968300	-0.67277500	-2.38271200
C	-3.71552600	-2.74483000	2.22484700
C	-5.92156200	0.60271200	-0.80746500
C	1.17074600	4.43780200	-2.59158600
C	-2.69842100	5.72603200	0.30413000
F	-2.24731000	6.11340400	1.51040900
F	-3.93900500	5.25659400	0.48447500
F	-2.77479800	6.81643300	-0.46438900
F	2.25784800	4.86837000	-1.92146800
F	0.79624100	5.43360600	-3.40321300
F	1.55990500	3.40780500	-3.34714200
F	-2.67939800	-3.56048600	1.99136500
F	-3.64591500	-2.40001500	3.52424900
F	-4.84318900	-3.44889700	2.06529900
F	-6.38858300	1.74032100	-0.27101200
F	-6.92825800	-0.27919700	-0.81957700
F	-5.60746100	0.87922800	-2.08406200
C	4.51559900	3.15301500	-0.69136000
C	4.65992000	2.63950800	-2.12739000
C	5.02155200	4.59332600	-0.55040000
H	3.44801100	3.14742300	-0.44447700
H	4.28958000	1.61457400	-2.20611500
H	4.08455500	3.27246900	-2.80674100
H	5.70609100	2.65976300	-2.44957800
H	4.87583400	4.96164500	0.46879000
H	6.08940200	4.65359000	-0.78482300
H	4.48645800	5.24978800	-1.23972300
C	2.96218200	-2.89256700	0.39219700
C	2.49384800	-1.57630700	1.00484100
H	4.06326000	-2.88766400	0.36355700
C	2.54611900	-0.34614800	0.29779700
H	2.87546800	-1.41275200	2.01864700
C	2.55154600	-4.07266200	1.28926200
C	3.13696500	-3.99047800	2.69870600
H	2.88741700	-5.00165700	0.81676200
H	1.45900600	-4.11771200	1.36682600
H	4.22766900	-3.89097400	2.66442000
H	2.74177700	-3.13894700	3.26153100
O	2.77636300	-0.06062100	-0.88134300
H	-0.62750900	-0.16695400	-1.23503500



C	-1.37814700	-2.72221900	-1.63110200
C	1.06328800	-2.83128500	-1.36352800
C	0.57445100	-1.89714200	-2.24469800
N	-0.78405000	-1.83892100	-2.38996700
O	1.29312900	-1.00563100	-2.95452400
S	-0.29213400	-3.64313100	-0.64154900
C	2.52240400	-3.08016900	-1.09227800
H	3.03135100	-2.28541100	-1.64542100
C	-2.83742800	-2.91550800	-1.63201500
C	-3.62818700	-2.06335600	-2.41316200
C	-3.45041300	-3.94056700	-0.90365000
C	-5.00649000	-2.23399300	-2.45888400
H	-3.14283700	-1.27797500	-2.98305700
C	-4.83147100	-4.09932300	-0.94241600
H	-2.84947300	-4.61344900	-0.29888400
C	-5.61356200	-3.24708600	-1.71897200
H	-5.61070000	-1.56365600	-3.06125900
H	-5.29548700	-4.89034500	-0.36263500
H	-6.69148300	-3.37063600	-1.74929300
C	3.07913400	-4.38378500	-1.66145500
C	2.29585600	-5.48344600	-2.01080900
C	4.46549700	-4.47944000	-1.83178500
C	2.88192400	-6.65024400	-2.49988700
H	1.21701500	-5.43494100	-1.91551000
C	5.05339700	-5.64065100	-2.31836600
H	5.09065500	-3.62320400	-1.58833000
C	4.26070000	-6.73659500	-2.65203900
H	2.25137900	-7.49287000	-2.76630800
H	6.13050800	-5.68758900	-2.44576500
C	0.55937700	-1.64391400	3.51162000
O	1.25228000	-0.64575700	3.73527400
O	0.29947900	-2.09324000	2.31819500
H	1.26018300	-1.72868300	1.52177300
C	-0.08090700	-2.43947800	4.63110500
H	-1.15697800	-2.51655100	4.45503800
H	0.32057100	-3.45647200	4.61588200
H	0.11702300	-1.97358200	5.59556700
H	4.71488600	-7.64485400	-3.03477900
H	2.90314200	-4.89456800	3.26723100

