

Electronic Supplementary Information for

**Exploring the general mechanistic map on NHC-catalyzed
activation/transformation reactions of saturated carboxylic anhydrides**

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Contents

Part 1: Generation of active NHC.....	S2
Part 2: Addition modes of NHC and R1	S3
Part 3: Possible β -H elimination pathways.....	S4
Part 4: Stereochemistry for reaction between M4 and R2.....	S5
Part 5: Configurations of TS5s associated with Michael-type addition process	S6
Part 6: Energy profiles of reaction between E-M4 and R2 associated with RR, RS, and SR pathways	S7
Part 7: Possible pathways for decarboxylation.....	S8
Part 8: Barriers for chemoselective pathways	S9
Part 9: NCI analysis for TS5RR and TS5SS	S10
Part 10: Cartesian coordinates for all stationary points	S11

Part 1: Generation of active NHC

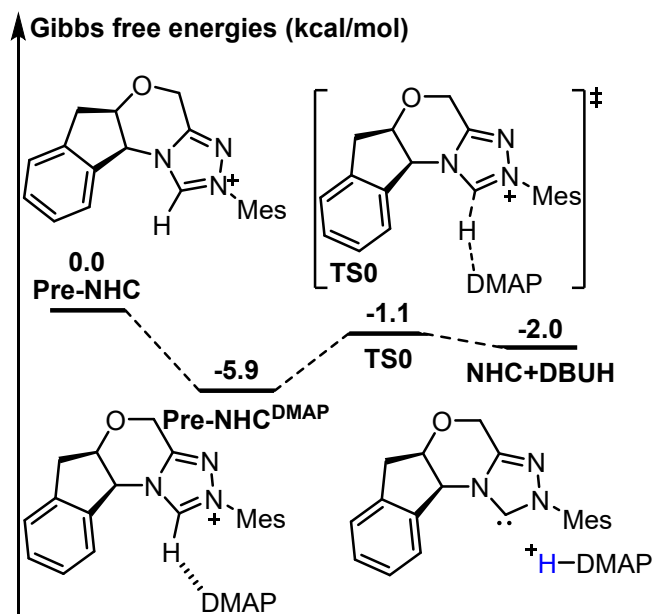


Fig.S1 Deprotonation of pre-NHC for generation of active NHC

Part 2: Addition modes of NHC and R1

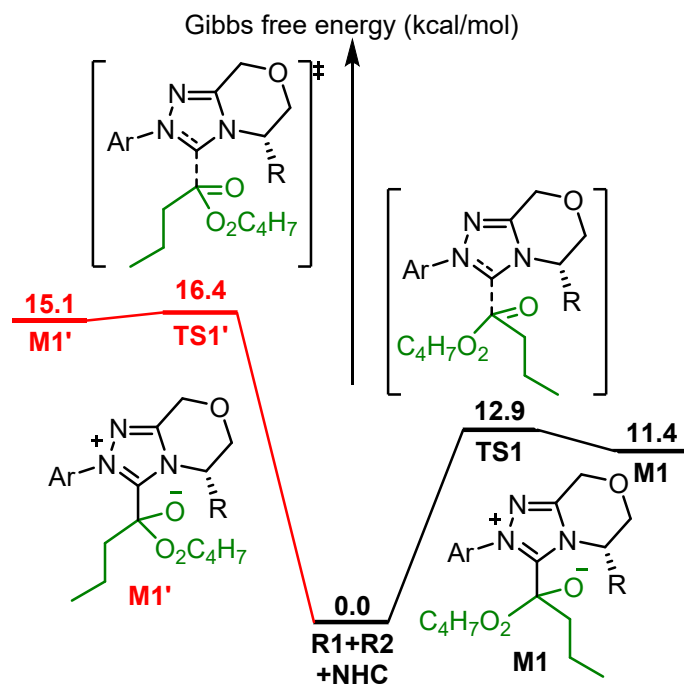
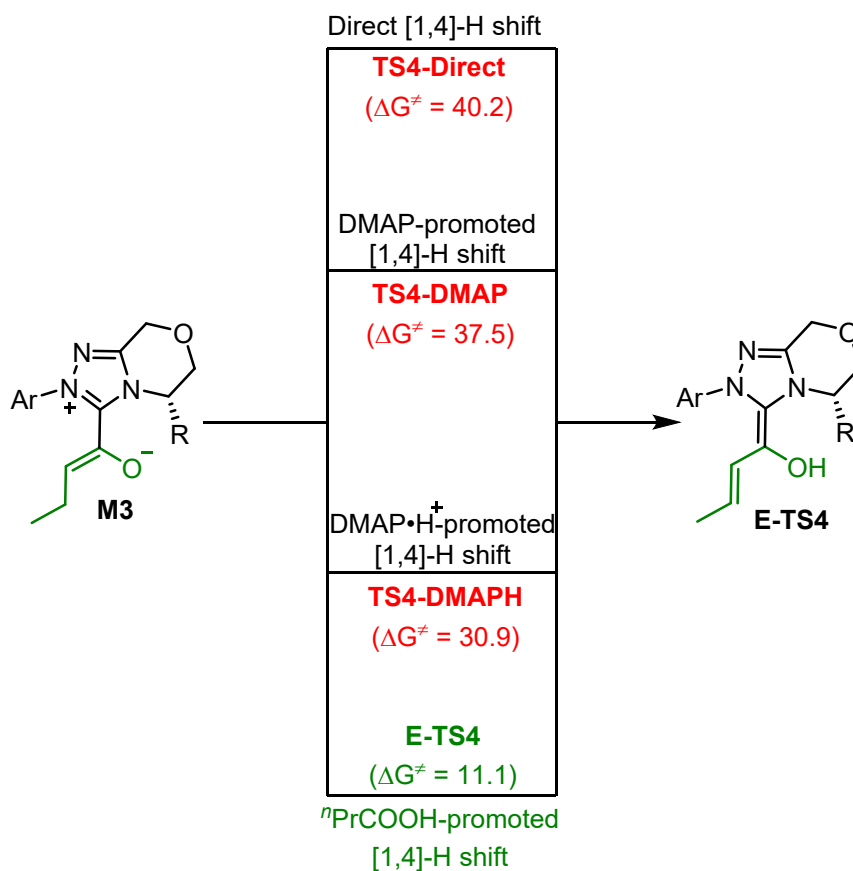


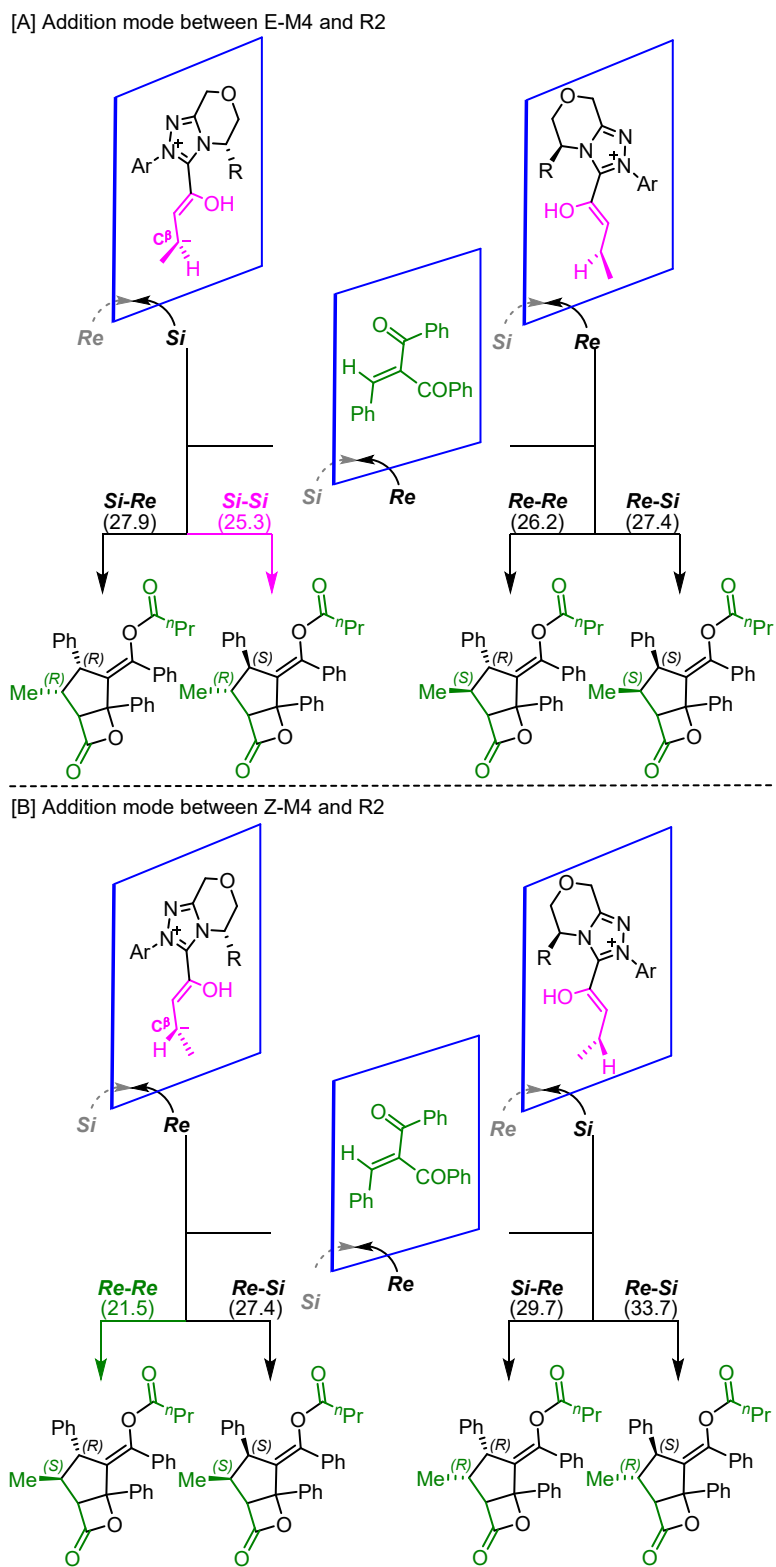
Fig. S2 Energy profile for NHC adsorption process

Part 3: Possible β -H elimination pathways



Scheme S1. Possible pathways involved in β -H elimination process

Part 4: Stereochemistry for reaction between M4 and R2



Scheme S2. Illustration of stereochemistry

Part 5: Configurations of TS5s associated with Michael-type addition process

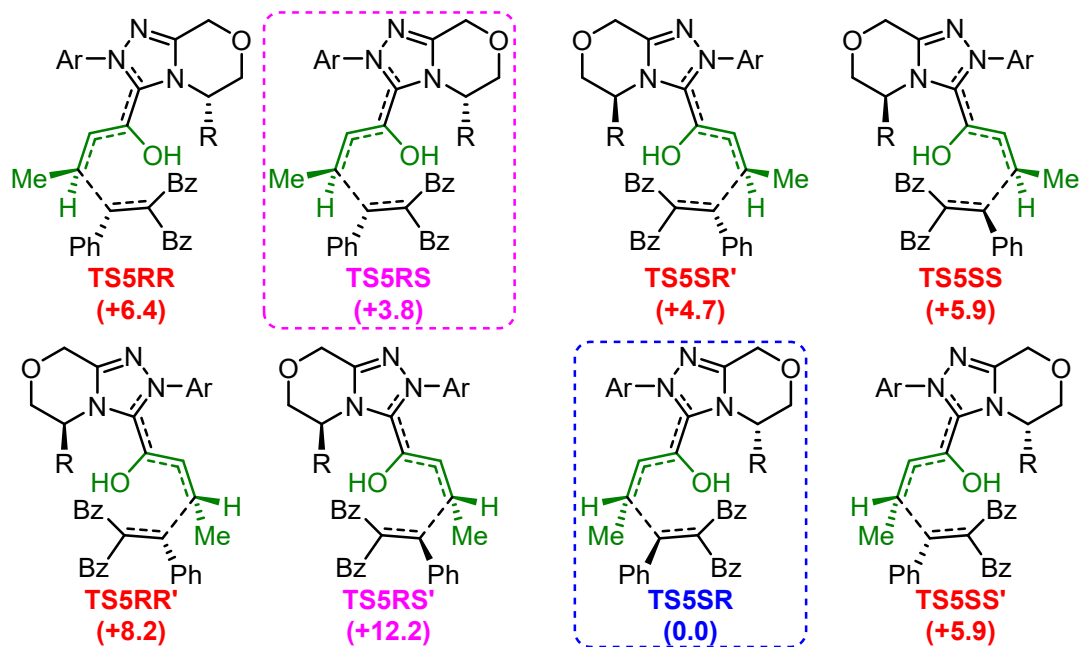


Fig. S3 Configurations involved in C-C bond formation process

Part 6: Energy profiles of reaction between E-M4 and R2 associated with RR, RS, and SR pathways

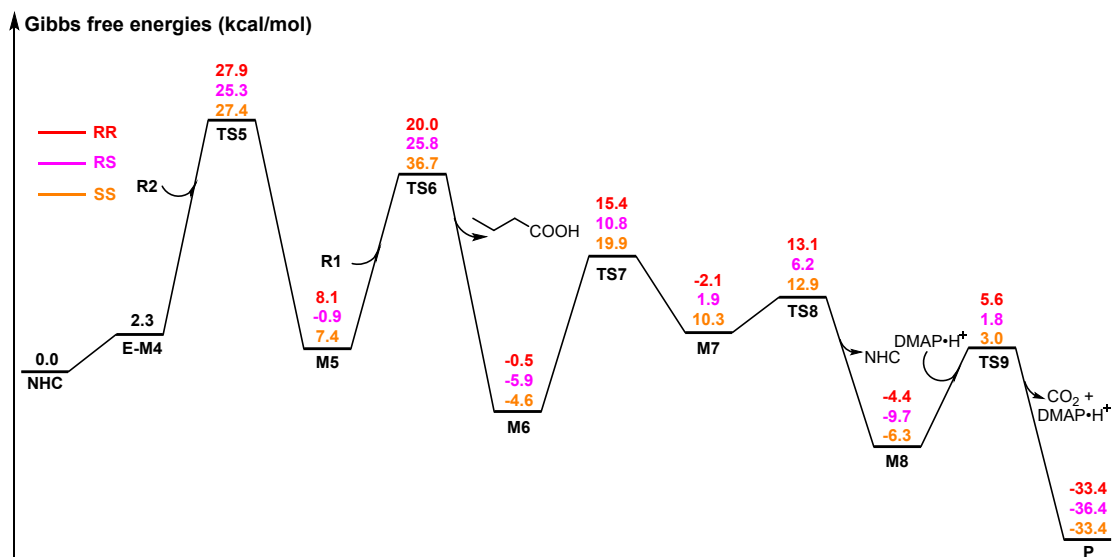
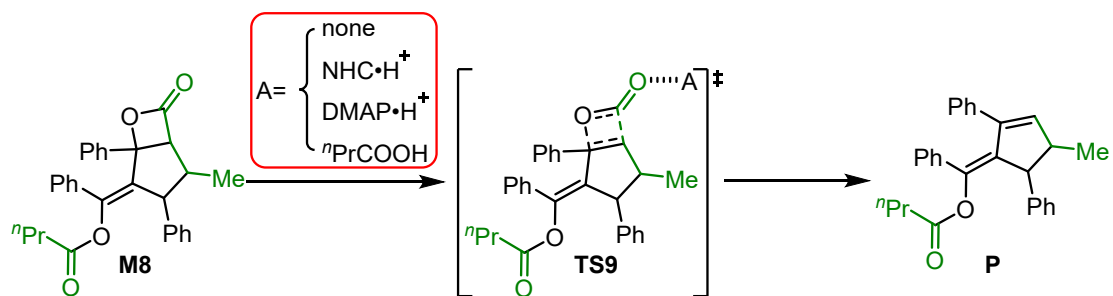


Fig. S4 Energy profiles of reaction between E-M4 and R2 associated with RR, RS, and SR pathways

Part 7: Possible pathways for decarboxylation



Scheme S3. Possible pathways for decarboxylation

Table S1. Energy barriers for decarboxylation process (Energy in kcal/mol)

TS9	ΔG^\ddagger			
	RR	RS	SR	SS
Direct	22.5	24.3	26.4	22.0
NHC·H ⁺	11.9	15.7	15.1	12.1
DMAP·H ⁺	10.0	11.5	13.6	9.3
ⁿ PrCOOH	23.0	23.6	23.4	23.4

Part 8: Barriers for chemoselective pathways

Table S2. Energy barriers for HAD pathway (Energy in kcal/mol)

	ΔG^\ddagger			
	RR	RS	SR	SS
TS4	26.8	22.2	23.4	22.3

Table S3. Energy barriers for Stetter pathway (Energy in kcal/mol)

	TS5			
	R	S	R'	S'
ΔG^\ddagger	23.6	22.9	25.1	26.1

Part 9: NCI analysis for TS5RR and TS5SS

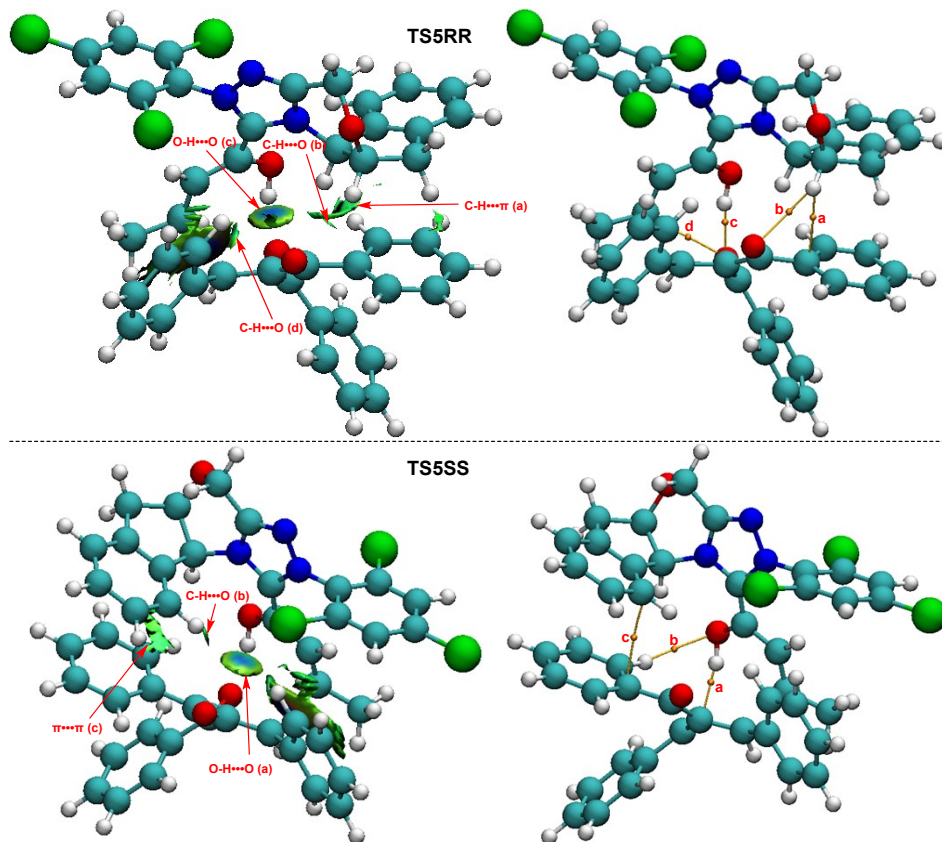


Fig. S5 NCI analysis and topological analysis of bond critical points (BCPs) along the bond paths for the stereoselective transition states **TS5RR** and **TS5SS**

Table S4. Summary of distances and Laplacian of electron density ($\nabla^2\rho$) involved in different types of interactions in **TS5RR** and **TS5SS**