**3(S7)**

O	-0.79503600	-0.13722100	-1.65523100
N	1.53665700	1.93875400	1.92548800
N	0.57393400	2.02528900	2.89681100

N	-0.05145200	0.70367800	1.24267500
C	3.48639700	2.21160200	3.29569500
H	3.02019300	1.50532000	3.97459100
C	4.73747500	2.74950800	3.55850900
H	5.27111000	2.46791200	4.45937400
C	5.29692600	3.64327800	2.64803600
H	6.27974500	4.06430800	2.83310300
C	4.59918100	3.99985600	1.50109900
H	5.04637600	4.70424200	0.80594900
C	3.33081100	3.48359400	1.20663000
C	2.81048000	2.57676700	2.13317500
C	1.18857500	1.11536500	0.92528500
C	-0.37814900	1.26598200	2.44650600
C	-1.69956200	0.78517000	2.93830700
H	-2.44659400	1.57840800	2.85109100
H	-1.64458100	0.48641900	3.98586500
C	-1.96612000	-0.41586400	1.99118500
H	-3.01404600	-0.49036100	1.69897600
H	-1.71042600	-1.35065000	2.49798700
C	-1.03723600	-0.27790300	0.74616100
H	-0.50557200	-1.21179800	0.55139100
C	-1.68436600	0.14380500	-0.62373500
C	-2.90528800	-0.75535900	-0.87165100
C	-4.13973900	-0.27417300	-1.29956400
C	-2.73822200	-2.13796600	-0.73121500
C	-5.19646400	-1.15233000	-1.53807100
H	-4.29981000	0.78662800	-1.45764900
C	-3.80514200	-2.99894500	-0.95636700
H	-1.76551000	-2.55554000	-0.47199900
C	-5.04786600	-2.51913700	-1.35684700
C	-2.02912000	1.63450900	-0.56113100
C	-3.02861100	2.11649100	0.28378500
C	-1.28069800	2.55341900	-1.29988900
C	-3.25805800	3.48359600	0.41107400
H	-3.65877300	1.42955000	0.84266600
C	-1.53943100	3.91619200	-1.18351400
H	-0.48354400	2.20420700	-1.94818500
C	-2.51865500	4.40021000	-0.32174900
H	-5.87607600	-3.19578500	-1.53342800
H	-2.70029100	5.46458200	-0.22588900
H	-0.02485800	-1.66471000	-2.33870200
C	-3.61203800	-4.46761700	-0.70251000
C	-6.50058400	-0.59820500	-2.04128900
C	-0.79106100	4.88379000	-2.05755100

C	-4.30740100	3.92648600	1.38953500
F	-3.94592500	3.61217100	2.65017800
F	-5.47529300	3.31118000	1.16545000
F	-4.51864100	5.24421900	1.35100500
F	0.44013600	4.43783000	-2.34806500
F	-0.66042400	6.08181600	-1.46569100
F	-1.42212200	5.08538100	-3.22035700
F	-2.39855400	-4.88077000	-1.08669800
F	-3.71826600	-4.74996100	0.61189200
F	-4.52395100	-5.21216500	-1.33750300
F	-6.77564200	0.58775600	-1.47843300
F	-7.52296500	-1.42260000	-1.77651300
F	-6.47561200	-0.40666600	-3.36686600
C	2.60453100	3.94446000	-0.04477900
C	3.41541300	3.63403000	-1.30756300
C	2.29283500	5.44335000	0.06005200
H	1.65437500	3.40613900	-0.13297400
H	3.63035400	2.56558400	-1.37862800
H	2.84678800	3.92908800	-2.19195800
H	4.36120200	4.18603000	-1.31076200
H	1.67417300	5.66075100	0.93543000
H	3.21540900	6.02623900	0.14684200
H	1.76360800	5.78148100	-0.83213500
C	4.20287600	-0.32854700	-0.94581500
C	3.23563700	0.25520700	0.04667500
H	4.43869300	0.43395500	-1.70491900
C	2.00198100	0.71382700	-0.25830500
H	3.52834500	0.24273400	1.09279200
C	5.51916600	-0.66865500	-0.23461800
C	6.19510500	0.57910100	0.33908800
H	6.20599600	-1.15864800	-0.93263700
H	5.33071600	-1.38822000	0.57725300
C	7.48763500	0.25896700	1.08352100
H	6.40142100	1.27510600	-0.48515400
H	5.50911200	1.10868200	1.01258000
H	7.95418800	1.16493200	1.48067500
H	7.29485700	-0.41445700	1.92494700
H	8.21098800	-0.23260200	0.42572100
O	1.43343600	0.83525300	-1.42150700
H	0.16722100	0.30457100	-1.52528600
C	1.15463000	-3.28111700	0.78266500
C	2.60903800	-2.34276600	-0.95978300
C	1.29133700	-2.52212900	-1.28777400
N	0.48272200	-3.04458900	-0.31123500