TS5RR				TS5SS			
BCP index	Type of interaction	Distance (Å)	$\nabla^2\rho \times 10^{-1}$ (a.u.)	BCP index	Type of interaction	Distance (Å)	$\nabla^2\rho \times 10^{-1}$ (a.u.)
a	C-H... π	2.89	0.2501	a	O-H...O	1.85	0.9279
b	C-H...O	2.59	0.2709	b	C-H...O	2.50	0.3144
c	O-H...O	1.81	1.0474	c	π ... π	3.18	0.2605
d	C-H...O	2.37	0.4414	-	-	-	-

Part 10: Cartesian coordinates for all stationary points

Coordinates for substrates

R1

C	-1.18346300	0.30565200	-0.20925500
O	-1.22583500	1.40754600	-0.67009100
O	0.00001100	-0.38161000	-0.00037800
C	1.18336500	0.30538900	0.20897600
O	1.22578800	1.40710000	0.67033000
C	2.35821100	-0.55461800	-0.17078700
C	3.69251800	0.08767200	0.18558300
H	2.28212100	-0.74865700	-1.24831900
H	2.23409100	-1.52905900	0.31612100
C	4.86936300	-0.79421100	-0.21990700
H	3.76031000	1.06380300	-0.30438400
H	3.71738900	0.28425100	1.26219000
H	5.82079800	-0.32577600	0.04198300
H	4.82381200	-1.76610700	0.28136500
H	4.87046600	-0.97616700	-1.29904400
C	-2.35815100	-0.55452200	0.17058500
C	-3.69261900	0.08773100	-0.18532300
H	-2.28177900	-0.74860100	1.24809500
H	-2.23401300	-1.52888100	-0.31645100
C	-4.86925000	-0.79447400	0.22014300
H	-3.76040800	1.06370400	0.30497100
H	-3.71779500	0.28458000	-1.26186900
H	-5.82083900	-0.32586300	-0.04087300
H	-4.82393000	-1.76598000	-0.28190400
H	-4.86978400	-0.97725000	1.29913800

R2

C	-0.75779900	-1.50591300	-0.90093700
O	-0.65970800	-2.05539600	-1.98432900
C	0.43446200	-0.82928700	-0.28126800
C	1.64963200	-1.29703600	-0.61804400
H	1.65321300	-2.17775900	-1.25986000
C	-2.06525000	-1.48662500	-0.17662000
C	-2.14285100	-1.43444600	1.21820400
C	-3.23484500	-1.57647200	-0.93726200
C	-3.38656800	-1.46022300	1.84275200
H	-1.23877800	-1.39760100	1.81781600
C	-4.47402100	-1.58409600	-0.31148500
H	-3.14819500	-1.63664900	-2.01732000
C	-4.54979500	-1.52538300	1.08013300

H	-3.44597700	-1.43113000	2.92561000
H	-5.38150700	-1.63847000	-0.90381000
H	-5.51809700	-1.53525700	1.57062200
C	2.97062300	-0.77378300	-0.24587900
C	4.04031700	-1.67399900	-0.15963100
C	3.21413400	0.58836500	-0.02317700
C	5.31289400	-1.23440200	0.18603600
H	3.86293500	-2.72771600	-0.35614000
C	4.48882600	1.02893200	0.30801500
H	2.41197400	1.31067200	-0.13867900
C	5.53879900	0.11909800	0.42307200
H	6.12854700	-1.94584500	0.26206500
H	4.66600300	2.08692700	0.47068500
H	6.53276000	0.46718000	0.68484700
C	0.22484600	0.33028500	0.65927600
O	0.63730500	0.29399300	1.80273800
C	-0.51300900	1.51866200	0.13379400
C	-0.78590400	1.66839700	-1.22918300
C	-0.91429600	2.50590100	1.03915800
C	-1.46102800	2.79824800	-1.68114500
H	-0.46018000	0.91220200	-1.93835700
C	-1.59283600	3.62865600	0.58607600
H	-0.68505000	2.36714700	2.09059200
C	-1.86646400	3.77440900	-0.77469300
H	-1.66906200	2.91683300	-2.73918800
H	-1.91156300	4.39181600	1.28849500
H	-2.39701400	4.65314300	-1.12781800

NHC·H⁺

C	-3.35255900	0.51355800	0.92560500
C	-4.07003900	0.82056800	-0.23509100
C	-4.62850400	2.08371300	-0.38739700
C	-4.45211400	3.02333500	0.62840600
C	-3.73941500	2.70816800	1.78649900
C	-3.18386600	1.44002400	1.94813100
C	-2.85197300	-0.90251700	0.84971000
C	-3.77359700	-1.53196000	-0.22276600
C	-4.11739600	-0.36323200	-1.17194100
H	-5.19832200	2.33527900	-1.27617100
H	-4.88677600	4.01163200	0.52197900
H	-3.62959400	3.44975200	2.57001300
H	-2.65511700	1.18143700	2.86169900
H	-4.68259700	-1.85143000	0.29106400
H	-3.36718000	-0.25058500	-1.96456900

H	-2.84030000	-1.45742000	1.78953600
H	-5.08568400	-0.50333600	-1.65532700
C	-1.07466300	-1.69462100	-0.78676300
C	-0.38622000	-0.28704200	0.71211100
N	0.19144700	-1.51553600	-1.04503800
N	-1.46535900	-0.94838300	0.29800500
N	0.60271600	-0.63516200	-0.09675300
C	-2.06170600	-2.53201800	-1.54464500
H	-2.25788000	-2.06081500	-2.51576700
H	-1.63866100	-3.52182500	-1.72279300
C	1.95454300	-0.18329500	-0.05349900
C	2.32779900	0.96194300	-0.75925700
C	2.90760700	-0.90674700	0.66525200
C	3.64538300	1.39582500	-0.74081700
C	4.22952700	-0.48630200	0.69285000
C	4.57885300	0.66211700	-0.01323100
H	3.93702300	2.28429600	-1.28714900
H	4.97148300	-1.04532700	1.24992200
Cl	1.14001200	1.84325700	-1.65275000
Cl	6.22281000	1.19086700	0.01228700
Cl	2.43289200	-2.32670400	1.52617600
O	-3.23511700	-2.70536200	-0.78848100
H	-0.32420400	0.40956700	1.53581800

DMAP

C	-1.94825400	1.12930800	-0.00032900
C	-0.56393400	1.19675400	-0.00047700
C	0.18346700	-0.00000800	-0.00019200
C	-0.56389800	-1.19673500	0.00030800
C	-1.94826500	-1.12927800	0.00042700
N	-2.66376500	-0.00001600	0.00011800
H	-2.51983700	2.05564500	-0.00054500
H	-0.08181900	2.16586500	-0.00097300
H	-0.08183500	-2.16587300	0.00078100
H	-2.51978900	-2.05566000	0.00081400
N	1.54976800	0.00000600	-0.00048300
C	2.26934700	-1.25760800	-0.00049800
H	3.33975000	-1.05616900	-0.00266400
H	2.03518700	-1.85539800	0.88877400
H	2.03202900	-1.85673700	-0.88798000
C	2.26939000	1.25759200	0.00085700
H	3.33978600	1.05610800	0.00232800
H	2.03494500	1.85637700	-0.88765500
H	2.03244100	1.85576400	0.88909500

NHC

C	-3.35313800	0.51615000	0.90241300
C	-4.22804800	0.73546300	-0.16327200
C	-4.88789200	1.95348800	-0.28470000
C	-4.65041200	2.94443200	0.66669300
C	-3.76355300	2.72436500	1.72209300
C	-3.10418200	1.50333800	1.84752200
C	-2.77001900	-0.87349100	0.83213500
C	-3.73566600	-1.58719800	-0.14927300
C	-4.28626100	-0.47216600	-1.06587700
H	-5.57690500	2.13124400	-1.10512300
H	-5.16052300	3.89916700	0.58543100
H	-3.58890900	3.50925700	2.45061300
H	-2.40132500	1.32511100	2.65469700
H	-4.56238500	-1.98445100	0.44527700
H	-3.64218500	-0.31765300	-1.94022000
H	-2.72544700	-1.37401900	1.80244800
H	-5.28835000	-0.70406300	-1.43383000
C	-1.05296700	-1.60574600	-0.83730900
C	-0.34623700	-0.20347200	0.79283100
N	0.20704100	-1.44882600	-1.09783400
N	-1.41704900	-0.87646100	0.26769500
N	0.60207500	-0.58947900	-0.08909000
C	-2.04569700	-2.43276600	-1.59425200
H	-2.33207300	-1.91802800	-2.52096000
H	-1.60035700	-3.39135200	-1.86517900
C	1.95330300	-0.17473100	-0.05323400
C	2.37193700	0.94765400	-0.77069400
C	2.90184500	-0.88348600	0.68651600
C	3.69564600	1.36838200	-0.74931900
C	4.23238100	-0.48511800	0.72760800
C	4.60766600	0.64030900	0.00443300
H	4.00366900	2.24305400	-1.30820500
H	4.95623900	-1.04275800	1.30862300
Cl	1.21769100	1.84263900	-1.70059700
Cl	6.26855400	1.15186100	0.04171500
Cl	2.41475300	-2.28666300	1.57538300
O	-3.17189000	-2.71222800	-0.78817200

DMAP·H⁺

C	1.87770200	-1.17900800	0.00019100
C	0.51479400	-1.21657200	0.00004300
C	-0.23602600	-0.00005200	-0.00015400

C	0.51475800	1.21651400	-0.00025500
C	1.87765400	1.17903100	-0.00010200
N	2.54200800	0.00000700	0.00006900
H	2.48525400	-2.07482100	0.00028700
H	0.02823700	-2.18125800	0.00008700
H	0.02809900	2.18115500	-0.00057000
H	2.48520700	2.07484200	-0.00025700
N	-1.56912300	-0.00000800	-0.00030400
C	-2.30533700	1.26350000	0.00041100
H	-3.37112900	1.04984200	0.00117300
H	-2.06851100	1.84953800	0.89293000
H	-2.06976800	1.84977800	-0.89231100
C	-2.30547400	-1.26344300	-0.00012200
H	-3.37124600	-1.04967900	-0.00053800
H	-2.06908300	-1.84986300	-0.89251800
H	-2.06961000	-1.84939100	0.89272400
H	3.55392600	0.00003500	0.00056200

Pre-NHC^{DMAP}

C	3.70452900	1.34000200	-0.71907000
C	4.49030500	1.61678100	0.40320100
C	4.51484100	2.90426400	0.92658000
C	3.73860400	3.89139100	0.31983600
C	2.95022500	3.60451400	-0.79638100
C	2.92828100	2.31758300	-1.33146400
C	3.82717500	-0.11576700	-1.08004700
C	5.11890500	-0.55021900	-0.34814200
C	5.20579500	0.37700600	0.88517100
H	5.12747300	3.14090000	1.79072100
H	3.75302400	4.90090400	0.71720200
H	2.36215500	4.39026100	-1.25837000
H	2.32505600	2.09294900	-2.20734500
H	5.95346500	-0.32948500	-1.01692500
H	4.68329400	-0.04848900	1.75112400
H	3.83974300	-0.33792100	-2.14837300
H	6.24015800	0.55469300	1.18540000
C	2.84376900	-1.97110100	0.35212500
C	1.40479300	-0.64042500	-0.59164000
N	1.67901600	-2.39652200	0.75755000
N	2.70871200	-0.88932800	-0.48232100
N	0.79876600	-1.55365100	0.15362200
C	4.20404100	-2.47541500	0.73320100
H	4.39786100	-2.22634900	1.78389800
H	4.23759800	-3.56097700	0.62884200

C	-0.60647800	-1.62840500	0.37386300
C	-1.20006300	-0.79607700	1.32531000
C	-1.39680900	-2.47869100	-0.39848200
C	-2.57677400	-0.79213000	1.49413100
C	-2.77483800	-2.50206600	-0.22988000
C	-3.34270100	-1.64952000	0.71010900
H	-3.03870900	-0.13359500	2.21977100
H	-3.39029400	-3.15958500	-0.83141500
Cl	-0.21295700	0.23671600	2.29634300
Cl	-5.06376300	-1.63299900	0.89314900
Cl	-0.66084900	-3.47792300	-1.60097200
O	5.18249300	-1.94255500	-0.12842900
H	0.87042100	0.15695400	-1.13293100
C	-0.98769700	2.14115100	-0.47047500
C	-2.24000300	2.53429700	-0.03578000
C	-3.38926500	1.90566000	-0.56992500
C	-3.15337000	0.89922500	-1.53781700
C	-1.85383100	0.58497000	-1.88459500
N	-0.76247200	1.17990800	-1.37756600
H	-0.10278000	2.62684600	-0.06215800
H	-2.31762200	3.32584300	0.69775400
H	-3.96913900	0.36597300	-2.00928500
H	-1.67403800	-0.19863600	-2.61919900
N	-4.64449000	2.24377200	-0.17736800
C	-5.79263600	1.69987800	-0.88517500
H	-6.70227400	2.11786500	-0.45757800
H	-5.76342900	1.95143900	-1.95193500
H	-5.83959000	0.61114100	-0.78193200
C	-4.83290500	3.32533400	0.77464800
H	-5.89383200	3.41933900	0.99983000
H	-4.30614600	3.11506100	1.71119700
H	-4.47374200	4.28411600	0.38105700
TS0			
C	3.24083800	1.68084000	-0.22488700
C	4.23292500	1.58270100	0.75488500
C	4.32699800	2.54894500	1.74923900
C	3.41700700	3.60521700	1.74935500
C	2.43174500	3.70212400	0.76506000
C	2.33725300	2.73682400	-0.23744800
C	3.34090100	0.51239700	-1.17204100
C	4.78850200	0.01493700	-0.93602000
C	5.08696800	0.35767600	0.54076100
H	5.09903700	2.48690000	2.50987800

H	3.48391700	4.36926300	2.51696700
H	1.74499300	4.54256300	0.77101600
H	1.58313100	2.81908300	-1.01582500
H	5.44087500	0.61465900	-1.57448000
H	4.77101200	-0.44663800	1.21640200
H	3.13824000	0.74875900	-2.21868900
H	6.15133900	0.52904100	0.71270900
C	2.81920300	-1.86868600	-0.51472900
C	1.09834600	-0.47875800	-0.55858400
N	1.80856400	-2.59834000	-0.14606100
N	2.42438700	-0.57595200	-0.76918000
N	0.76301700	-1.71772900	-0.18734200
C	4.25503500	-2.28442500	-0.63056800
H	4.66884000	-2.45279500	0.37152000
H	4.32328500	-3.22040500	-1.18722300
C	-0.53736900	-2.12100400	0.21624600
C	-1.06866700	-1.66953100	1.42742100
C	-1.30204400	-2.96752100	-0.58945500
C	-2.33838400	-2.05451000	1.83611200
C	-2.56970300	-3.37351000	-0.19375500
C	-3.06974000	-2.90892800	1.01817700
H	-2.74163700	-1.70305900	2.77781900
H	-3.15420000	-4.03521000	-0.82111900
Cl	-0.13736300	-0.62413800	2.44680200
Cl	-4.65006800	-3.40550000	1.52161500
Cl	-0.67490900	-3.49948500	-2.10967400
O	4.98996000	-1.31821100	-1.34695100
H	0.14964600	0.52818000	-0.59229700
C	-1.08037900	2.27569200	0.30855000
C	-2.18969000	3.08663400	0.29945300
C	-3.17637300	2.91754100	-0.70961500
C	-2.94399600	1.88317400	-1.65585500
C	-1.80244300	1.12479300	-1.55997700
N	-0.87647400	1.31180100	-0.60553000
H	-0.30720200	2.38760200	1.06339700
H	-2.28922500	3.84416000	1.06460500
H	-3.64590300	1.67623400	-2.45182300
H	-1.59855600	0.32608900	-2.26963000
N	-4.27405800	3.69680200	-0.76685400
C	-5.25113100	3.50528300	-1.83019600
H	-6.03925100	4.24739100	-1.72239100
H	-4.79072100	3.63391600	-2.81502900
H	-5.70464500	2.50995600	-1.77744500
C	-4.48273400	4.73861900	0.22910900

H	-5.42328700	5.24384100	0.02014700
H	-4.53753500	4.31484100	1.23700300
H	-3.67850100	5.48118100	0.19881500

Coordinates for the formation of enolate M3

TS1

C	3.61897000	-0.63362700	0.53459000
C	4.91182100	-0.97821300	0.15221700
C	5.50368700	-2.12760800	0.66932700
C	4.77630400	-2.91064200	1.56344600
C	3.48022400	-2.55048900	1.94312700
C	2.88275300	-1.40074700	1.43204500
C	3.16161800	0.62888400	-0.16114300
C	4.27698800	0.91077300	-1.23265900
C	5.48085900	0.03585100	-0.80907000
H	6.51070300	-2.41206700	0.37829900
H	5.22226400	-3.81300900	1.97029400
H	2.93301600	-3.17260800	2.64392800
H	1.88288300	-1.08613000	1.72470000
H	4.53101700	1.97136500	-1.24686700
H	5.94642100	-0.40767400	-1.69489300
H	3.04129900	1.45092100	0.54649600
H	6.24212700	0.65185200	-0.31839600
C	1.79856500	-0.28389200	-1.99457500
C	0.62384100	0.62684800	-0.33968000
N	0.57088400	-0.53047000	-2.32302600
N	1.86779100	0.41243600	-0.81342600
N	-0.13679800	0.03954300	-1.28347100
C	3.08198600	-0.53439800	-2.71470200
H	3.59015200	-1.41820600	-2.30427800
H	2.90193100	-0.68636900	-3.77895600
C	-1.54021000	-0.15947800	-1.23448500
C	-2.05734200	-1.42982800	-0.95124600
C	-2.43101200	0.88097600	-1.50715500
C	-3.43034100	-1.64755700	-0.90251200
C	-3.80635600	0.68739300	-1.45382600
C	-4.28579400	-0.58068700	-1.14948200
H	-3.81940600	-2.63442400	-0.68125500
H	-4.48326000	1.50508100	-1.66810600
Cl	-0.99451600	-2.76117500	-0.67502000
Cl	-6.00198700	-0.84467900	-1.09869200
Cl	-1.83068700	2.43285000	-1.98000400
O	3.86110500	0.63807100	-2.56493200
C	0.42163800	1.58135400	1.41119600

O	1.30385100	1.17000900	2.15419600
O	-0.95983600	1.21118800	1.66653000
C	-1.25150600	-0.07258800	1.93612900
O	-0.47083100	-0.98986100	1.84800000
C	-2.71325500	-0.22948900	2.28740500
C	-3.09767000	-1.67193800	2.58870700
H	-3.29124500	0.15986500	1.43723300
H	-2.93936100	0.43610100	3.12825200
C	-4.60939400	-1.83886500	2.69914100
H	-2.69807500	-2.31766500	1.79920500
H	-2.60478100	-1.99244000	3.51229800
H	-4.88469600	-2.87855400	2.89202000
H	-5.01786000	-1.22617200	3.50889800
H	-5.09850700	-1.52366700	1.77037200
C	0.39754600	3.02537900	0.93631800
C	0.23901900	3.96330900	2.13568700
H	-0.40744100	3.18192800	0.21478000
H	1.34993500	3.22800300	0.43192900
C	0.24566900	5.43042200	1.71790700
H	-0.69766300	3.72423100	2.65138500
H	1.04926100	3.76224600	2.84339000
H	0.13413600	6.09074300	2.58183100
H	1.18321100	5.69061000	1.21609400
H	-0.57291100	5.64441900	1.02335800
MI			
C	3.63731500	-0.69976300	0.51258200
C	4.92563800	-0.99928200	0.07827800
C	5.51492100	-2.20822600	0.43799100
C	4.78741000	-3.09782900	1.22578200
C	3.49506700	-2.78405600	1.65574300
C	2.90080300	-1.57315100	1.30759000
C	3.19483900	0.64998900	-0.00565100
C	4.29657600	1.05460900	-1.04904300
C	5.49589600	0.12519200	-0.75015400
H	6.51907500	-2.45648900	0.10690500
H	5.23065900	-4.04761900	1.50915600
H	2.94812400	-3.49092900	2.27121100
H	1.90504900	-1.29137500	1.64508200
H	4.55776800	2.10706900	-0.93309700
H	5.95130300	-0.20585600	-1.68891900
H	3.07797400	1.37184200	0.80260200
H	6.26570600	0.66918200	-0.19251500
C	1.79629100	0.00074400	-1.93037500

C	0.64573400	0.68608600	-0.18805800
N	0.56206900	-0.17420200	-2.28265900
N	1.88681200	0.52907400	-0.67015200
N	-0.14727600	0.24988300	-1.18457900
C	3.07038600	-0.17872000	-2.68787700
H	3.56408600	-1.11572200	-2.39537000
H	2.87466500	-0.19473300	-3.75998200
C	-1.55287600	0.01817600	-1.18678900
C	-2.03647800	-1.29180100	-1.07268000
C	-2.46284100	1.06067000	-1.37137800
C	-3.40473100	-1.54123600	-1.05158100
C	-3.83272900	0.83037400	-1.34541100
C	-4.28353200	-0.47211300	-1.17019800
H	-3.77181100	-2.55552900	-0.95068700
H	-4.52808100	1.64985400	-1.47682200
Cl	-0.95347900	-2.63118400	-0.99678600
Cl	-5.99193500	-0.77463200	-1.12760000
Cl	-1.89867200	2.65979700	-1.70617800
O	3.86603100	0.95417600	-2.40208400
C	0.43324100	1.35048900	1.24932700
O	1.29433600	0.92673300	2.07794600
O	-1.02823700	1.01063900	1.56345800
C	-1.29839900	-0.26853800	1.80631700
O	-0.52629200	-1.18323600	1.60670100
C	-2.72596000	-0.46502700	2.27100000
C	-3.09807200	-1.93270400	2.43684500
H	-3.37280500	0.02395400	1.52901300
H	-2.86710700	0.09678000	3.20150700
C	-4.59934000	-2.11903600	2.62919600
H	-2.75516200	-2.48659600	1.55575900
H	-2.54469300	-2.35170500	3.28344100
H	-4.85704400	-3.17171900	2.77004500
H	-4.95824100	-1.56536400	3.50254800
H	-5.14968400	-1.75087600	1.75559600
C	0.36362800	2.88068100	1.05298100
C	0.28966400	3.57983600	2.40669100
H	-0.48770900	3.16161200	0.42847300
H	1.27892300	3.18946600	0.52742600
C	0.29716400	5.09951600	2.27063400
H	-0.62014300	3.25070200	2.92051700
H	1.13243900	3.23701100	3.01247200
H	0.24527400	5.58735300	3.24783700
H	1.20976700	5.44471500	1.77314300
H	-0.55450300	5.44825500	1.67724400

TS1'

C	-0.18759600	1.40215400	-0.07069000
O	-0.34955100	1.34060700	1.14091700
O	1.19593200	1.67920100	-0.52973400
C	1.66683600	2.90731700	-0.24360400
O	0.98187400	3.82784900	0.13152800
C	3.16198100	2.97364900	-0.46188600
C	3.74164200	4.35244700	-0.17594600
H	3.36725900	2.66317800	-1.49452900
H	3.61640100	2.20736800	0.18052500
C	5.25300000	4.38750400	-0.38006000
H	3.25150400	5.08715900	-0.82273700
H	3.48815300	4.63581600	0.85024300
H	5.65859900	5.38026900	-0.17075000
H	5.75452900	3.67363900	0.28105800
H	5.51724300	4.12813200	-1.41031600
C	-1.21394700	2.03930300	-1.01643300
C	-2.44128600	2.54362700	-0.26196900
H	-1.50251200	1.31865700	-1.78800100
H	-0.72886700	2.87645500	-1.52821500
C	-3.52915500	3.02692600	-1.21570000
H	-2.82946300	1.74751500	0.38183900
H	-2.13085000	3.34886900	0.41070100
H	-4.41799800	3.35799200	-0.67126700
H	-3.17818800	3.86340300	-1.82858200
H	-3.83324800	2.22437100	-1.89812100
C	3.11504800	-0.92926800	0.36559800
C	4.29817700	-1.66056000	0.31725800
C	5.10616700	-1.74581700	1.44789500
C	4.69980100	-1.09908700	2.61333200
C	3.49675700	-0.38929300	2.65791000
C	2.68363000	-0.29909300	1.52996600
C	2.40856600	-0.95829900	-0.97112100
C	3.15419200	-2.07322700	-1.78514300
C	4.49741700	-2.28140500	-1.04350400
H	6.03039100	-2.31573600	1.42696700
H	5.31831300	-1.15931800	3.50332000
H	3.18826900	0.08930300	3.58157700
H	1.72620500	0.22025100	1.55751400
H	3.31113300	-1.74704700	-2.81431000
H	4.73570900	-3.34883000	-1.00242000
H	2.46312000	0.00606800	-1.47683900
H	5.31115700	-1.78964900	-1.58706300

C	0.60334600	-2.58154100	-0.60551300
C	-0.06532700	-0.46059800	-0.65275200
N	-0.66569400	-2.65487500	-0.35396700
N	0.99554500	-1.28050900	-0.80676500
N	-1.05068000	-1.33261400	-0.38258900
C	1.64203400	-3.64028200	-0.78267800
H	2.26184100	-3.72357900	0.12140500
H	1.17784900	-4.60464500	-0.98839400
C	-2.37333300	-0.97686500	-0.02035700
C	-3.34161600	-0.71851600	-0.99176900
C	-2.71942900	-0.87230800	1.32995100
C	-4.62412700	-0.31961600	-0.63744300
C	-3.99582300	-0.47378100	1.70708900
C	-4.92666600	-0.19399800	0.71310900
H	-5.36650700	-0.11355100	-1.39846000
H	-4.25273300	-0.37944600	2.75486300
Cl	-2.94979200	-0.89671400	-2.67061500
Cl	-6.52004300	0.31991400	1.17202500
Cl	-1.55720500	-1.25230500	2.54687900
O	2.41005100	-3.27667300	-1.91532700
MI'			
C	-0.16715700	1.14393000	-0.18957500
O	-0.33174500	1.13434300	1.06667500
O	1.23431800	1.60850800	-0.62636200
C	1.58385400	2.85298200	-0.28349500
O	0.81451400	3.71436700	0.07391200
C	3.08146300	3.05270800	-0.41184500
C	3.52170900	4.47322900	-0.08580700
H	3.37481400	2.77342000	-1.43228900
H	3.56372000	2.32264600	0.25230000
C	5.02968600	4.65235800	-0.23066600
H	2.99014100	5.16975000	-0.74212400
H	3.20486600	4.71711000	0.93285100
H	5.33282000	5.67465300	0.00865200
H	5.57180600	3.97646200	0.43843500
H	5.35528100	4.43736700	-1.25378500
C	-1.19388300	1.88849100	-1.08933900
C	-2.30017500	2.53984000	-0.26793300
H	-1.62489000	1.19538600	-1.82141000
H	-0.67190400	2.65290000	-1.67069700
C	-3.40424000	3.10361100	-1.15682400
H	-2.71318900	1.80638300	0.43301300
H	-1.85001100	3.32361700	0.34735000

H	-4.20340800	3.55775900	-0.56424300
H	-3.01561400	3.86790700	-1.83770100
H	-3.85214100	2.31349500	-1.77257100
C	3.12314400	-0.91000700	0.41518700
C	4.26744600	-1.70264900	0.39881600
C	5.01260000	-1.86760100	1.56324600
C	4.58327100	-1.23709500	2.72884800
C	3.42209200	-0.45935400	2.73722900
C	2.67147800	-0.28551100	1.57634000
C	2.48186000	-0.86453300	-0.95238300
C	3.24283500	-1.95229800	-1.79318500
C	4.51252900	-2.28478800	-0.97092500
H	5.90691400	-2.48369200	1.56583800
H	5.15144700	-1.36033400	3.64556800
H	3.09720400	0.01128200	3.65939500
H	1.74960000	0.29813100	1.57960400
H	3.49582400	-1.54784600	-2.77381800
H	4.67213600	-3.36783100	-0.95898700
H	2.56819000	0.11631900	-1.41334200
H	5.39498800	-1.83650200	-1.43901500
C	0.63365000	-2.48306500	-0.78165500
C	-0.02312900	-0.38956700	-0.63174800
N	-0.63964500	-2.56944800	-0.56117900
N	1.04787000	-1.17334100	-0.85321600
N	-1.03117100	-1.26080100	-0.47015900
C	1.65177900	-3.54776600	-1.02230600
H	2.23507100	-3.73175600	-0.10848900
H	1.16500900	-4.47364600	-1.32871800
C	-2.35026300	-0.94518300	-0.04798700
C	-3.36247000	-0.70017600	-0.97549800
C	-2.64281000	-0.89538900	1.31867300
C	-4.63217100	-0.31929500	-0.56111100
C	-3.90675000	-0.51709700	1.75254800
C	-4.87638200	-0.21486500	0.80304700
H	-5.40948200	-0.11519200	-1.28692700
H	-4.12693600	-0.46126800	2.81121600
Cl	-3.04904200	-0.88872500	-2.66882200
Cl	-6.45043500	0.28234600	1.33715000
Cl	-1.45448600	-1.36040800	2.47650200
O	2.46491000	-3.10240200	-2.08800900
TS2			
C	3.52916100	-0.76744700	0.55704800
C	4.79946900	-1.17347700	0.15910300

C	5.23133700	-2.46534000	0.44585200
C	4.36635900	-3.32527800	1.11975700
C	3.08892100	-2.90697200	1.50260100
C	2.64983800	-1.61448100	1.22565000
C	3.25452900	0.65042300	0.10637100
C	4.43829700	0.99445000	-0.86696100
C	5.52426300	-0.06419400	-0.56152800
H	6.21807800	-2.80093200	0.14100800
H	4.68676900	-4.33801800	1.34371900
H	2.42824500	-3.59579900	2.01844800
H	1.65593400	-1.27075200	1.51063000
H	4.79636000	2.00797100	-0.68339000
H	6.00699700	-0.38173600	-1.49098100
H	3.19806500	1.35252500	0.93855100
H	6.30182300	0.37134300	0.07497200
C	1.88955900	0.21902900	-1.89349200
C	0.71876200	0.86358600	-0.14819700
N	0.65815600	0.11154900	-2.27283900
N	1.96920900	0.68671700	-0.60969700
N	-0.07109300	0.50955900	-1.18097900
C	3.17092700	-0.02271100	-2.62138400
H	3.56275400	-1.02098000	-2.38123900
H	3.01452400	0.05318200	-3.69733400
C	-1.46164200	0.18405100	-1.23016200
C	-1.83669800	-1.16542500	-1.20561100
C	-2.44448500	1.16029800	-1.36881900
C	-3.18078400	-1.51934000	-1.21708400
C	-3.79103000	0.82488600	-1.37947000
C	-4.13864500	-0.51571400	-1.28076500
H	-3.46835200	-2.56275100	-1.17353100
H	-4.54642000	1.59507100	-1.46822000
Cl	-0.66056600	-2.42995400	-1.18718900
Cl	-5.81857600	-0.95166300	-1.25617300
Cl	-2.00224600	2.81795600	-1.58951700
O	4.05855600	1.00720200	-2.23553200
C	0.58632000	1.56448100	1.22831700
O	1.21215200	1.06465800	2.13890000
O	-1.54745200	1.03820700	1.46511300
C	-1.55527600	-0.21901800	1.67201100
O	-0.61602400	-0.99435900	1.41427400
C	-2.84288200	-0.79959600	2.26414700
C	-2.84557600	-2.31857600	2.36822500
H	-3.67210800	-0.45980600	1.62781800
H	-3.01185800	-0.32690400	3.23935200

C	-4.21812400	-2.87089900	2.74137500
H	-2.51407900	-2.73436400	1.40893800
H	-2.09329300	-2.63191200	3.09961300
H	-4.21836600	-3.96398100	2.77760300
H	-4.54043900	-2.50416900	3.72153500
H	-4.97299700	-2.55863400	2.01064500
C	0.26899800	3.04070100	1.15468600
C	0.07664000	3.64012600	2.54240300
H	-0.60759400	3.20507900	0.53065800
H	1.12466900	3.51196400	0.64219200
C	0.04768800	5.16474300	2.50719400
H	-0.86516700	3.24570300	2.92993400
H	0.87123400	3.28177000	3.20233000
H	-0.10753500	5.57938600	3.50623200
H	0.98880600	5.56868100	2.11972600
H	-0.75976700	5.53003600	1.86471400
M2			
C	-3.64091900	-0.18911800	0.27016100
C	-4.92477700	-0.62366100	-0.04992500
C	-5.85599300	0.27894700	-0.55408000
C	-5.47220600	1.60674800	-0.73280000
C	-4.17890800	2.02731200	-0.41421600
C	-3.24004700	1.13114400	0.09536500
C	-2.81997400	-1.33351700	0.82273100
C	-3.65494700	-2.61753000	0.47696100
C	-5.08913600	-2.09496700	0.23902200
H	-6.85983500	-0.04589600	-0.81109800
H	-6.18588000	2.32133400	-1.13065700
H	-3.89735800	3.06513700	-0.56616100
H	-2.22202300	1.44584800	0.32977800
H	-3.61089700	-3.32975300	1.30191400
H	-5.55746400	-2.65504700	-0.57575200
H	-2.66327500	-1.24294400	1.89480800
H	-5.69931200	-2.25085700	1.13541800
C	-1.37919300	-1.91367400	-1.07429900
C	-0.27339600	-0.95697900	0.55285100
N	-0.15691800	-1.85730900	-1.50458900
N	-1.49084600	-1.39579100	0.18892700
N	0.51950000	-1.25697200	-0.48408700
C	-2.58972400	-2.55526700	-1.66623200
H	-3.28818800	-1.79600300	-2.04160400
H	-2.30027300	-3.21756200	-2.48191500
C	1.90595700	-0.99179600	-0.65800100

C	2.32074800	0.02272700	-1.52199200
C	2.85916300	-1.77934300	-0.00932000
C	3.67366300	0.29773200	-1.67729200
C	4.21213400	-1.51667000	-0.14883400
C	4.59629200	-0.46605900	-0.97744100
H	3.99223500	1.10413600	-2.32527400
H	4.94775300	-2.12075200	0.36690400
Cl	1.17088100	0.91104500	-2.44763900
Cl	6.28716100	-0.12240500	-1.15941300
Cl	2.34968200	-3.11187900	0.97737400
O	-3.15656200	-3.34435300	-0.63862200
C	0.02835100	-0.33692600	1.91947200
O	-0.91659000	-0.28088100	2.67486000
O	2.01343500	2.21226100	0.36498800
C	0.78636100	2.41061600	0.29547700
O	-0.13218800	1.55068100	0.50372400
C	0.32799500	3.82464400	-0.09294700
C	-1.16826300	3.98208400	-0.32197200
H	0.89089200	4.10375800	-0.99209800
H	0.67193600	4.50719300	0.69485100
C	-1.55158600	5.39615200	-0.75050400
H	-1.48913300	3.25664000	-1.08025600
H	-1.69931800	3.70985300	0.59782800
H	-2.62983500	5.49444800	-0.91109900
H	-1.26027300	6.12773500	0.01029500
H	-1.04824500	5.67312700	-1.68252700
C	1.43146700	0.01634500	2.31346500
C	1.42588600	1.11593800	3.37558900
H	1.98327000	0.38012900	1.44505100
H	1.90711200	-0.89543300	2.70290500
C	2.83522600	1.65035100	3.60394000
H	0.77395200	1.91872000	3.01638400
H	0.98709300	0.73826400	4.30427700
H	2.84263700	2.43105600	4.36917300
H	3.51476500	0.85547600	3.93023900
H	3.21640400	2.07389900	2.67073100
TS3			
C	-3.74056300	-0.14313100	0.27228900
C	-5.02941300	-0.56944600	-0.04099500
C	-5.96985700	0.34745400	-0.49848900
C	-5.59002300	1.68128200	-0.64171300
C	-4.29274000	2.09355700	-0.33047400
C	-3.34613000	1.18259100	0.13649100

C	-2.90460800	-1.30958000	0.75408400
C	-3.73177900	-2.57207500	0.33192700
C	-5.17824100	-2.05255200	0.19344300
H	-6.97723600	0.02967400	-0.75056200
H	-6.31041500	2.40635800	-1.00731300
H	-4.01404600	3.13505200	-0.45528400
H	-2.32937400	1.48933200	0.37080700
H	-3.64565300	-3.35589800	1.08572000
H	-5.68817400	-2.58123100	-0.61671300
H	-2.73451200	-1.27510500	1.82834200
H	-5.73604600	-2.24673700	1.11635600
C	-1.49089600	-1.72659400	-1.20032200
C	-0.35516300	-0.95610200	0.50766500
N	-0.27099200	-1.64800300	-1.63596400
N	-1.58291400	-1.32521200	0.10463600
N	0.42275600	-1.15876200	-0.56686600
C	-2.71410100	-2.30777400	-1.82923400
H	-3.41368300	-1.51640000	-2.12767100
H	-2.43897000	-2.89877200	-2.70246700
C	1.82695600	-0.97662500	-0.72019100
C	2.32558400	0.12132800	-1.42213300
C	2.71184700	-1.94822800	-0.24534100
C	3.69665600	0.30034400	-1.56165800
C	4.08219300	-1.78880100	-0.37778900
C	4.55381900	-0.65048900	-1.02398100
H	4.08129900	1.16610400	-2.08595900
H	4.76398300	-2.53556500	0.00911600
Cl	1.24989700	1.23490700	-2.17921300
Cl	6.26616800	-0.43220700	-1.18997100
Cl	2.09356900	-3.37006000	0.52944800
O	-3.26937100	-3.18373900	-0.86707100
C	-0.04225500	-0.45395400	1.92715500
O	-1.04225000	-0.23518900	2.60262600
O	1.86382000	2.01918000	0.94172900
C	0.74033500	2.54145000	0.58226600
O	-0.33463800	1.93128000	0.55038300
C	0.81005800	4.00559900	0.17281000
C	-0.50037500	4.54559900	-0.38419300
H	1.62285300	4.10427200	-0.55720400
H	1.12784200	4.57988900	1.05213700
C	-0.39658000	6.01328300	-0.78848300
H	-0.80093100	3.93472300	-1.24343900
H	-1.28468500	4.41082400	0.36818800
H	-1.34358500	6.38949100	-1.18482800

H	-0.12130500	6.63646400	0.06844800
H	0.36897800	6.15571400	-1.55813000
C	1.31824900	-0.18546900	2.26304900
C	1.54813000	0.27331100	3.69131900
H	1.58373700	0.90724200	1.50656100
H	2.04059600	-0.91428600	1.89788400
C	2.99032900	0.73045200	3.89713900
H	0.86169100	1.10224300	3.89747100
H	1.29264700	-0.51739000	4.40992200
H	3.15909900	1.07707000	4.92034000
H	3.69217000	-0.08744800	3.70090500
H	3.22890600	1.54851500	3.21104800
M3			
C	3.53004900	-0.63013600	0.02417700
C	4.79277400	-0.16677100	-0.33295100
C	5.57753900	-0.89972900	-1.21980800
C	5.07405700	-2.09315700	-1.73223700
C	3.81174800	-2.55802900	-1.35345200
C	3.02475100	-1.83214900	-0.46339700
C	2.84733700	0.32694400	0.97682300
C	3.79303100	1.58503600	1.01715100
C	5.12252200	1.12186200	0.37649400
H	6.56354600	-0.54744800	-1.50825800
H	5.67288200	-2.67289300	-2.42775100
H	3.44555900	-3.49929600	-1.75051800
H	2.05789800	-2.18340800	-0.11186400
H	3.93016600	1.91537800	2.04703200
H	5.50728500	1.90402600	-0.28569000
H	2.68287200	-0.12577400	1.95450600
H	5.87892400	0.95548100	1.15046900
C	1.39221200	1.65793100	-0.51898900
C	0.30656400	0.20063900	0.71127500
N	0.16152100	1.77640300	-0.91045400
N	1.52476400	0.71216100	0.46209000
N	-0.50351400	0.85260700	-0.14354900
C	2.60966600	2.44814500	-0.86740600
H	3.25439000	1.88686400	-1.55786300
H	2.32797500	3.39544400	-1.32698900
C	-1.86639400	0.57575300	-0.42246200
C	-2.21883100	-0.59247300	-1.10340600
C	-2.86471600	1.47119800	-0.03987700
C	-3.54818300	-0.87835100	-1.37970800
C	-4.20075400	1.20952400	-0.31675500