O	0.77999000	-2.20055600	-2.48691000
S	2.85056400	-2.92154700	0.65815600
C	3.55662100	-1.50682600	-1.76768100
H	2.88609800	-1.01744500	-2.48424100
C	0.50682200	-3.73678500	2.02024100
C	-0.77757000	-4.29346100	1.94586300
C	1.09720100	-3.56421200	3.27405800
C	-1.45294400	-4.65164300	3.10299000
H	-1.22259300	-4.45815500	0.97087100
C	0.41618100	-3.93912300	4.42751400
H	2.08497900	-3.11721500	3.35195500
C	-0.86807900	-4.48277500	4.36365700
H	-2.44900400	-5.07947200	3.02340500
H	0.88699100	-3.79696900	5.39650400
C	4.60525400	-2.26336500	-2.56043100
C	5.06418100	-3.52904800	-2.19515800
C	5.17761900	-1.64103200	-3.67421200
C	6.07920100	-4.15284700	-2.91781700
H	4.61898200	-4.03811800	-1.34513100
C	6.19200400	-2.25952300	-4.39628100
H	4.81598100	-0.66131600	-3.97803500
C	6.64972000	-3.51962300	-4.01719300
H	6.42143200	-5.13938600	-2.62074600
H	6.62023700	-1.76181300	-5.26083700
H	7.43863200	-4.00701700	-4.58094000
C	-1.60264300	-4.90085500	5.61061500
H	-1.64901900	-5.99187800	5.68624000
H	-1.10812300	-4.52478300	6.50886400
H	-2.63197700	-4.53160200	5.60553100

**TS4(S7)**

O	-0.09727600	0.27465100	-0.43659500
N	3.43665900	1.58115600	1.43911600
N	3.02739800	2.67874500	2.14698400
N	1.33524900	1.39475100	1.55124700
C	5.44670400	0.40638600	2.06869500
H	4.87171800	-0.02983900	2.88031400
C	6.78432300	0.09515300	1.86952200
H	7.28427800	-0.60434700	2.52986900
C	7.47328700	0.69255000	0.81500400
H	8.51947500	0.45622100	0.64990800
C	6.83079000	1.58769800	-0.03145300
H	7.38277200	2.04008900	-0.85009000
C	5.48244500	1.92026400	0.13804400

C	4.82833600	1.30744700	1.20577300
C	2.42794800	0.78843500	1.08512900
C	1.73650900	2.52769600	2.20265000
C	0.57434900	3.20440600	2.85364700
H	0.24741200	4.06585600	2.26356000
H	0.82327300	3.54802100	3.85775800
C	-0.46710000	2.05136600	2.85999400
H	-1.49572600	2.40326400	2.77691700
H	-0.36956900	1.49630400	3.79563600
C	-0.08465100	1.07677700	1.72108900
H	-0.12628900	0.04348500	2.04310700
C	-0.83767800	1.15995700	0.36812800
C	-2.25466400	0.60309000	0.55007000
C	-3.38434300	1.16577600	-0.04156000
C	-2.39677900	-0.60775900	1.24081100
C	-4.63316400	0.56664900	0.11635800
H	-3.30771100	2.05813400	-0.65463200
C	-3.65300300	-1.17102800	1.41708300
H	-1.53080500	-1.15201300	1.61486500
C	-4.78868200	-0.58855800	0.86789500
C	-0.74919900	2.58117500	-0.18435700
C	-1.54542400	3.62018100	0.30040800
C	0.24039900	2.87525600	-1.12721800
C	-1.34830200	4.92523300	-0.13930800
H	-2.33332000	3.42562700	1.02209000
C	0.41112200	4.18282400	-1.57232100
H	0.86798000	2.07387300	-1.50948600
C	-0.37321800	5.22121800	-1.08238600
H	-5.76190600	-1.05135000	0.98204200
H	-0.23563900	6.23732400	-1.43517100
H	1.96350100	-0.63214000	-2.49736600
C	-3.75095800	-2.42010200	2.24921800
C	-5.81783100	1.19783600	-0.55841900
C	1.50533800	4.49692400	-2.55501800
C	-2.14931200	6.02408200	0.49962200
F	-1.63144400	6.34420900	1.69880800
F	-3.41795900	5.65196300	0.71014700
F	-2.16041300	7.13559200	-0.24189400
F	2.64682000	4.81650700	-1.91379000
F	1.18957300	5.54227100	-3.32852200
F	1.78040400	3.45882500	-3.34848400
F	-2.80567300	-3.31100800	1.92404500
F	-3.58015000	-2.13939900	3.55424600
F	-4.94369200	-3.01725400	2.12818700