C	-4.52134100	0.03158700	-0.98082500
H	-3.81610700	-1.78885400	-1.90100400
H	-4.97113300	1.90604800	-0.00978900
Cl	-0.99069900	-1.69880400	-1.60734200
Cl	-6.18568600	-0.31391300	-1.32699800
Cl	-2.43919700	2.90220900	0.83201400
O	3.25788200	2.72683600	0.35795700
C	0.03506000	-0.91756300	1.67441600
O	1.02756900	-1.69939200	1.84441500
C	-1.21412900	-0.91118700	2.23006400
C	-1.66986400	-2.00499700	3.14355900
H	-1.91251900	-0.11468200	1.99299400
C	-2.76802200	-2.86223500	2.50027200
H	-0.80424000	-2.62924300	3.38426100
H	-2.04652500	-1.59299900	4.08918300
H	-3.11024200	-3.65493900	3.17300900
H	-3.63516700	-2.24859500	2.23219900
H	-2.39411900	-3.32528800	1.58227100

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O	2.04151000	-0.93314100	-0.27537800
C	1.18879600	-0.14726300	0.05862500
O	1.42663700	1.17646900	0.14504800
C	-0.23233800	-0.48877700	0.42482000
C	-1.26606300	0.31195800	-0.37479400
H	-0.36011300	-0.28246500	1.49436300
H	-0.35689300	-1.56278000	0.27055100
C	-2.69077600	-0.07610800	0.00843500
H	-1.10282600	1.37912900	-0.19946800
H	-1.10736500	0.13855400	-1.44500900
H	-3.42340300	0.49308100	-0.56863900
H	-2.87056400	-1.13973500	-0.17451800
H	-2.87490000	0.11625400	1.06991800
H	2.35316700	1.31247700	-0.10708100

Coordinates for the formation of M4

Z-TS4

C	-2.52011200	-2.18683500	-0.58808600
C	-3.52919400	-3.01981300	-0.11315900
C	-3.93524700	-4.12058700	-0.86342000
C	-3.31272600	-4.36879000	-2.08424900
C	-2.30468100	-3.52453000	-2.55635400
C	-1.89932000	-2.42019000	-1.81162900
C	-2.22084000	-1.07663300	0.39645100

C	-3.05449700	-1.45218700	1.68037900
C	-4.04991500	-2.54264000	1.21833500
H	-4.71948900	-4.77826000	-0.50031300
H	-3.61438100	-5.22718000	-2.67608700
H	-1.83666800	-3.72875200	-3.51383300
H	-1.13527700	-1.73946700	-2.17427100
H	-3.56986200	-0.56648500	2.05364100
H	-4.11116300	-3.33311200	1.97305900
H	-2.51236900	-0.09419100	0.02305400
H	-5.05388200	-2.11855200	1.11340000
C	-0.23421000	-1.84597200	1.65284700
C	0.20205600	-0.23491200	0.20911000
N	1.03332300	-1.64238300	1.80218700
N	-0.79045300	-1.01923400	0.71036500
N	1.30917300	-0.64210000	0.89005300
C	-1.17065400	-2.70802200	2.43071000
H	-1.48493100	-3.57815700	1.83748100
H	-0.69535100	-3.04928500	3.35002800
C	2.65800000	-0.37224300	0.56437100
C	3.23380300	-0.93637100	-0.57869700
C	3.44924600	0.42249200	1.39723100
C	4.56036800	-0.69161800	-0.90677500
C	4.78251600	0.66948900	1.09661900
C	5.31615800	0.11030400	-0.05865400
H	4.99479200	-1.12566700	-1.79872000
H	5.38644100	1.29118100	1.74581500
Cl	2.28356300	-1.96195400	-1.59630900
Cl	6.97671200	0.42196900	-0.45280400
Cl	2.74890400	1.13112700	2.80967200
O	-2.26456500	-1.88196100	2.77947400
C	0.08137100	0.73441900	-0.81627400
O	-0.99788800	0.56624300	-1.64555000
C	0.92520700	1.82269200	-0.89594900
C	0.78914100	2.93819600	-1.75980800
H	1.67226900	1.90933400	-0.10774300
C	0.15892500	2.82883600	-3.14447700
H	1.65042000	3.60508700	-1.71849900
H	-0.18327000	3.59190400	-1.06984800
H	0.60415800	2.02810600	-3.74461900
H	-0.91657800	2.64213400	-3.09597600
H	0.30519900	3.77156600	-3.67746000
O	-1.14460000	4.24307300	-0.54470000
C	-2.26259000	3.63247200	-0.46004800
O	-2.50001700	2.46998500	-0.84632200

C	-3.38687500	4.44397500	0.16830300
C	-4.66144000	3.65235900	0.42825700
H	-3.58522700	5.28946900	-0.50270600
H	-2.99698600	4.88598300	1.09225900
C	-5.75287700	4.51541900	1.05451100
H	-5.00964300	3.21902400	-0.51432400
H	-4.42829600	2.80430900	1.08204600
H	-6.66202700	3.93850400	1.24339500
H	-5.41992500	4.93853800	2.00779000
H	-6.01684900	5.35078300	0.39802900
H	-1.59457100	1.35522300	-1.47384400

E-TS4

C	-2.81359400	-1.93824000	-0.61598100
C	-3.95613400	-2.53097200	-0.08551000
C	-4.54812200	-3.61179700	-0.73232600
C	-3.97493300	-4.08631900	-1.90945000
C	-2.83067600	-3.48430700	-2.43849400
C	-2.23872700	-2.39875900	-1.79671200
C	-2.34051900	-0.79874000	0.26121800
C	-3.21709200	-0.91606200	1.56609600
C	-4.39278400	-1.84226100	1.18156200
H	-5.43832400	-4.08031100	-0.32303400
H	-4.42246000	-4.93204500	-2.42191000
H	-2.40198300	-3.86380100	-3.36031000
H	-1.36183900	-1.90488900	-2.20488100
H	-3.56236400	0.07413300	1.86545200
H	-4.60576700	-2.53242700	2.00380500
H	-2.48853900	0.17894600	-0.20239400
H	-5.29952800	-1.25263600	1.00967300
C	-0.48859800	-1.71821100	1.61736500
C	0.16808700	-0.28706500	0.07210300
N	0.78737200	-1.63309700	1.80819000
N	-0.91860600	-0.92137400	0.58746300
N	1.19922300	-0.74817400	0.83163400
C	-1.54431100	-2.39112600	2.42728600
H	-1.97403800	-3.24318500	1.88264000
H	-1.13287400	-2.73605900	3.37542100
C	2.58057400	-0.58921800	0.58182600
C	3.19077900	-1.26520700	-0.47979300
C	3.36518500	0.21836700	1.40936700
C	4.54819400	-1.12051700	-0.73290200
C	4.72761000	0.36592900	1.18421700
C	5.29713300	-0.30509600	0.10844300

H	5.01176900	-1.64123100	-1.56152100
H	5.32680200	0.99614400	1.82960600
Cl	2.24510000	-2.30323600	-1.48818900
Cl	6.99680300	-0.12348900	-0.19083700
Cl	2.62071400	1.07088200	2.71599000
O	-2.51211200	-1.39606700	2.70290500
C	0.18574800	0.59822200	-1.03018300
O	-0.85254500	0.46000600	-1.91785600
C	1.10085800	1.62199700	-1.15553300
C	0.98353700	2.65274000	-2.11491700
H	1.85547700	1.72884900	-0.37526100
C	2.15158000	3.59574900	-2.33592700
H	0.43636700	2.35962000	-3.01364100
H	0.01131400	3.37836300	-1.47975300
H	1.81851900	4.52652700	-2.80334200
H	2.62108900	3.86242700	-1.38307800
H	2.92829400	3.16479100	-2.97870200
O	-0.84719200	4.07577100	-0.85234400
C	-1.98588800	3.52909100	-0.66544700
O	-2.31313800	2.37696500	-1.01388100
C	-3.00919000	4.40736800	0.04078900
C	-4.28733700	3.68068700	0.43768300
H	-3.23286600	5.24273400	-0.63511100
H	-2.51782400	4.85553400	0.91165500
C	-5.28593900	4.60743100	1.12468900
H	-4.73256900	3.23238700	-0.45566800
H	-4.03163600	2.84533100	1.09968200
H	-6.19451800	4.07305600	1.41455500
H	-4.85454500	5.05053300	2.02797500
H	-5.57794100	5.42834400	0.46197200
H	-1.43316800	1.26120600	-1.77063600

Z-M4

C	-3.28386700	0.63813700	0.02979500
C	-4.48890700	0.37349600	-0.61427400
C	-5.05991800	1.32885200	-1.45206900
C	-4.40500700	2.54413900	-1.63266800
C	-3.20078800	2.80899500	-0.97483700
C	-2.63210600	1.85839600	-0.13091600
C	-2.82882800	-0.54067300	0.86434200
C	-3.88463300	-1.67306800	0.55637500
C	-5.01309300	-0.99409600	-0.25984400
H	-5.99846400	1.12761600	-1.96054800
H	-4.83477600	3.29434500	-2.28900900

H	-2.70817400	3.76522000	-1.11975600
H	-1.70342700	2.05649500	0.39573600
H	-4.26455100	-2.07838200	1.49477800
H	-5.25482200	-1.60359100	-1.13709600
H	-2.82979700	-0.29814000	1.92648900
H	-5.92785800	-0.92170100	0.33727200
C	-1.25742200	-1.83157000	-0.53669800
C	-0.24193300	-0.53352900	0.96383100
N	-0.01707800	-2.02628700	-0.80281400
N	-1.48385900	-0.98565200	0.52033100
N	0.66784300	-1.23733500	0.14840400
C	-2.45735300	-2.46038700	-1.16142300
H	-2.92401900	-1.76594700	-1.87600300
H	-2.17892500	-3.37585300	-1.68286400
C	1.87692200	-0.67127500	-0.32046000
C	1.89466600	0.47044000	-1.13116000
C	3.10444500	-1.26588000	-0.01225400
C	3.08169400	1.03090500	-1.58409500
C	4.30882800	-0.73697000	-0.46038500
C	4.27686400	0.41429700	-1.23659200
H	3.07089200	1.92002200	-2.20222100
H	5.24771700	-1.21176300	-0.20385900
Cl	0.39461700	1.20290600	-1.60067000
Cl	5.77407900	1.09915700	-1.79525000
Cl	3.13539000	-2.68919900	0.97340200
O	-3.34411600	-2.79874800	-0.11263400
C	0.05235900	0.35316000	1.94722800
O	-1.01389000	1.07214400	2.48750500
C	1.39632500	0.56232600	2.45572300
C	1.86840600	1.60776700	3.15771300
H	2.07069300	-0.27878200	2.30388700
C	1.18366800	2.91201600	3.45501500
H	-0.92828300	1.03039400	3.44959400
H	2.88405500	1.51724400	3.53722000
H	1.00239000	3.03494900	4.52995800
H	1.82757500	3.74556000	3.15509200
H	0.23409000	3.00851600	2.92964500
E-M4			
C	3.58977800	0.53688100	0.06924600
C	4.84590300	-0.04179500	0.23318500
C	5.69582200	0.40581100	1.24107200
C	5.26688100	1.43323600	2.07834800
C	4.00512500	2.00879700	1.91135000

C	3.15548400	1.56546700	0.90079700
C	2.83114400	-0.10790300	-1.07057000
C	3.71562000	-1.34204600	-1.48325000
C	5.08266500	-1.12663500	-0.78751700
H	6.67535800	-0.04324500	1.37803100
H	5.91750100	1.78737800	2.87165100
H	3.68446700	2.80477600	2.57557700
H	2.16588200	1.99650900	0.77511300
H	3.82178100	-1.37555900	-2.56812300
H	5.42863500	-2.06764800	-0.34748200
H	2.71798200	0.57803800	-1.90969300
H	5.83786700	-0.81724900	-1.51782900
C	1.33623900	-1.69917500	0.05067700
C	0.33499600	0.20748100	-0.52536200
N	0.17141400	-1.83199400	0.57175100
N	1.49749500	-0.54633100	-0.68245800
N	-0.48939600	-0.64579200	0.21615200
C	2.50477100	-2.62735100	0.10881600
H	3.19302500	-2.32352100	0.91214100
H	2.17100700	-3.64812800	0.29653300
C	-1.89071600	-0.64089800	0.26288100
C	-2.55124400	-0.55040900	1.49567000
C	-2.67971300	-0.74510900	-0.89159100
C	-3.93675900	-0.54200500	1.58663700
C	-4.06717800	-0.70794600	-0.83117900
C	-4.67679500	-0.60943400	0.41277600
H	-4.42400600	-0.46792500	2.55090800
H	-4.65654800	-0.77696900	-1.73723500
Cl	-1.61698200	-0.41093000	2.94819400
Cl	-6.41337900	-0.57806600	0.50376900
Cl	-1.92387700	-0.95278100	-2.43435900
O	3.13518500	-2.59490000	-1.15534200
C	0.07565000	1.46944400	-0.95754800
O	1.00305600	2.04285600	-1.82279500
C	-1.08712100	2.25044300	-0.59747500
C	-1.42575200	3.41148600	-1.18205900
H	-1.68267900	1.89432500	0.24152700
C	-2.57607000	4.26631100	-0.74514100
H	1.21073100	2.92235600	-1.47472600
H	-0.84955500	3.75529900	-2.03958400
H	-2.24369000	5.26429700	-0.43687300
H	-3.29580000	4.41225600	-1.55831200
H	-3.10481300	3.81249400	0.09752700

TS4-Direct

C	3.45256700	0.50569000	-0.04781200
C	4.63616200	-0.01066000	0.47292400
C	5.38513500	0.73667600	1.37854000
C	4.92766800	1.99743600	1.75166600
C	3.74425200	2.51353900	1.21715600
C	2.99643500	1.77394000	0.30515000
C	2.79106900	-0.47136200	-0.99217000
C	3.74266600	-1.72660700	-1.00221700
C	4.94219700	-1.37585400	-0.08557900
H	6.31152500	0.34292600	1.78659400
H	5.49988900	2.58919200	2.45922400
H	3.40961100	3.50349700	1.50940600
H	2.09036100	2.17748900	-0.13798400
H	4.07414000	-1.90206000	-2.02584100
H	5.05979300	-2.13746100	0.69331000
H	2.64853300	-0.04037500	-1.98375700
H	5.87355700	-1.37206700	-0.65947900
C	1.21850600	-1.92550700	0.29425500
C	0.29130500	-0.14625000	-0.61884500
N	-0.01035200	-1.99199200	0.68802900
N	1.45363000	-0.85127600	-0.52365100
N	-0.59311300	-0.87865800	0.11531400
C	2.35600100	-2.85472300	0.55542900
H	2.96241700	-2.48487100	1.39519000
H	1.98475700	-3.85013800	0.79950600
C	-1.97898200	-0.66110900	0.26060200
C	-2.50102100	-0.19460300	1.47063500
C	-2.85977000	-0.93243900	-0.79189200
C	-3.86466300	0.00962200	1.63520500
C	-4.22507600	-0.71923200	-0.65590100
C	-4.70724700	-0.25208100	0.56133800
H	-4.25600400	0.37477100	2.57649300
H	-4.89704700	-0.92441500	-1.48002200
Cl	-1.42681000	0.16781100	2.77786400
Cl	-6.41329000	0.00990900	0.74704600
Cl	-2.24474600	-1.54038500	-2.28687200
O	3.10724400	-2.94171800	-0.63611300
C	0.07284400	1.03711100	-1.35350300
O	1.00607200	1.45632900	-2.21003600
C	-0.86851900	2.00653200	-1.02051000
C	-0.60987500	3.22372800	-1.72319400
H	-1.52166300	1.92795600	-0.15431200
C	-1.09926800	4.53452300	-1.14868100

H	0.68579200	2.68212600	-1.99292800
H	-0.72620700	3.14525000	-2.81015800
H	-0.59076900	5.38141100	-1.61834900
H	-2.17701600	4.68495000	-1.29374800
H	-0.90130100	4.59349300	-0.07402100

TS4-DMAP

C	-0.65006100	3.51857400	-0.72172700
C	-0.96464600	4.81962700	-0.34136800
C	-1.78966000	5.60203700	-1.14679500
C	-2.28413600	5.05855200	-2.32977400
C	-1.93987100	3.76017800	-2.71773500
C	-1.10977100	2.97614400	-1.91980400
C	0.21642700	2.82711000	0.30698900
C	0.41378600	3.90226900	1.44255600
C	-0.28191300	5.19757200	0.94767800
H	-2.04241400	6.61882300	-0.85920600
H	-2.93338300	5.65473200	-2.96385100
H	-2.31584300	3.36414900	-3.65612800
H	-0.77720900	1.98222100	-2.21104900
H	1.48135500	4.06602100	1.59472100
H	-0.97405900	5.56847500	1.71172300
H	1.15502800	2.49179800	-0.12922900
H	0.45575800	5.98966700	0.78442500
C	-1.30486600	1.68954500	1.89971900
C	-0.52897700	0.36299700	0.29248500
N	-1.93670200	0.58761700	2.11398100
N	-0.43865000	1.63014700	0.84311800
N	-1.47016400	-0.26167300	1.10751400
C	-1.36257700	2.95847400	2.68066800
H	-2.07367000	3.65821100	2.21701000
H	-1.68055900	2.75871500	3.70412900
C	-2.33543600	-1.31099000	0.74199000
C	-3.27646900	-1.15903200	-0.28549600
C	-2.31872800	-2.52145200	1.44181500
C	-4.13711700	-2.18890300	-0.63949800
C	-3.17971500	-3.56325200	1.11969600
C	-4.07293600	-3.38133800	0.07227600
H	-4.85451500	-2.05503900	-1.43959000
H	-3.14678400	-4.49474000	1.67087900
Cl	-3.38269400	0.35223500	-1.12296100
Cl	-5.15211200	-4.67830000	-0.35378100
Cl	-1.17720400	-2.74075100	2.72665300
O	-0.05682200	3.49649100	2.71879200

C	0.21010800	-0.09949000	-0.81385000
O	0.95031300	0.73395200	-1.50370000
C	0.12397500	-1.47744800	-1.12131100
C	0.82789200	-2.04446100	-2.18927100
H	-0.38497000	-2.14640400	-0.42864000
C	0.58257800	-3.47681500	-2.61104600
H	1.09218600	-1.33245900	-2.97460000
H	2.17013700	-1.98231200	-1.56166600
H	1.45491700	-3.91050600	-3.11327700
H	0.35823700	-4.10608700	-1.74230400
H	-0.26219200	-3.57379800	-3.30553800
C	4.21153700	-2.72154300	-0.87054100
C	5.46364800	-2.43616200	-0.37776000
C	5.81348700	-1.08705100	-0.11104500
C	4.82899800	-0.10534400	-0.38216600
C	3.60060400	-0.47937400	-0.88301100
N	3.30633600	-1.76752300	-1.11675300
H	3.90482100	-3.74239100	-1.07928200
H	6.15554800	-3.24767000	-0.19901000
H	5.02106300	0.94463800	-0.20709100
H	2.78168700	0.21926700	-1.11730900
N	7.03275600	-0.75786700	0.38097500
C	7.34704500	0.63166800	0.66834300
H	8.34756400	0.68812700	1.09346900
H	7.32320200	1.24338100	-0.24046800
H	6.64242000	1.05473500	1.39231700
C	8.02012900	-1.79389700	0.63024000
H	8.93272400	-1.33224700	1.00297200
H	7.66654200	-2.51099000	1.37977100
H	8.26358800	-2.34008300	-0.28779600

TS4-DMAP·H+

C	2.79129700	-2.94713100	-0.62394600
C	3.58891000	-3.99754600	-0.18083900
C	4.75529400	-4.32251300	-0.86990400
C	5.10315900	-3.57733200	-1.99358200
C	4.29731700	-2.52269200	-2.43088700
C	3.12842000	-2.19888500	-1.74863600
C	1.59056300	-2.75536700	0.27356800
C	1.83135900	-3.74098700	1.48144100
C	3.00787700	-4.64981500	1.04740800
H	5.38631200	-5.13967600	-0.53392000
H	6.01175200	-3.81744300	-2.53599200
H	4.58403200	-1.95507900	-3.30985000

H	2.48941800	-1.38832800	-2.08770900
H	0.92572400	-4.31871700	1.66741700
H	3.72645500	-4.74377700	1.86805600
H	0.65492800	-2.98156000	-0.23272600
H	2.64681700	-5.65859900	0.82405300
C	2.28433100	-0.94790800	1.80502700
C	0.93474600	-0.25571000	0.20167900
N	2.21789900	0.32664500	1.99221400
N	1.51199500	-1.36363700	0.74515200
N	1.37888400	0.76356100	0.98877500
C	2.97956600	-1.99914500	2.60480100
H	3.92109400	-2.29331500	2.11958100
H	3.19320100	-1.62879900	3.60717800
C	1.34867700	2.15073600	0.70985900
C	2.25136300	2.69341800	-0.21010800
C	0.45290300	2.99704200	1.36465000
C	2.25216100	4.05269100	-0.49076000
C	0.43890000	4.36091500	1.10489300
C	1.34242900	4.86791300	0.17515400
H	2.95221000	4.46603600	-1.20633800
H	-0.25931700	5.01252300	1.61593400
Cl	3.37479000	1.64915000	-1.00973100
Cl	1.33349600	6.56590600	-0.16305200
Cl	-0.68303200	2.32396100	2.48248900
O	2.07813200	-3.08138600	2.71096400
C	0.09839500	-0.18720600	-0.93770400
O	0.07674000	-1.33868500	-1.70797700
C	-0.63748700	0.91887100	-1.31442600
C	-1.51839600	0.95968300	-2.41463100
H	-0.63313500	1.78068700	-0.65070600
C	-2.03555200	2.30500900	-2.89462900
H	-1.30136900	0.23752100	-3.20590500
H	-2.66907700	0.38960600	-1.81495400
H	-2.97574100	2.19423900	-3.44259400
H	-2.23007000	2.96957000	-2.04622300
H	-1.32623700	2.81112100	-3.55767300
C	-3.92194000	0.01456900	0.02917500
C	-5.02587300	-0.48361300	0.67910900
C	-6.01561900	-1.18448200	-0.06209000
C	-5.78557200	-1.32103100	-1.45802600
C	-4.64846800	-0.78574100	-2.01363500
N	-3.72732400	-0.13292400	-1.28926600
H	-3.14698000	0.55815600	0.56484600
H	-5.12114100	-0.32998300	1.74513400

H	-6.49007700	-1.83343400	-2.09831200
H	-4.44855000	-0.86949400	-3.07806400
N	-7.11556100	-1.69372500	0.52628800
C	-8.10620300	-2.40374000	-0.27122100
H	-8.89689000	-2.76200800	0.38456300
H	-8.55218900	-1.74716000	-1.02584200
H	-7.65907800	-3.26784900	-0.77302700
C	-7.32989200	-1.51138000	1.95523200
H	-8.27761700	-1.96882300	2.23130400
H	-6.53462800	-1.98786700	2.53807400
H	-7.37207500	-0.44870700	2.21560300
H	-0.84327200	-1.55276700	-1.91480000

M04-DMAP·H+

C	-0.74202600	-3.43663500	-0.58723700
C	-1.10202400	-4.73132100	-0.22114900
C	-1.19627200	-5.72651100	-1.18997000
C	-0.92071200	-5.40129400	-2.51578800
C	-0.56106500	-4.09961200	-2.87410200
C	-0.47114400	-3.09927100	-1.90991600
C	-0.70025700	-2.53105600	0.62480700
C	-0.82425000	-3.51030400	1.85356000
C	-1.35878800	-4.83205400	1.26053900
H	-1.47387800	-6.73977200	-0.91636800
H	-0.98590000	-6.16855700	-3.28034800
H	-0.35254200	-3.86678200	-3.91291100
H	-0.21153600	-2.07910200	-2.17627000
H	-1.50159800	-3.09278300	2.59876500
H	-0.85858900	-5.68043800	1.73695800
H	-1.49609800	-1.78472900	0.61706300
H	-2.42988700	-4.93320900	1.46408000
C	1.71621400	-2.42677400	1.13750000
C	0.91121700	-0.55513900	0.34638900
N	2.74335300	-1.63412300	1.07755700
N	0.57639300	-1.80448300	0.69609500
N	2.23085600	-0.47454000	0.57059400
C	1.54922000	-3.78416000	1.73903300
H	1.44812300	-4.55096600	0.95992700
H	2.39985200	-4.02268000	2.37659200
C	3.10368500	0.60260500	0.24983200
C	3.40623400	0.88669900	-1.08437100
C	3.67347200	1.37023800	1.26656700
C	4.25674400	1.93495500	-1.40603500
C	4.53203900	2.41815000	0.96314500

C	4.80851400	2.68733700	-0.37359400
H	4.48767900	2.15509500	-2.44113900
H	4.97081500	3.01399300	1.75399900
Cl	2.70545000	-0.06142400	-2.34873400
Cl	5.86652700	3.99937600	-0.76286700
Cl	3.27803500	1.03736100	2.91536600
O	0.39696900	-3.68824700	2.55492900
C	0.01865600	0.46507400	-0.22401000
O	-0.90663600	-0.07538300	-1.02936600
C	0.20651900	1.76118300	0.07818200
C	-0.52177800	2.90613100	-0.55327000
H	0.97374900	2.00905700	0.80821400
C	0.47274000	3.97368100	-1.02143200
H	-1.11929500	2.54149800	-1.39364600
H	-1.22603000	3.34566300	0.16467300
H	-0.04849700	4.81981000	-1.47382400
H	1.06597800	4.34998400	-0.18241300
H	1.16183700	3.55908800	-1.76257300
C	-3.46969500	1.28381400	0.72996000
C	-4.65329700	1.86486700	1.13079500
C	-5.62649800	2.20348400	0.15750700
C	-5.29422500	1.90889200	-1.18818800
C	-4.07935900	1.32590000	-1.47632400
N	-3.16512200	1.00760700	-0.54740100
H	-2.71203300	1.02439000	1.46660700
H	-4.81670500	2.05518600	2.18285500
H	-5.97313800	2.13116000	-2.00004300
H	-3.81539000	1.09687500	-2.50494600
N	-6.80425000	2.77771300	0.49374800
C	-7.76768700	3.11866100	-0.54111500
H	-8.63810200	3.57860500	-0.07730100
H	-7.34461400	3.83101400	-1.25747300
H	-8.09818600	2.22759700	-1.08591800
C	-7.10436700	3.05693000	1.88885300
H	-8.09411200	3.50439600	1.95596900
H	-7.10296000	2.13919800	2.48697900
H	-6.38080800	3.75802300	2.31916400
H	-1.84047200	0.39507100	-0.89032300

Coordinates for the reaction between M4 and R2

TS5RR

C	-1.47344300	-3.16803700	-0.17238100
C	-2.43358800	-3.84323200	0.57749800
C	-3.15294700	-4.88649000	0.00159900

C	-2.89118500	-5.23565100	-1.32241700
C	-1.92963800	-4.54818700	-2.06734600
C	-1.21124100	-3.49984700	-1.49686200
C	-0.85522200	-2.05537600	0.63793800
C	-1.34727000	-2.30358800	2.10688700
C	-2.55865500	-3.24923300	1.95864900
H	-3.90580000	-5.42113700	0.57353700
H	-3.44135200	-6.05096800	-1.78188700
H	-1.74428300	-4.83091900	-3.09857900
H	-0.47468100	-2.93876200	-2.06485700
H	-1.61935000	-1.34728500	2.56105700
H	-2.55526800	-3.99319200	2.76085100
H	-1.19148600	-1.07884000	0.29042700
H	-3.48822600	-2.67265300	2.03805000
C	1.38102200	-2.73198500	1.42778200
C	1.37122000	-1.07227900	-0.02793300
N	2.61497000	-2.34326900	1.40765100
N	0.59316100	-2.01207600	0.56987900
N	2.61516800	-1.31508700	0.47876400
C	0.64988900	-3.64142100	2.35734800
H	0.22109600	-4.49210100	1.81014600
H	1.31425000	-4.00553000	3.14031000
C	3.84253400	-0.83851100	-0.02982300
C	4.63203900	0.03605500	0.72104900
C	4.30552300	-1.25657900	-1.28208900
C	5.85450400	0.49183700	0.24423800
C	5.51707900	-0.80304400	-1.78567600
C	6.27637900	0.06533000	-1.00923400
H	6.45623000	1.17057300	0.83567400
H	5.86457400	-1.13122100	-2.75727400
Cl	4.06174600	0.58330500	2.25784700
Cl	7.79693200	0.63103400	-1.62428500
Cl	3.36296000	-2.36379700	-2.21927600
O	-0.34824000	-2.84466400	2.97001100
C	0.95712700	-0.09687600	-0.95414800
O	-0.07069100	-0.48819000	-1.78112900
C	1.55378300	1.15643500	-0.98215700
C	1.06615300	2.25370700	-1.67916000
H	2.34670400	1.33284400	-0.25606400
C	1.86655200	3.52283900	-1.76089800
H	-0.61398300	0.28194600	-2.05321800
H	0.37419400	2.06882700	-2.49562900
H	2.52658300	3.52126100	-2.63587400
H	1.21860200	4.40327500	-1.84832000

H	2.48346000	3.65657000	-0.86652200
C	-2.07450700	1.14099500	0.94834100
O	-1.53190900	1.19015600	2.05733000
C	-1.64756200	1.87307900	-0.23035000
C	-0.60528900	2.82796900	-0.31772800
H	-0.76631800	3.56166700	-1.10845000
C	-3.30366600	0.25368700	0.84190000
C	-3.57175900	-0.58868100	-0.24179900
C	-4.17468200	0.24900400	1.93605700
C	-4.70090300	-1.40514500	-0.24035100
H	-2.88446800	-0.63768400	-1.08423900
C	-5.31924500	-0.54048600	1.92479400
H	-3.93766200	0.87956800	2.78695900
C	-5.58537500	-1.36965000	0.83422900
H	-4.87803200	-2.07521000	-1.07590800
H	-6.00076000	-0.51726100	2.76934300
H	-6.47288900	-1.99457400	0.82939000
C	0.17118600	3.40579900	0.80437300
C	0.29993800	4.80002200	0.85065000
C	0.84279300	2.64262100	1.77033100
C	1.05641800	5.42261300	1.84025200
H	-0.20739300	5.40314500	0.10179000
C	1.60824200	3.26302200	2.74869900
H	0.75238100	1.56356600	1.75093300
C	1.71557300	4.65374400	2.79257300
H	1.13310400	6.50508700	1.86042900
H	2.12033100	2.65732700	3.48998200
H	2.30949500	5.13115700	3.56565500
C	-2.44713400	1.79329200	-1.48192300
O	-1.91358700	1.44339300	-2.53935100
C	-3.87677300	2.23048000	-1.51179000
C	-4.43086500	2.99162500	-0.47982700
C	-4.65370700	1.90061200	-2.62654200
C	-5.75443500	3.41256600	-0.56036900
H	-3.81985900	3.25818100	0.37741800
C	-5.97646100	2.31568000	-2.70227000
H	-4.19991100	1.31498100	-3.41939500
C	-6.52756800	3.07261600	-1.66813200
H	-6.18243400	4.00712100	0.24005900
H	-6.58022000	2.05135400	-3.56434200
H	-7.56119100	3.39916300	-1.72713900
TS5RS			
C	-0.75689800	-3.52009800	-0.70378600

C	-1.60200200	-4.48221000	-0.15495700
C	-2.15106700	-5.46658900	-0.97107100
C	-1.83738700	-5.46795000	-2.32961300
C	-0.99431500	-4.49457400	-2.87101600
C	-0.44760900	-3.50315900	-2.05870800
C	-0.32331200	-2.53823300	0.35607100
C	-0.74196200	-3.19900900	1.71166500
C	-1.81539800	-4.23491600	1.31871300
H	-2.81195100	-6.22293600	-0.55760300
H	-2.25397500	-6.23400300	-2.97620000
H	-0.76704000	-4.50972000	-3.93203700
H	0.19494300	-2.72635000	-2.46357000
H	-1.12848800	-2.42643200	2.38085700
H	-1.71932700	-5.13227900	1.93667800
H	-0.83706400	-1.58865100	0.23453100
H	-2.81286900	-3.81206000	1.48849700
C	2.00174900	-2.98050100	1.02595000
C	1.67245900	-1.02567600	0.04852800
N	3.13988100	-2.38337300	1.16563000
N	1.08994900	-2.21880100	0.34372500
N	2.94429000	-1.16186600	0.53712000
C	1.45633100	-4.21546900	1.66095000
H	1.18151300	-4.95498100	0.89674700
H	2.18436700	-4.64812300	2.34628300
C	4.06907600	-0.38553000	0.18634800
C	4.71592000	0.40514200	1.13981100
C	4.57788100	-0.41511200	-1.11679700
C	5.83582500	1.15883900	0.81116900
C	5.68622400	0.34136700	-1.47289700
C	6.30077500	1.11851700	-0.49757100
H	6.32627500	1.76856600	1.55976100
H	6.06740400	0.31321600	-2.48612100
Cl	4.09308000	0.46890000	2.75162200
Cl	7.69134700	2.06311800	-0.92725400
Cl	3.82636100	-1.42064800	-2.30812700
O	0.33864000	-3.79954800	2.42562700
C	1.08723000	0.05997900	-0.62016800
O	0.12484400	-0.28026500	-1.54876200
C	1.50501300	1.36160800	-0.35935300
C	0.91988900	2.52164200	-0.83910900
H	2.28107500	1.47247000	0.39713900
C	1.64013300	3.83489700	-0.68087400
H	-0.52586600	0.44158300	-1.65824400
H	0.22830600	2.44329200	-1.67591000

H	2.46009200	3.91682400	-1.40517500
H	0.97571800	4.68664700	-0.84199900
H	2.07307100	3.93000600	0.32141800
C	-1.88365300	0.36697700	1.27892400
O	-1.18397500	0.23152500	2.28932600
C	-1.76019000	1.47525900	0.34714200
C	-0.85498500	2.50512400	0.63975300
H	-0.27189300	2.29197900	1.53495500
C	-2.98582300	-0.64476600	1.04380200
C	-3.24413400	-1.22490300	-0.20301400
C	-3.75445800	-1.02973300	2.14662900
C	-4.26781400	-2.15816400	-0.34794200
H	-2.62522400	-0.97442200	-1.06210900
C	-4.79924500	-1.93558300	1.99520700
H	-3.52437600	-0.59729800	3.11550500
C	-5.05967100	-2.49995500	0.74589900
H	-4.43914900	-2.61913900	-1.31555600
H	-5.40667500	-2.20878200	2.85232500
H	-5.86803900	-3.21488600	0.62949100
C	-1.10811500	3.94669400	0.43108800
C	-0.65546100	4.82464900	1.42613700
C	-1.76683300	4.49068600	-0.68306800
C	-0.86168300	6.19647400	1.32667100
H	-0.13718100	4.41691600	2.28990800
C	-1.96957700	5.86227200	-0.78213800
H	-2.09321700	3.85185900	-1.49572200
C	-1.52171400	6.72207300	0.22018300
H	-0.50400600	6.85366600	2.11299400
H	-2.47539700	6.26399800	-1.65451800
H	-1.68184800	7.79190900	0.13403700
C	-2.60027300	1.54787500	-0.87530100
O	-2.06228500	1.45957200	-1.98334700
C	-4.07126300	1.76910100	-0.78720200
C	-4.66591400	2.18170500	0.40748800
C	-4.85416700	1.58642100	-1.93124800
C	-6.03825300	2.40338100	0.45860400
H	-4.04593500	2.33654900	1.28595000
C	-6.22435500	1.80203900	-1.87626000
H	-4.36788200	1.26930700	-2.84824300
C	-6.81651200	2.21028100	-0.68028400
H	-6.49987400	2.72876400	1.38502900
H	-6.83437000	1.65209000	-2.76124800
H	-7.88793100	2.37988800	-0.63815900

TS5SR'

C	-0.86695400	0.15731000	-0.84367800
O	0.07334500	0.03464700	-1.84293500
C	-1.21449300	1.37118300	-0.24346500
C	-0.67083700	2.61393200	-0.51176700
H	-1.93595100	1.31153900	0.56899000
C	-1.39017800	3.84393000	-0.01486400
H	0.73781100	0.75011300	-1.78739700
H	-0.07491200	2.72365800	-1.41657700
H	-1.63870400	3.75108700	1.04895500
H	-2.32984900	3.99402700	-0.56062900
H	-0.78873300	4.74613600	-0.14016300
C	1.94879800	0.22481200	1.17880600
O	1.27385700	0.15330400	2.21314900
C	2.00941100	1.43100100	0.36674300
C	1.19964200	2.50615900	0.74603700
H	0.65991200	2.29925800	1.66863900
C	2.75303900	-0.98447400	0.77289100
C	2.94260400	-1.37016500	-0.55715300
C	3.26145700	-1.79453800	1.79268800
C	3.62579700	-2.54670300	-0.85994700
H	2.51719500	-0.78327900	-1.36528900
C	3.95569900	-2.95947700	1.49244600
H	3.07681400	-1.50244700	2.82159100
C	4.13589600	-3.34077200	0.16295000
H	3.75529600	-2.84154600	-1.89733500
H	4.34270200	-3.58152000	2.29335300
H	4.66961000	-4.25647800	-0.07331700
C	1.53355800	3.94072400	0.57281900
C	1.32603100	4.77466800	1.68071800
C	2.02653300	4.51803300	-0.60760400
C	1.61654800	6.13370000	1.62616800
H	0.93202200	4.34381300	2.59719100
C	2.31225700	5.87794500	-0.66121700
H	2.15910100	3.91378700	-1.49707500
C	2.11271400	6.69223100	0.45199800
H	1.44881900	6.75560500	2.49994900
H	2.68680200	6.30596100	-1.58583600
H	2.33456700	7.75329300	0.40075700
C	2.85924000	1.53131900	-0.83929000
O	2.33362500	1.69127600	-1.94738300
C	4.34383700	1.48444700	-0.72943700
C	4.97808900	1.58844300	0.51096900
C	5.10664900	1.36108300	-1.89516500

C	6.36678700	1.56050000	0.58503400
H	4.37851400	1.70236400	1.40900600
C	6.49233800	1.33058400	-1.81875700
H	4.59097700	1.28674300	-2.84713700
C	7.12258000	1.42895800	-0.57741600
H	6.85912700	1.64541400	1.54811900
H	7.08470900	1.23004900	-2.72250000
H	8.20629100	1.40553100	-0.51809500
C	0.35559600	-3.42337800	0.40901200
C	0.81585400	-4.73740900	0.34163700
C	1.13822100	-5.42347000	1.50744400
C	0.97785300	-4.77663300	2.73289700
C	0.50785900	-3.46411700	2.79227700
C	0.19087800	-2.77113900	1.62501000
C	0.00029100	-2.91279000	-0.97449800
C	-0.04072200	-4.20646900	-1.84653300
C	0.85618100	-5.20923300	-1.09116900
H	1.49208000	-6.44962600	1.46661600
H	1.21607400	-5.30343900	3.65183000
H	0.39519200	-2.97109000	3.75232500
H	-0.14577200	-1.73814800	1.67493300
H	0.31676200	-4.01077800	-2.85854700
H	0.49451100	-6.23107900	-1.23657700
H	0.71763600	-2.19041000	-1.36479300
H	1.88005700	-5.15640000	-1.48153000
C	-2.40206800	-3.07363800	-0.67683600
C	-1.63929700	-0.99455600	-0.63706900
N	-3.40299200	-2.40420900	-0.21931400
N	-1.31586700	-2.28214200	-0.96737700
N	-2.93280800	-1.09662900	-0.17932200
C	-2.24628700	-4.54110000	-0.93431600
H	-1.87738900	-5.04687500	-0.03185000
H	-3.20522000	-4.97706500	-1.21744800
C	-3.88118700	-0.05843800	-0.06249200
C	-4.34544400	0.62007000	-1.19467200
C	-4.38131600	0.30659400	1.18986700
C	-5.25545300	1.66266200	-1.08348600
C	-5.30386600	1.33647600	1.32542800
C	-5.72035000	2.00587100	0.18116700
H	-5.60118700	2.18603500	-1.96644100
H	-5.67862800	1.61430600	2.30271800
Cl	-3.78007300	0.15296700	-2.76035200
Cl	-6.86113300	3.30603800	0.33380200
Cl	-3.81226200	-0.51541800	2.60202900