F	-6.20297200	2.32062800	0.06652700
F	-6.87549000	0.37552000	-0.59109600
F	-5.53008900	1.54039400	-1.82437100
C	4.79878000	2.89962100	-0.79434100
C	4.86016000	2.41323200	-2.24555600
C	5.41769900	4.29343000	-0.63679000
H	3.74167600	2.96849000	-0.51405500
H	4.41342800	1.42021100	-2.33529700
H	4.31132300	3.10321800	-2.89053700
H	5.89424900	2.36603800	-2.60210700
H	5.33007700	4.64653300	0.39438200
H	6.47993800	4.27739800	-0.90206200
H	4.91549100	5.00578400	-1.29464000
C	2.79071500	-3.01642200	0.19345700
C	2.46227000	-1.68256100	0.85827000
H	3.88616500	-3.11637200	0.14188900
C	2.58957000	-0.43970900	0.18432500
H	2.89690700	-1.58098700	1.85886900
C	2.27773300	-4.18167600	1.05493100
C	2.87583700	-4.23372900	2.46123000
H	2.50585100	-5.12483100	0.54376300
H	1.18702500	-4.11753000	1.15485300
C	2.37520600	-5.44730800	3.24016700
H	3.97155400	-4.26043600	2.39230900
H	2.62260100	-3.32359400	3.01819000
H	2.78436400	-5.47461600	4.25386700
H	1.28276800	-5.42947900	3.31504600
H	2.65499500	-6.37848600	2.73768500
O	2.80150400	-0.13460100	-0.99366300
H	-0.60407000	0.02878900	-1.23119800
C	-1.56275400	-2.41456400	-1.70877800
C	0.86823300	-2.73309200	-1.51248100
C	0.43640500	-1.73700700	-2.35414800
N	-0.91648000	-1.56144600	-2.45965300
O	1.20902700	-0.88834200	-3.05981200
S	-0.53193500	-3.45135200	-0.77506100
C	2.30741600	-3.11084000	-1.28663000
H	2.86985800	-2.34159400	-1.82372800
C	-3.03114100	-2.48251800	-1.66348300
C	-3.77612300	-1.54086100	-2.38077000
C	-3.70928300	-3.47520200	-0.94636500
C	-5.16508800	-1.58865000	-2.36938400
H	-3.25038500	-0.77804200	-2.94578700
C	-5.09678200	-3.50487300	-0.92944900

H	-3.15150200	-4.22191000	-0.38862600
C	-5.84877200	-2.56160300	-1.63789200
H	-5.73004300	-0.84350600	-2.92235100
H	-5.60707800	-4.27071200	-0.35130800
C	2.73963600	-4.43519800	-1.91352700
C	1.85678300	-5.44453200	-2.29642900
C	4.10995800	-4.64770400	-2.10704600
C	2.33018500	-6.63802000	-2.84020300
H	0.78775200	-5.30302600	-2.18428300
C	4.58562700	-5.83572600	-2.64842400
H	4.81240500	-3.86195800	-1.83808300
C	3.69391700	-6.84149800	-3.01476000
H	1.62348200	-7.40890100	-3.13150800
H	5.65280700	-5.97361500	-2.79260300
H	4.06033300	-7.77034800	-3.43987000
C	0.65473100	-1.63395800	3.45312900
O	1.42596000	-0.68841500	3.64645300
O	0.30062300	-2.05067400	2.27181300
H	1.24089500	-1.74704100	1.43407400
C	0.03657300	-2.40402100	4.60213600
H	-1.03737300	-2.51709800	4.43733500
H	0.47015400	-3.40855100	4.62320300
H	0.23279900	-1.90151800	5.54846000
C	-7.35402300	-2.59889600	-1.60384000
H	-7.78162300	-1.71855500	-2.08698400
H	-7.73614100	-3.48853600	-2.11408000
H	-7.72215400	-2.63203500	-0.57352500