O	-1.36686700	-4.69465900	-2.03064800
TS5SS			
C	0.62265800	0.22728200	-1.47198500
O	-0.50395500	0.27953300	-2.26319100
C	1.42627800	-0.90774800	-1.39411500
C	1.13788200	-2.14423800	-1.95547500
H	2.29455000	-0.86866700	-0.74632700
C	2.22441100	-3.18027000	-2.06767200
H	-0.88873100	-0.61599600	-2.36302000
H	0.36327500	-2.19057300	-2.71512000
H	2.94539700	-3.08847900	-1.24836000
H	2.76571200	-3.07456400	-3.01443800
H	1.81794100	-4.19783300	-2.03724300
C	-1.71736900	-1.43785300	0.91831500
O	-1.06897100	-1.39703100	1.96854100
C	-1.36119500	-2.21653700	-0.25531100
C	-0.17143900	-2.96167900	-0.44222700
H	-0.28713300	-3.76343200	-1.17279100
C	-2.96251200	-0.58322200	0.86445100
C	-3.32958100	0.15153600	-0.26473400
C	-3.69369000	-0.43227800	2.04407200
C	-4.40274500	1.03738000	-0.20755800
H	-2.75001500	0.07183800	-1.18031500
C	-4.77831300	0.43371200	2.09590000
H	-3.37970200	-0.98949000	2.92112000
C	-5.12701400	1.18225100	0.97189200
H	-4.66563600	1.62346500	-1.08395800
H	-5.34270100	0.54230800	3.01702600
H	-5.96052900	1.87632100	1.01724600
C	0.83002000	-3.31716600	0.59737500
C	1.21842400	-4.65781000	0.69360300
C	1.47236900	-2.38003600	1.41903700
C	2.20622300	-5.06164000	1.58998900
H	0.73780700	-5.39585100	0.05623100
C	2.46557400	-2.77853500	2.30251100
H	1.17748400	-1.33952400	1.36625300
C	2.83721900	-4.12116600	2.39520600
H	2.48466900	-6.10902000	1.64935400
H	2.94146800	-2.03620400	2.93755400
H	3.61118700	-4.42819800	3.09166000
C	-2.31978400	-2.34424100	-1.37218700
O	-1.96657000	-2.11470800	-2.53687400
C	-3.71222900	-2.84061300	-1.13633400

C	-4.06502200	-3.50105900	0.04312000
C	-4.65954900	-2.68437700	-2.15247900
C	-5.35686600	-3.99022100	0.20805300
H	-3.32169600	-3.63909200	0.82246100
C	-5.95055500	-3.16806000	-1.98462500
H	-4.36122100	-2.17826100	-3.06482200
C	-6.30009400	-3.82166300	-0.80298000
H	-5.62644600	-4.50705900	1.12324200
H	-6.68652500	-3.03836200	-2.77155600
H	-7.30798600	-4.20314700	-0.67221200
C	-1.69092300	2.93878300	0.51113400
C	-2.52638700	4.04296500	0.66144100
C	-3.09533700	4.32295700	1.89929800
C	-2.80937200	3.48229400	2.97417100
C	-1.97067300	2.37780100	2.81454000
C	-1.39879700	2.09548700	1.57621800
C	-1.17541400	2.84929000	-0.91146500
C	-1.50280500	4.25613000	-1.51126900
C	-2.66788400	4.78151500	-0.64716100
H	-3.74470200	5.18406800	2.02863900
H	-3.24542600	3.68708400	3.94701200
H	-1.77057400	1.71900700	3.65348300
H	-0.76052700	1.22155400	1.45454500
H	-1.76772300	4.18086700	-2.56681400
H	-2.60916200	5.86973400	-0.55472700
H	-1.64939200	2.05065300	-1.48347900
H	-3.62551300	4.54113500	-1.12464900
C	1.06757300	3.62932900	-0.42784200
C	1.00484600	1.46890900	-0.92802500
N	2.24647500	3.21776600	-0.11194300
N	0.27121300	2.62746200	-0.92967500
N	2.21486700	1.86967100	-0.41383700
C	0.47804800	5.00361700	-0.37569600
H	-0.04719900	5.16198100	0.57525500
H	1.26631000	5.75017800	-0.47623100
C	3.37874100	1.10949600	-0.17870600
C	4.27563600	0.82838400	-1.21355300
C	3.65275400	0.62400800	1.10302700
C	5.40408200	0.05136200	-0.99162500
C	4.78057600	-0.14772700	1.35164000
C	5.63698300	-0.42754600	0.29319500
H	6.08655400	-0.17162300	-1.80216900
H	4.98335500	-0.52351100	2.34698800
Cl	3.95135700	1.42904800	-2.80124100

Cl	7.04336300	-1.40156100	0.58494800
Cl	2.55382500	0.96797800	2.39385100
O	-0.38285400	5.13453900	-1.48986700

TS5RR'

C	-0.84660400	0.18837700	-0.85153300
O	0.07934800	0.10265400	-1.86644600
C	-1.17207800	1.34954100	-0.14678800
C	-0.71921000	2.64388200	-0.37827100
H	-1.75062000	1.17953200	0.75995300
C	-0.37977700	3.16774000	-1.75296100
H	0.76834400	0.79297600	-1.76028000
H	-1.12658500	3.38743000	0.30055600
H	0.57338200	3.70554500	-1.78183700
H	-1.16004900	3.87128500	-2.06303600
H	-0.34038400	2.37400300	-2.49924600
C	1.89866200	0.29007100	1.26598500
O	1.16792600	0.21184300	2.26328500
C	2.00481700	1.49810300	0.46573400
C	1.16128600	2.56585300	0.81506600
H	0.60507400	2.34287700	1.72268500
C	2.70005100	-0.93024600	0.88560800
C	2.90497700	-1.33305100	-0.43702200
C	3.18301600	-1.73595300	1.92066400
C	3.57865200	-2.52008900	-0.71741800
H	2.50225200	-0.74862900	-1.25882800
C	3.86772300	-2.91236500	1.64314300
H	2.98580600	-1.43232300	2.94400500
C	4.06367000	-3.30988900	0.32094900
H	3.72097200	-2.82674700	-1.74990100
H	4.23468100	-3.53048300	2.45650800
H	4.58874800	-4.23495600	0.10246200
C	1.45824900	4.00999000	0.66540400
C	0.76833500	4.89767500	1.50714600
C	2.40132700	4.55025900	-0.22163000
C	1.00218700	6.26535000	1.46926200
H	0.04180000	4.49462100	2.20870300
C	2.63596100	5.92224800	-0.26050800
H	2.95988800	3.91224200	-0.89495700
C	1.94066800	6.78602300	0.57945900
H	0.45636700	6.92460600	2.13683300
H	3.37077900	6.31522700	-0.95594300
H	2.12866700	7.85421100	0.54411000
C	2.85408800	1.55831300	-0.73717500

O	2.34002200	1.74172200	-1.84829400
C	4.33837000	1.44065100	-0.62922100
C	4.98268000	1.53668900	0.60657000
C	5.09015900	1.26257300	-1.79473200
C	6.36870600	1.44114600	0.67679700
H	4.39256800	1.69570100	1.50420700
C	6.47338400	1.16552500	-1.72242600
H	4.56770900	1.19753100	-2.74384700
C	7.11305600	1.25294700	-0.48531800
H	6.86827800	1.51830500	1.63689900
H	7.05590500	1.02021000	-2.62657500
H	8.19457100	1.17716300	-0.42894900
C	0.33948400	-3.42498200	0.34328600
C	0.78135900	-4.74466400	0.26440000
C	1.06748200	-5.45449400	1.42520800
C	0.88938500	-4.82516800	2.65734600
C	0.44029600	-3.50604400	2.72808000
C	0.16173100	-2.78837800	1.56580000
C	0.01203800	-2.89017000	-1.03823900
C	-0.02512300	-4.17007800	-1.93088200
C	0.84855900	-5.19241900	-1.17494400
H	1.40717900	-6.48497400	1.37516600
H	1.09906400	-5.37012100	3.57263500
H	0.31640700	-3.02573200	3.69318700
H	-0.15698200	-1.74973700	1.62591800
H	0.35126300	-3.96291300	-2.93362700
H	0.48352000	-6.20895500	-1.34638100
H	0.73645300	-2.16286500	-1.40668500
H	1.88099500	-5.13975100	-1.54257900
C	-2.39682400	-3.04276700	-0.77511400
C	-1.62128100	-0.97396100	-0.68622800
N	-3.39863400	-2.37149200	-0.31845400
N	-1.30243500	-2.25389400	-1.03657900
N	-2.92029100	-1.07065700	-0.25907300
C	-2.24847300	-4.50601200	-1.05984500
H	-1.89908800	-5.03321300	-0.16202500
H	-3.20574500	-4.92803200	-1.36837500
C	-3.85364600	-0.02731600	-0.07303700
C	-4.27870200	0.76395100	-1.14661300
C	-4.39856400	0.21019700	1.19192800
C	-5.19788600	1.78797000	-0.96108100
C	-5.33558000	1.21494000	1.39631300
C	-5.71590300	1.99610800	0.31191300
H	-5.51126400	2.39960600	-1.79801900

H	-5.74862400	1.38791400	2.38230100
Cl	-3.65626400	0.47142600	-2.73286100
Cl	-6.87244800	3.26802700	0.55350700
Cl	-3.86922300	-0.74038200	2.53664600
O	-1.35244400	-4.64271200	-2.14488500

TS5RS'

C	0.78611400	0.01508300	-1.24133600
O	-0.19616300	0.11798500	-2.19759400
C	1.37481300	-1.17601800	-0.82733500
C	1.11180000	-2.46501100	-1.29276800
H	1.99161500	-1.09659300	0.06401200
C	0.82314800	-2.78247500	-2.74267700
H	-0.71359200	-0.71616700	-2.23891400
H	1.68463900	-3.23740000	-0.78641900
H	0.02722600	-3.52447400	-2.86226600
H	1.73307600	-3.19367700	-3.19352800
H	0.53860900	-1.90440800	-3.32129000
C	-2.13062900	-1.11388900	0.91050700
O	-1.66015700	-1.13554500	2.05122700
C	-1.74055000	-2.02349400	-0.15580600
C	-0.66240400	-2.94498700	-0.12898000
H	-0.77927800	-3.73190800	-0.87358300
C	-3.14729100	-0.02698600	0.61792900
C	-3.30585100	0.57956000	-0.63132900
C	-3.87567300	0.46996000	1.70296000
C	-4.18252500	1.65069800	-0.79340600
H	-2.71905600	0.25182900	-1.48400500
C	-4.75374600	1.53402600	1.54392000
H	-3.71278500	0.01921400	2.67639200
C	-4.90933000	2.12968400	0.29233800
H	-4.29118100	2.11255300	-1.77096300
H	-5.30826700	1.91029000	2.39803000
H	-5.59205400	2.96497100	0.16649000
C	0.03485200	-3.45457600	1.08780000
C	0.10543700	-4.84285500	1.25023300
C	0.68971700	-2.64519900	2.02536200
C	0.78340800	-5.41067000	2.32682800
H	-0.38243300	-5.48741100	0.52337900
C	1.38162800	-3.20968200	3.08851200
H	0.64374700	-1.56820700	1.92218200
C	1.42748000	-4.59478200	3.24970000
H	0.81294900	-6.49030000	2.43558500
H	1.88518400	-2.56238500	3.80019800

H	1.96361800	-5.03158400	4.08635000
C	-2.53331300	-2.09206800	-1.39364100
O	-1.98147500	-2.02450500	-2.50069000
C	-4.01017800	-2.33215700	-1.34256500
C	-4.63388200	-2.83554500	-0.19838900
C	-4.76750400	-2.08182700	-2.49058600
C	-6.00534400	-3.07145600	-0.19955600
H	-4.04094900	-3.05249900	0.68505400
C	-6.13687600	-2.31229300	-2.48888600
H	-4.26067600	-1.70112900	-3.37157100
C	-6.75744700	-2.80667400	-1.34140000
H	-6.48599400	-3.46582200	0.68978300
H	-6.72334300	-2.10637800	-3.37860300
H	-7.82771100	-2.98827100	-1.33941400
C	-1.19904300	2.76880100	0.79364200
C	-1.95880200	3.90487400	1.06451400
C	-2.39185300	4.15798200	2.36163900
C	-2.04660700	3.26134600	3.37281000
C	-1.28316500	2.12687200	3.09369700
C	-0.84725800	1.87316100	1.79531300
C	-0.78639100	2.73742100	-0.66478200
C	-1.08901000	4.18434100	-1.16749900
C	-2.15966300	4.71700500	-0.19133100
H	-2.97804200	5.04416500	2.58713200
H	-2.37526900	3.44897400	4.39036100
H	-1.03745900	1.42587400	3.88429700
H	-0.27017900	0.97835800	1.57354900
H	-1.43788600	4.17608600	-2.20094200
H	-2.04390100	5.79540600	-0.05021800
H	-1.32089900	1.98908400	-1.25002600
H	-3.15956500	4.53715300	-0.60490700
C	1.51909600	3.39222700	-0.27443900
C	1.27430200	1.25153300	-0.76827600
N	2.66621000	2.88518600	0.02630800
N	0.64379100	2.46078200	-0.77856300
N	2.51953900	1.54189900	-0.28063300
C	1.00744900	4.79511300	-0.15427800
H	0.55895500	4.94670200	0.83673300
H	1.82157200	5.50784000	-0.28928900
C	3.67768200	0.73333000	-0.29314600
C	4.36019100	0.47908300	-1.48615700
C	4.18449600	0.20793800	0.89825800
C	5.51513300	-0.29234900	-1.49894400
C	5.34468100	-0.55427600	0.91308900

C	5.99281600	-0.79389500	-0.29339400
H	6.03365300	-0.48816000	-2.42936200
H	5.72651300	-0.95816100	1.84241100
Cl	3.75701500	1.13047600	-2.96829700
Cl	7.44034000	-1.74967600	-0.29410500
Cl	3.32260700	0.48131600	2.37441800
O	0.07699300	5.00258400	-1.19789000

TS5SR

C	3.89386400	-1.60990500	0.11741700
C	5.07492800	-1.33729500	-0.56916500
C	6.23662000	-2.04434700	-0.26698800
C	6.19187900	-3.02551600	0.71988000
C	5.00290100	-3.29564200	1.40221800
C	3.84153700	-2.58582500	1.10907100
C	2.77393200	-0.71051800	-0.35218300
C	3.36503600	0.05668400	-1.59570500
C	4.88238600	-0.24747700	-1.59089300
H	7.16153800	-1.83795700	-0.79791800
H	7.08874300	-3.58718300	0.96177400
H	4.98606100	-4.06190600	2.17070000
H	2.91509700	-2.77002800	1.64365500
H	3.15643400	1.12189300	-1.47839700
H	5.20336100	-0.54450400	-2.59514500
H	2.47948000	0.00665200	0.40861600
H	5.44489000	0.65179400	-1.32177300
C	1.35079700	-1.90225600	-1.97314800
C	0.38765700	-1.52274200	-0.02736900
N	0.13725600	-2.31061600	-2.15460900
N	1.56049100	-1.43718700	-0.70406700
N	-0.45844700	-2.09633800	-0.92869800
C	2.44327500	-1.66423100	-2.95943400
H	3.30789000	-2.31225400	-2.75595300
H	2.08372700	-1.84090000	-3.97270400
C	-1.78318400	-2.54137300	-0.72973800
C	-2.84629300	-1.89179200	-1.36645700
C	-2.05818400	-3.64462000	0.08446100
C	-4.15710200	-2.31227400	-1.18487100
C	-3.36273300	-4.07390900	0.28936300
C	-4.39514000	-3.39787000	-0.35053200
H	-4.97216500	-1.79804300	-1.67880200
H	-3.56586800	-4.92486300	0.92756100
Cl	-2.52997300	-0.52087600	-2.37520000
Cl	-6.02936300	-3.92951900	-0.10488000

Cl	-0.76171100	-4.49738900	0.84544900
O	2.76723000	-0.29373000	-2.83585600
C	0.14041300	-1.12156300	1.31349100
O	1.23936400	-1.13722800	2.13135600
C	-1.12677500	-0.72365600	1.70656900
C	-1.49647700	-0.03805100	2.86487400
H	-1.88016700	-0.73785400	0.92338700
C	-0.80116000	-0.12301600	4.20228600
H	1.31947300	-0.24703600	2.56754000
H	-2.56030100	0.17247400	2.93188200
H	-0.46402900	0.85751000	4.55590500
H	-1.49853600	-0.52330100	4.94503500
H	0.07173700	-0.77398300	4.17636500
C	-0.05674600	2.09800200	-0.34678400
O	0.59680600	1.31587900	-1.03240500
C	0.00731300	2.04601700	1.13939000
C	-1.10517700	1.97992000	2.01290400
H	-0.87159600	2.24596900	3.04207800
C	-0.86786100	3.15351600	-1.04257000
C	-1.27426700	4.32233800	-0.39486000
C	-1.19489200	2.95784700	-2.38670300
C	-2.02466500	5.27352100	-1.07791700
H	-1.00734700	4.47478100	0.64685000
C	-1.95361800	3.90318800	-3.06611900
H	-0.84243000	2.05527000	-2.87644000
C	-2.37295800	5.06019700	-2.40995600
H	-2.34095000	6.17896400	-0.57022600
H	-2.21672000	3.74278800	-4.10688600
H	-2.96634200	5.79905500	-2.93956500
C	-2.49542400	2.27082100	1.59820800
C	-3.28702200	3.11345500	2.38735000
C	-3.06162100	1.72293100	0.43957200
C	-4.58809900	3.43178700	2.00759800
H	-2.86876600	3.53471400	3.29774500
C	-4.35898200	2.03720900	0.05886700
H	-2.46678000	1.06217800	-0.18346700
C	-5.12796600	2.89966700	0.83965200
H	-5.18141300	4.09762300	2.62654400
H	-4.76702500	1.61096500	-0.85299300
H	-6.14129300	3.15020000	0.54295500
C	1.29871900	1.90000300	1.75080800
O	1.42748100	1.38203500	2.88752200
C	2.55258200	2.40925400	1.09088700
C	2.56204300	3.44801700	0.15588700

C	3.76888100	1.83497700	1.47905700
C	3.76018800	3.87484100	-0.41036300
H	1.63409100	3.93717500	-0.12619900
C	4.96484000	2.25202700	0.90647400
H	3.75355800	1.04747900	2.22729200
C	4.96223100	3.27226400	-0.04490000
H	3.75458400	4.68367000	-1.13390600
H	5.89793300	1.78215400	1.20308000
H	5.89472200	3.60453900	-0.49094500

TS5SS'

C	0.78082700	-3.43585300	0.76977200
C	1.61294800	-4.41375400	0.23028900
C	2.20422900	-5.35644700	1.06659800
C	1.94494400	-5.30053600	2.43500000
C	1.11294100	-4.31198900	2.96654400
C	0.52410700	-3.36254600	2.13428000
C	0.29763900	-2.50031400	-0.30954800
C	0.69795800	-3.19538400	-1.65824800
C	1.76227600	-4.24050800	-1.26077700
H	2.85605700	-6.12448500	0.66036400
H	2.39515800	-6.03334300	3.09741700
H	0.92787700	-4.28238100	4.03537200
H	-0.11049200	-2.57435900	2.52974900
H	1.08718000	-2.43957900	-2.34431700
H	1.60792900	-5.16451800	-1.82615900
H	0.78595900	-1.53080800	-0.23177500
H	2.76223300	-3.86237900	-1.50251100
C	-2.03509300	-3.00063900	-0.92740400
C	-1.71309100	-1.02080000	-0.00819400
N	-3.17876100	-2.41326100	-1.07320300
N	-1.12378500	-2.21543500	-0.27164500
N	-2.98561200	-1.17848100	-0.47586100
C	-1.48099900	-4.23308600	-1.55874900
H	-1.16623600	-4.95767400	-0.79570500
H	-2.21557100	-4.68974500	-2.22108800
C	-4.10692400	-0.37569100	-0.17230100
C	-4.77406200	0.32479200	-1.18100000
C	-4.59911200	-0.30098300	1.13562800
C	-5.89928300	1.09013800	-0.90298700
C	-5.71076500	0.47286800	1.44004400
C	-6.34742900	1.15669400	0.41041200
H	-6.40614900	1.62804600	-1.69442200
H	-6.07830200	0.52871600	2.45706500

Cl	-4.17252700	0.25740900	-2.80093100
Cl	-7.74410100	2.11967900	0.77695200
Cl	-3.82405000	-1.19354500	2.39863400
O	-0.39535400	-3.79092300	-2.35442100
C	-1.13787400	0.10727300	0.60547300
O	-0.20829700	-0.17710200	1.58364900
C	-1.52125900	1.37614000	0.18088200
C	-1.03713500	2.60625100	0.60977400
H	-2.14043900	1.37628600	-0.71576000
C	-0.60470200	2.90033700	2.02246300
H	0.48764400	0.51266800	1.61014100
H	-1.43284000	3.46230500	0.07099900
H	0.34401500	3.44569300	2.06959200
H	-1.36192400	3.53287900	2.49928700
H	-0.50504600	1.99723900	2.62416600
C	1.85276900	0.40524500	-1.36089900
O	1.13034300	0.27553900	-2.35598600
C	1.75774700	1.51798500	-0.42937200
C	0.84860600	2.55131200	-0.71020300
H	0.27708000	2.34468800	-1.61350700
C	2.94191500	-0.62576900	-1.14375000
C	3.22431000	-1.20559100	0.09804300
C	3.67717500	-1.02757700	-2.26356100
C	4.24245100	-2.14779000	0.22277500
H	2.63272300	-0.94497400	0.97321900
C	4.71442700	-1.94545700	-2.13437900
H	3.42745100	-0.59760300	-3.22867700
C	5.00261100	-2.50411100	-0.88858400
H	4.43175100	-2.60585900	1.18850700
H	5.29608000	-2.23023900	-3.00551600
H	5.80689700	-3.22614000	-0.78833900
C	1.08377800	3.99573400	-0.48849700
C	0.41298900	4.89390100	-1.33561200
C	1.95588500	4.53020800	0.47210700
C	0.60327400	6.26483400	-1.23589600
H	-0.26393000	4.49597100	-2.08772600
C	2.14361700	5.90622900	0.57456800
H	2.49509100	3.88435700	1.15472100
C	1.47279000	6.77962100	-0.27501200
H	0.07633900	6.93257300	-1.91024800
H	2.82466900	6.29416500	1.32534000
H	1.62606100	7.85069600	-0.19190800
C	2.59903900	1.55525100	0.79043600
O	2.06145400	1.48413800	1.89924900

C	4.08088100	1.71744100	0.70080200
C	4.69363100	2.10273900	-0.49380300
C	4.85459200	1.50842500	1.84616200
C	6.07410400	2.26611000	-0.54452500
H	4.08162300	2.28098400	-1.37342000
C	6.23280100	1.66901400	1.79274800
H	4.35436300	1.21497600	2.76354000
C	6.84302900	2.04639800	0.59606100
H	6.54977000	2.56762100	-1.47197400
H	6.83450900	1.49849400	2.67972700
H	7.92054700	2.17182300	0.55438500

M5RR

C	1.18253800	3.19105600	0.11439700
C	2.09455500	3.88783400	0.90390400
C	2.73519200	5.00987700	0.38761500
C	2.44466500	5.41181900	-0.91569000
C	1.53531700	4.69958700	-1.70109500
C	0.89507500	3.57216100	-1.19048800
C	0.65198300	1.99614400	0.86528800
C	1.09645200	2.21851400	2.34648100
C	2.26619200	3.21780800	2.24546500
H	3.45002400	5.56420000	0.98845300
H	2.93393800	6.28862300	-1.32804100
H	1.33039600	5.02395800	-2.71599800
H	0.20116400	2.99275000	-1.79425400
H	1.38639400	1.25586400	2.77332600
H	2.25129000	3.90806700	3.09368600
H	1.04413800	1.05408700	0.49153900
H	3.21677600	2.67046400	2.26840800
C	-1.62494600	2.64300000	1.57245600
C	-1.54638400	1.02056900	0.11258400
N	-2.87020000	2.30460900	1.40189400
N	-0.79685500	1.88931800	0.78963100
N	-2.80538500	1.29681300	0.47568400
C	-0.93676600	3.51813200	2.57193100
H	-0.50151700	4.39763200	2.07896700
H	-1.63657900	3.84015700	3.34263500
C	-3.99379700	0.72966900	-0.05698700
C	-4.74265500	-0.17712800	0.69442000
C	-4.43313600	1.09990000	-1.32988800
C	-5.92064200	-0.71069700	0.18888500
C	-5.60496600	0.57257100	-1.85452000
C	-6.33469300	-0.32415200	-1.08132000

H	-6.49800000	-1.41591900	0.77374000
H	-5.94111700	0.85983700	-2.84296100
Cl	-4.18546600	-0.65963900	2.25695700
Cl	-7.80412600	-0.98071400	-1.72121000
Cl	-3.50723700	2.22045000	-2.26601500
O	0.04296500	2.70153700	3.18441900
C	-1.04665600	-0.05218900	-0.75175100
O	-0.17988700	0.38762600	-1.68930600
C	-1.40361900	-1.30588100	-0.44682400
C	-0.83061400	-2.50059000	-1.13270300
H	-2.09844700	-1.44847000	0.37789800
C	-1.82665400	-3.66185800	-1.15523600
H	0.36624700	-0.35321000	-2.08401400
H	-0.61899700	-2.21179600	-2.16831400
H	-2.72350400	-3.39275600	-1.72068300
H	-1.37501600	-4.54023600	-1.62610300
H	-2.12609600	-3.94671900	-0.14263400
C	1.93827200	-1.11543900	0.68756300
O	1.22308700	-1.09489900	1.71977600
C	1.66867500	-1.86889700	-0.47656600
C	0.56897400	-2.93204800	-0.57041500
H	0.91837800	-3.60867400	-1.36292100
C	3.13315000	-0.17191800	0.72167900
C	3.38119100	0.80248900	-0.24969700
C	3.97787000	-0.23501800	1.83550000
C	4.47233000	1.66118400	-0.14088300
H	2.70878300	0.90167800	-1.10010400
C	5.08427500	0.60306600	1.93571500
H	3.75874700	-0.96193000	2.61213300
C	5.33802900	1.55210800	0.94372800
H	4.63634100	2.41756000	-0.90266300
H	5.74831700	0.52228100	2.79119300
H	6.19799800	2.20988800	1.02433100
C	0.49933000	-3.81561900	0.66837500
C	1.21148300	-5.01727000	0.66129500
C	-0.26222900	-3.51130900	1.80209200
C	1.16905000	-5.89508400	1.74270400
H	1.81131400	-5.26818300	-0.21079000
C	-0.32158600	-4.39025500	2.87821900
H	-0.77897700	-2.56033100	1.85452100
C	0.39342700	-5.58668300	2.85490300
H	1.73500100	-6.82115100	1.70960600
H	-0.92026700	-4.13327800	3.74703600
H	0.34809300	-6.26824800	3.69871800

C	2.28855700	-1.58082500	-1.75031900
O	1.56539700	-1.38145800	-2.75927500
C	3.77172600	-1.59054500	-1.96111700
C	4.62754800	-2.23286400	-1.06360100
C	4.29965400	-0.97430900	-3.09827900
C	6.00102000	-2.22581100	-1.28196700
H	4.20030800	-2.72660100	-0.19572700
C	5.67166500	-0.96902600	-3.31816000
H	3.61399600	-0.49657800	-3.79076400
C	6.52452200	-1.59012800	-2.40602200
H	6.66387000	-2.71965200	-0.57847900
H	6.08042200	-0.48063400	-4.19736300
H	7.59701700	-1.58362700	-2.57520400

M5RS

C	-0.57448600	-3.20740000	-0.37714500
C	-1.34010000	-4.18193200	0.25808900
C	-1.82305700	-5.26340900	-0.47243900
C	-1.52935500	-5.34263000	-1.83274200
C	-0.77174500	-4.35156000	-2.46242700
C	-0.28666600	-3.26626300	-1.73627200
C	-0.18133400	-2.12209100	0.59569400
C	-0.58787100	-2.68269700	2.00638900
C	-1.57355300	-3.83076300	1.70525700
H	-2.42369700	-6.03023000	0.00771200
H	-1.89761400	-6.18301800	-2.41279100
H	-0.56407600	-4.42664800	-3.52468700
H	0.28518100	-2.47303000	-2.21125200
H	-1.04006900	-1.88519700	2.60042800
H	-1.40541800	-4.66106700	2.39757800
H	-0.66797300	-1.16429600	0.38479400
H	-2.60368500	-3.48033600	1.84311700
C	2.16189400	-2.66666700	1.20223400
C	1.91711300	-0.82347900	0.05810600
N	3.36759300	-2.18713300	1.10455200
N	1.25637100	-1.86706100	0.56191700
N	3.19780200	-1.03845500	0.37478300
C	1.57299100	-3.75163100	2.04677200
H	1.21105400	-4.58140800	1.42540500
H	2.30858700	-4.12170800	2.76010600
C	4.31101100	-0.23803600	0.00471900
C	4.98656100	0.51450300	0.96742800
C	4.74652500	-0.20907900	-1.32243400
C	6.09093100	1.28083800	0.61979700

C	5.84377500	0.55797000	-1.68962800
C	6.50383000	1.28923500	-0.70801800
H	6.61137800	1.86269200	1.37032900
H	6.17582500	0.58020000	-2.72012800
Cl	4.43067500	0.51500600	2.60378400
Cl	7.87917300	2.24212900	-1.15370300
Cl	3.91003500	-1.12624800	-2.52513600
O	0.53105000	-3.12665700	2.77366500
C	1.27033700	0.33236700	-0.57974200
O	0.50949600	-0.00852600	-1.62211700
C	1.38085200	1.49834200	0.07339900
C	0.50737400	2.69357900	-0.15638900
H	2.03560200	1.52251600	0.94408400
C	1.22924500	3.95850600	0.31728200
H	-0.23692900	0.70561400	-1.83361100
H	0.27572800	2.78339000	-1.22183900
H	2.20177900	4.05501500	-0.17416100
H	0.64256000	4.85303400	0.10164500
H	1.39541200	3.91904900	1.40037300
C	-2.31722800	0.56312800	1.28323000
O	-2.01697400	0.74693700	2.48073700
C	-1.74538000	1.32360500	0.21238900
C	-0.80951800	2.45983200	0.64492200
H	-0.50823500	2.21580900	1.66948000
C	-3.24773700	-0.60920200	1.01262400
C	-3.23708500	-1.39603700	-0.14358500
C	-4.14639300	-0.93769300	2.03430500
C	-4.13101000	-2.45400300	-0.29466400
H	-2.51967000	-1.19705200	-0.93527900
C	-5.04230800	-1.99048900	1.88711000
H	-4.12277700	-0.34145100	2.94014900
C	-5.04093400	-2.75035500	0.71618400
H	-4.09851200	-3.05528500	-1.19841000
H	-5.74407700	-2.21941400	2.68341100
H	-5.74056600	-3.57206900	0.59763400
C	-1.66858700	3.71383500	0.72387700
C	-2.15848900	4.14350600	1.95854900
C	-2.05582800	4.40595200	-0.43113300
C	-3.00885300	5.24530500	2.04346100
H	-1.88835000	3.58400600	2.84993900
C	-2.90053700	5.50749200	-0.34697200
H	-1.70524900	4.06326300	-1.40242700
C	-3.37901400	5.93344800	0.89208000
H	-3.38290800	5.56457300	3.01175400

H	-3.19163800	6.03340100	-1.25129600
H	-4.03903000	6.79294300	0.95554100
C	-2.20334400	1.31268200	-1.13472800
O	-1.40766900	1.47544800	-2.11587200
C	-3.65334500	1.22921400	-1.48778900
C	-4.63530400	1.71410900	-0.62042400
C	-4.02397000	0.71774600	-2.73478900
C	-5.97786500	1.64673900	-0.98080500
H	-4.33487500	2.15484800	0.32647900
C	-5.36440000	0.64164100	-3.08963500
H	-3.24356300	0.37257700	-3.40582300
C	-6.34397500	1.10171900	-2.20892000
H	-6.73775500	2.02520800	-0.30471500
H	-5.65075700	0.22630300	-4.05097000
H	-7.39226700	1.04432500	-2.48598200

M5SR'

C	-1.12327700	0.20935200	-0.78566400
O	-0.37779800	0.16097600	-1.88269700
C	-1.25385500	1.17434400	0.14044100
C	-0.48225500	2.46083500	0.16740800
H	-1.90161100	0.96733500	0.99195900
C	-1.29206500	3.51134000	0.93479500
H	0.32586600	0.98550100	-1.95621400
H	-0.31858800	2.80733400	-0.85703300
H	-2.29653600	3.60747200	0.51115000
H	-0.80644600	4.48819700	0.90075200
H	-1.39117900	3.22208800	1.98819300
C	2.63537300	0.42191800	1.02485100
O	2.59500200	0.55321900	2.25760100
C	1.89133300	1.28580400	0.13579300
C	0.89795800	2.21139600	0.84533100
H	0.68426500	1.74167400	1.81361500
C	3.33732100	-0.82116400	0.49595100
C	3.10542600	-1.38614600	-0.76409800
C	4.17473600	-1.50082200	1.38284400
C	3.72224000	-2.57653200	-1.13681900
H	2.43015600	-0.89920500	-1.46013000
C	4.79201000	-2.69272500	1.01656100
H	4.31318200	-1.07584500	2.37115000
C	4.57118200	-3.23415400	-0.24751300
H	3.53958800	-2.99167200	-2.12461600
H	5.44361700	-3.20248500	1.71995000
H	5.05455800	-4.16241900	-0.53831700

C	1.61660000	3.51870800	1.14844000
C	2.00068500	3.82850700	2.45303200
C	1.93582500	4.41732900	0.12195400
C	2.67577100	5.01556300	2.73511300
H	1.78909100	3.11495900	3.24440700
C	2.60512200	5.60330200	0.40236000
H	1.66565700	4.17389300	-0.90360300
C	2.97557700	5.90922700	1.71222400
H	2.97016300	5.23872100	3.75645100
H	2.84360400	6.29028600	-0.40412400
H	3.49981200	6.83461900	1.92960400
C	2.22323100	1.50520400	-1.21050000
O	1.35662200	1.85332800	-2.09713000
C	3.63444100	1.43745600	-1.70036300
C	4.71433800	1.73452200	-0.86473200
C	3.86984800	1.13359400	-3.04544500
C	6.01526700	1.68297700	-1.35840500
H	4.52567200	2.02322900	0.16530100
C	5.16768700	1.07535000	-3.53552400
H	3.01630100	0.93782400	-3.68690100
C	6.24404900	1.34505300	-2.68936500
H	6.85011800	1.91630600	-0.70529800
H	5.34593800	0.82296500	-4.57635000
H	7.25914900	1.30263600	-3.07231900
C	0.58309000	-2.77781900	0.90318400
C	1.17244300	-4.01599900	1.14268400
C	1.73318500	-4.28624500	2.38737100
C	1.69814800	-3.29871800	3.36949700
C	1.11682900	-2.05493200	3.11535000
C	0.54536000	-1.78552300	1.87593900
C	0.07281800	-2.69020600	-0.51664800
C	0.20895700	-4.14884400	-1.08148200
C	1.12457000	-4.89225400	-0.08235300
H	2.19965000	-5.24685500	2.58517900
H	2.14340300	-3.49168300	4.34042600
H	1.14002400	-1.27699700	3.86981400
H	0.12582100	-0.80474300	1.66175100
H	0.63625000	-4.12200900	-2.08419000
H	0.72938600	-5.89551300	0.10761300
H	0.61652500	-1.96091600	-1.11984700
H	2.12750600	-5.00747700	-0.50637500
C	-2.34609600	-3.15408700	-0.24179600
C	-1.85660800	-1.04809200	-0.54923300
N	-3.48160000	-2.53867100	-0.09744200

N	-1.33560600	-2.27888300	-0.53244700
N	-3.15756900	-1.22127600	-0.28669400
C	-1.97820600	-4.60368500	-0.21455200
H	-1.56271200	-4.87177500	0.76724200
H	-2.85128500	-5.22344000	-0.41817200
C	-4.16810300	-0.22202600	-0.27309500
C	-4.60380300	0.35394300	-1.46850800
C	-4.73910700	0.17994800	0.93507200
C	-5.59380300	1.32684000	-1.46208100
C	-5.73646800	1.14480900	0.96017800
C	-6.14758500	1.70546600	-0.24418000
H	-5.92588800	1.77589000	-2.38984300
H	-6.17374200	1.45808600	1.90000700
Cl	-3.90088800	-0.14067500	-2.96666600
Cl	-7.38734200	2.91763300	-0.22587500
Cl	-4.17511100	-0.50595500	2.41869900
O	-1.04735200	-4.79603700	-1.25951800

M5SS

C	-0.83146200	0.01974200	0.95227200
O	-0.03014300	0.10256800	2.03864500
C	-1.23813600	-1.07196800	0.28795900
C	-0.91074700	-2.45622700	0.74342800
H	-1.85417000	-0.93097700	-0.59729000
C	-2.09210300	-3.39972900	0.49784700
H	0.43555700	-0.75697000	2.23507900
H	-0.76619200	-2.38998800	1.82855500
H	-2.97101300	-3.06841600	1.06049100
H	-1.83908800	-4.41386600	0.82099100
H	-2.35871500	-3.44762000	-0.56092900
C	1.90409700	-1.12211700	-0.68855600
O	1.24079800	-1.04264800	-1.74985600
C	1.63577000	-2.05503900	0.33977000
C	0.45875600	-3.01962400	0.24087800
H	0.66873800	-3.79709000	0.98707200
C	2.95893900	-0.04335900	-0.50339400
C	3.15121400	0.66257900	0.68747700
C	3.68261800	0.35193000	-1.63274000
C	4.05242100	1.72391900	0.75355900
H	2.57778700	0.39923400	1.57239000
C	4.58996500	1.40326100	-1.57105700
H	3.49658800	-0.16888900	-2.56694200
C	4.77571100	2.09748600	-0.37591800
H	4.18819100	2.25660600	1.69131400

H	5.14327200	1.69361400	-2.45918200
H	5.47789500	2.92468000	-0.32701800
C	0.41734400	-3.77278000	-1.08257400
C	1.13851700	-4.96512400	-1.17350700
C	-0.30715100	-3.35803000	-2.20392500
C	1.14080400	-5.72767000	-2.33973600
H	1.71479300	-5.29539300	-0.31186700
C	-0.32376400	-4.12181800	-3.36625500
H	-0.83384700	-2.41037900	-2.17273700
C	0.40093800	-5.31037700	-3.44087800
H	1.71388700	-6.64903500	-2.38172400
H	-0.89552800	-3.78142800	-4.22461500
H	0.39041900	-5.90206900	-4.35108900
C	2.26049100	-2.02298900	1.63350900
O	1.55623600	-2.04391800	2.67718000
C	3.75052800	-2.04323000	1.80510800
C	4.59741200	-2.45736400	0.77445700
C	4.29544000	-1.67982300	3.03941500
C	5.97527900	-2.47601600	0.96627000
H	4.16153700	-2.76476700	-0.17139400
C	5.67143300	-1.69995100	3.23212200
H	3.61770400	-1.37805200	3.83176800
C	6.51415400	-2.09407700	2.19286500
H	6.62892400	-2.79494200	0.16055700
H	6.09089500	-1.40764700	4.19002900
H	7.58951200	-2.10934900	2.34221300
C	1.17790200	2.93988200	-0.96518500
C	1.87621600	4.13124900	-1.14957900
C	2.37584500	4.45496100	-2.40613200
C	2.15770800	3.56967700	-3.46143900
C	1.46755300	2.37337500	-3.26207000
C	0.96879400	2.04129100	-2.00395600
C	0.69726600	2.82076000	0.46507300
C	0.93624400	4.24542600	1.07307000
C	1.98581300	4.89321800	0.14647600
H	2.91936100	5.38167800	-2.56450700
H	2.53731100	3.81121800	-4.44949000
H	1.33282100	1.67932200	-4.08502200
H	0.49666900	1.07329800	-1.84387600
H	1.28317400	4.17066400	2.10414000
H	1.79727100	5.96677000	0.05554600
H	1.20960000	2.04162200	1.02986200
H	2.98633700	4.76461800	0.57550800
C	-1.66176300	3.45598900	0.15841800

C	-1.36737600	1.32964500	0.56928200
N	-2.84851300	2.94157700	0.03848200
N	-0.73433000	2.50501500	0.49054200
N	-2.65083500	1.61346400	0.29361900
C	-1.17180000	4.86769300	0.09320100
H	-0.71048600	5.06942300	-0.88248400
H	-1.99610400	5.56207800	0.25522000
C	-3.76346100	0.72922900	0.35187700
C	-4.24991800	0.28978500	1.58536000
C	-4.37897500	0.30163600	-0.82487400
C	-5.33736000	-0.57063500	1.64780400
C	-5.47251100	-0.55260300	-0.78187700
C	-5.93561600	-0.97614700	0.45912500
H	-5.70925100	-0.91504100	2.60489200
H	-5.94400600	-0.88629700	-1.69792200
Cl	-3.47965700	0.80141300	3.04443600
Cl	-7.29728000	-2.04457600	0.52688500
Cl	-3.74357900	0.80529300	-2.35129800
O	-0.25858200	5.01656900	1.16224900

M5RR'

C	-1.14894700	0.27278600	-0.67097200
O	-0.41260200	0.26493300	-1.76985300
C	-1.28979600	1.17586500	0.31697500
C	-0.53427500	2.47097000	0.44706600
H	-1.95548700	0.89708100	1.13168800
C	-0.77844100	3.42403400	-0.73070300
H	0.34624200	1.06585100	-1.85555700
H	-0.96842200	2.97944500	1.31763900
H	-0.31464400	4.39311200	-0.53034200
H	-1.85620500	3.58346200	-0.83721700
H	-0.38440100	3.05014300	-1.67317800
C	2.66028100	0.40273900	1.05532500
O	2.62564600	0.51894600	2.28791900
C	1.91485600	1.28552600	0.17581600
C	0.93615700	2.19635100	0.92354400
H	0.79626400	1.68842800	1.88332000
C	3.36079200	-0.83769700	0.51389800
C	3.13504300	-1.39587300	-0.75067100
C	4.19701300	-1.52225500	1.39862600
C	3.75705700	-2.58199900	-1.12869300
H	2.46626000	-0.90652500	-1.45091600
C	4.81803400	-2.71062600	1.02747200
H	4.33276400	-1.10318900	2.38967800

C	4.60374600	-3.24408700	-0.24081400
H	3.58098600	-2.98968200	-2.12078600
H	5.46816000	-3.22302600	1.73027400
H	5.09061300	-4.16899900	-0.53632100
C	1.62463400	3.51270000	1.26435300
C	1.69471200	3.93985400	2.59113200
C	2.19636500	4.32101100	0.27404200
C	2.30792400	5.14586300	2.92677000
H	1.27865600	3.30596700	3.37027900
C	2.80612700	5.52686400	0.60402300
H	2.15655000	4.00139800	-0.76455100
C	2.86368600	5.94496400	1.93303600
H	2.35865900	5.45484900	3.96664100
H	3.24232000	6.14060800	-0.17835900
H	3.34589100	6.88298400	2.19019100
C	2.25566100	1.49099400	-1.16675200
O	1.39338700	1.83025600	-2.06173800
C	3.66809500	1.42220900	-1.65207000
C	4.74404700	1.72178900	-0.81213600
C	3.90985200	1.11762100	-2.99589600
C	6.04734200	1.67001400	-1.29932600
H	4.54990100	2.01253700	0.21629700
C	5.21009800	1.06044700	-3.47981200
H	3.05985400	0.92015500	-3.64147800
C	6.28245900	1.33102200	-2.62888900
H	6.87889700	1.90402600	-0.64230600
H	5.39322100	0.80776700	-4.51969500
H	7.29930300	1.28885200	-3.00713900
C	0.58095800	-2.76499000	0.89889800
C	1.17783700	-4.00967100	1.07936400
C	1.74173400	-4.33512800	2.30935000
C	1.70354300	-3.39534900	3.33671000
C	1.11653600	-2.14334300	3.14150200
C	0.54225900	-1.81869900	1.91675200
C	0.07354000	-2.61075600	-0.51624700
C	0.23737100	-4.03516800	-1.15901200
C	1.14004800	-4.82724500	-0.18561100
H	2.21366700	-5.30143600	2.46125500
H	2.15103000	-3.63178400	4.29696000
H	1.13582000	-1.40350200	3.93367200
H	0.11659900	-0.83206200	1.74792200
H	0.68595000	-3.94511500	-2.14862500
H	0.73930500	-5.83665700	-0.04576900
H	0.60587600	-1.83860100	-1.07449500

H	2.14727000	-4.92742400	-0.60360900
C	-2.34555200	-3.12581200	-0.31178700
C	-1.88090300	-1.00031400	-0.50198500
N	-3.49463300	-2.53459700	-0.17319000
N	-1.34110100	-2.22251900	-0.52565200
N	-3.18537400	-1.20458900	-0.28748900
C	-1.95609500	-4.56888000	-0.36124400
H	-1.54954600	-4.88786400	0.60892600
H	-2.81604700	-5.18884600	-0.61355000
C	-4.21127700	-0.22184000	-0.25588400
C	-4.60307200	0.42588100	-1.42987200
C	-4.84377500	0.09039300	0.94825000
C	-5.61421700	1.37669400	-1.40536600
C	-5.86446900	1.02997500	0.98970500
C	-6.23373000	1.66045500	-0.19338300
H	-5.91133600	1.88283100	-2.31539700
H	-6.35169800	1.27018000	1.92640000
Cl	-3.81855400	0.05273700	-2.92195500
Cl	-7.50164700	2.84238800	-0.15487300
Cl	-4.32679800	-0.67503200	2.41106800
O	-1.00706400	-4.68392700	-1.40164300

M5RS'

C	0.88808200	-0.11891200	-0.81848900
O	0.19717700	-0.08614500	-1.97174700
C	1.13757200	-1.11043800	0.05229900
C	0.80466500	-2.56166500	-0.13017900
H	1.69645100	-0.82929000	0.94196100
C	1.42912200	-3.06405400	-1.44518700
H	-0.38815800	-0.90168300	-2.14825500
H	1.30767800	-3.09392700	0.68154500
H	1.33097600	-4.15183700	-1.50737100
H	2.49317300	-2.81039400	-1.49936100
H	0.92004400	-2.63319100	-2.31148700
C	-1.99626500	-0.92817100	0.78260900
O	-1.36336800	-0.95513800	1.86231400
C	-1.76402600	-1.85782400	-0.26214000
C	-0.71583100	-2.94624700	-0.07986900
H	-0.85121400	-3.60123400	-0.94750500
C	-2.92684100	0.25572100	0.59412000
C	-3.05647200	0.96943400	-0.60095600
C	-3.59173000	0.73309800	1.72764500
C	-3.83976900	2.12030100	-0.66582500
H	-2.52247700	0.64254300	-1.48916000

C	-4.37709800	1.87836800	1.66854400
H	-3.44885300	0.20168500	2.66339900
C	-4.50248400	2.57913500	0.46951800
H	-3.92834500	2.65838200	-1.60622000
H	-4.88220800	2.23492500	2.56122600
H	-5.11029900	3.47811000	0.42313600
C	-1.07196700	-3.81930300	1.12146300
C	-2.03064500	-4.82184400	0.94628100
C	-0.49801600	-3.67185300	2.38599500
C	-2.39504400	-5.66568400	1.99170800
H	-2.49562800	-4.93872300	-0.03074500
C	-0.85353900	-4.51586800	3.43411000
H	0.20909000	-2.86715100	2.55613400
C	-1.80073600	-5.51894200	3.24231900
H	-3.13744800	-6.44090700	1.82731700
H	-0.39507600	-4.38253100	4.40963500
H	-2.07604500	-6.17612600	4.06141300
C	-2.31105400	-1.77621700	-1.57920700
O	-1.54761500	-1.88215000	-2.58377600
C	-3.77767100	-1.64577100	-1.84483200
C	-4.72642200	-1.98101700	-0.87581000
C	-4.20179100	-1.22006000	-3.10692500
C	-6.08366000	-1.85944400	-1.15624600
H	-4.38576400	-2.33998500	0.09074700
C	-5.55711200	-1.09932800	-3.38707600
H	-3.44680100	-0.98496400	-3.85054200
C	-6.50039600	-1.41486500	-2.40921300
H	-6.81752000	-2.11742300	-0.39919700
H	-5.88272700	-0.75986600	-4.36553800
H	-7.56001400	-1.32083300	-2.62677300
C	-0.81536400	3.01574400	0.92342900
C	-1.39380700	4.27084600	1.09644600
C	-1.82284100	4.66845200	2.35836900
C	-1.65847600	3.79074300	3.42879000
C	-1.09070200	2.52904100	3.24111300
C	-0.66192100	2.12448800	1.97887500
C	-0.38890800	2.81692400	-0.51445300
C	-0.54875900	4.23211200	-1.17074900
C	-1.48116000	5.00756600	-0.21567000
H	-2.27462200	5.64467100	2.50741900
H	-1.98556200	4.08889900	4.42003700
H	-0.99999800	1.84371900	4.07728700
H	-0.27918800	1.11631900	1.82785400
H	-0.96722700	4.14271000	-2.17353700

H	-1.17953300	6.05790500	-0.16428500
H	-0.96403900	2.05224600	-1.03678800
H	-2.50877600	4.97417400	-0.59534000
C	2.02216800	3.29450700	-0.31874000
C	1.54459900	1.17496100	-0.55848000
N	3.16539300	2.69290600	-0.17927500
N	1.01477600	2.40178000	-0.56348100
N	2.85175400	1.37073500	-0.32749900
C	1.64630200	4.74230200	-0.33555600
H	1.24854300	5.04557500	0.64244600
H	2.51322200	5.35600900	-0.57974100
C	3.88318500	0.39137500	-0.31320600
C	4.28178000	-0.23251900	-1.49772300
C	4.51377800	0.06071200	0.88672900
C	5.29767600	-1.17868800	-1.48747800
C	5.53878200	-0.87511900	0.91396100
C	5.91473400	-1.48237500	-0.27877400
H	5.60002400	-1.66629600	-2.40604100
H	6.02311500	-1.13104100	1.84801500
Cl	3.49223500	0.15476900	-2.98314900
Cl	7.18719700	-2.65979400	-0.25789200
Cl	3.98436200	0.79056300	2.36230200
O	0.69700600	4.89339800	-1.37186000

M5SR

C	-0.13321100	3.75517900	-0.06220000
C	0.48272400	4.82472100	0.58177600
C	0.32631800	6.11600500	0.08464600
C	-0.45004100	6.30742500	-1.05658400
C	-1.05584800	5.22464700	-1.70057500
C	-0.90046000	3.93029900	-1.20945100
C	0.20423400	2.45221200	0.62101000
C	0.93031500	2.86915700	1.94778600
C	1.31237800	4.35313100	1.74885700
H	0.80293400	6.95956300	0.57556200
H	-0.58269500	7.30886100	-1.45410200
H	-1.64613600	5.39535300	-2.59518600
H	-1.32943800	3.06426200	-1.70877200
H	1.79878300	2.22670900	2.09782600
H	1.13648000	4.91318200	2.67274800
H	0.83847200	1.80597900	0.01451900
H	2.37860200	4.43345900	1.50854000
C	-1.77567400	1.95614300	2.02187200
C	-1.54041100	0.64579800	0.28705300

N	-2.79469200	1.15369000	2.09567000
N	-0.99794900	1.68277400	0.92994900
N	-2.63721900	0.34425400	0.99732000
C	-1.23600000	2.97503900	2.97224900
H	-1.40122100	3.99072200	2.58702900
H	-1.71062000	2.87500300	3.94804000
C	-3.66877200	-0.55308300	0.61772800
C	-3.90185000	-1.72338300	1.34041700
C	-4.48855100	-0.24689200	-0.47244700
C	-4.93336600	-2.58368800	0.98690600
C	-5.51728900	-1.09905900	-0.84829200
C	-5.72564900	-2.25658100	-0.10732300
H	-5.10755900	-3.49188300	1.55030400
H	-6.14474500	-0.85870500	-1.69729800
Cl	-2.88077900	-2.12129900	2.67726200
Cl	-7.01625500	-3.32458900	-0.56016900
Cl	-4.22496000	1.20907500	-1.36675400
O	0.13827700	2.67590900	3.11746100
C	-0.99740100	-0.00260000	-0.93890100
O	-0.67604400	0.82441600	-1.88347100
C	-0.84860300	-1.34489100	-0.80789700
C	-0.15155500	-2.22307600	-1.80518500
H	-1.16420300	-1.79456900	0.13062100
C	-0.67952500	-2.04506900	-3.23580100
H	0.52932700	0.48402000	-2.71654500
H	-0.38359800	-3.25523400	-1.52274000
H	-0.21901900	-2.78486000	-3.89871800
H	-1.76297900	-2.19319500	-3.25507400
H	-0.46333300	-1.05244100	-3.62895000
C	2.33392200	-0.85555300	0.37677500
O	1.61676100	-0.20473700	1.12534000
C	2.03483700	-0.87764900	-1.09951800
C	1.43523900	-2.12434000	-1.76862300
H	1.75151000	-2.04961000	-2.81419900
C	3.48811300	-1.62116100	0.94691900
C	4.51924100	-2.09585400	0.13437800
C	3.53434300	-1.83797500	2.32656700
C	5.57720900	-2.80494200	0.69358100
H	4.48131400	-1.90939800	-0.93516700
C	4.58914700	-2.54896600	2.88415500
H	2.72797300	-1.44943700	2.94007400
C	5.60891700	-3.03698200	2.06679100
H	6.37285600	-3.17911500	0.05767800
H	4.61929000	-2.72693300	3.95434500

H	6.43115000	-3.59602400	2.50275200
C	2.02097700	-3.40599900	-1.20699800
C	2.98664500	-4.11764900	-1.91854500
C	1.62334600	-3.88983000	0.04368800
C	3.56757300	-5.26643100	-1.38433600
H	3.29884200	-3.75584400	-2.89529800
C	2.20611700	-5.02879300	0.58688800
H	0.86578500	-3.34777400	0.60863700
C	3.18649800	-5.71879500	-0.12494700
H	4.32143800	-5.80437600	-1.95113300
H	1.89982400	-5.37668200	1.56856400
H	3.64363700	-6.60742300	0.29854100
C	2.13842100	0.26311200	-1.82189000
O	1.50881700	0.35658900	-3.01884400
C	2.83652200	1.51070900	-1.40615600
C	3.92032700	1.53510900	-0.51905200
C	2.37304700	2.72363500	-1.93308100
C	4.49879100	2.74263100	-0.14218600
H	4.33215200	0.60723300	-0.13571500
C	2.94880800	3.93146700	-1.55352200
H	1.53617800	2.70287000	-2.62239300
C	4.01377600	3.94586600	-0.65500300
H	5.34272500	2.74258700	0.54051800
H	2.55515200	4.86194700	-1.95240700
H	4.47005800	4.88689300	-0.36199900

M5SS'

C	-0.27341200	3.73257000	-1.15968500
C	0.17678100	5.02492500	-0.90323100
C	0.13424200	5.98605300	-1.90916900
C	-0.36201200	5.62572600	-3.16012800
C	-0.79704400	4.32179400	-3.41077800
C	-0.75261100	3.35482700	-2.40970700
C	-0.13843700	2.86525300	0.07079500
C	0.21285700	3.87116100	1.22749800
C	0.69365500	5.15096800	0.50855700
H	0.47935100	6.99865800	-1.72274300
H	-0.40715600	6.36631600	-3.95237600
H	-1.16631300	4.05924700	-4.39664800
H	-1.05269900	2.32522700	-2.58503300
H	0.97823800	3.44231800	1.87642300
H	0.32671600	6.03500800	1.03840900
H	0.62054000	2.09428700	-0.06581000
H	1.78834900	5.19989900	0.51473000

C	-2.42987400	2.82242300	0.99637300
C	-1.77777100	0.91090300	0.15019700
N	-3.45262600	2.03966400	1.15818700
N	-1.39259800	2.17392800	0.38101200
N	-3.03530200	0.85229500	0.61434000
C	-2.14978900	4.20167500	1.49401000
H	-2.17803800	4.92874500	0.67139900
H	-2.87516700	4.48562400	2.25597600
C	-3.95616700	-0.22102200	0.48367600
C	-4.35768600	-0.94500100	1.60700000
C	-4.48980000	-0.54030200	-0.76742400
C	-5.27964100	-1.97718300	1.49338200
C	-5.40349800	-1.57619500	-0.90253700
C	-5.78751200	-2.27827400	0.23511300
H	-5.58419300	-2.53868900	2.36782900
H	-5.80962500	-1.82469600	-1.87522000
Cl	-3.67107400	-0.58063200	3.15140900
Cl	-6.93342900	-3.56925900	0.07855800
Cl	-4.00668800	0.35358900	-2.16471200
O	-0.87547000	4.13312400	2.10540800
C	-0.96105000	-0.11684400	-0.53580400
O	-0.22237900	0.38777900	-1.48455800
C	-1.07196900	-1.38506600	-0.07721600
C	-0.32655000	-2.56118400	-0.64554800
H	-1.69670900	-1.55826100	0.79495000
C	-0.41012100	-2.65687100	-2.17528800
H	0.93359800	-0.29133800	-1.79702400
H	-0.86001500	-3.45150200	-0.28524200
H	-0.01265300	-3.61845700	-2.50905700
H	-1.46278200	-2.60240300	-2.47045000
H	0.12976000	-1.86940100	-2.69545100
C	2.74875400	-1.58503200	1.48397800
O	2.72482500	-2.57483300	2.20923000
C	2.09853600	-1.59675500	0.15214100
C	1.07583100	-2.73191400	0.03545600
H	0.81925600	-2.95560900	1.07458000
C	3.35777800	-0.32488300	2.05848200
C	2.98241600	0.96068700	1.66413200
C	4.30173700	-0.47276800	3.07721500
C	3.56932500	2.07763600	2.25011500
H	2.23664800	1.07425500	0.88424600
C	4.88835000	0.64155400	3.66615400
H	4.56616200	-1.47758700	3.38996600
C	4.52642700	1.92124200	3.25037800

H	3.29160700	3.07453700	1.91864500
H	5.63137900	0.51353900	4.44686800
H	4.98793500	2.79316100	3.70313600
C	1.76772000	-3.98616800	-0.48483900
C	1.63994200	-5.18725500	0.21408000
C	2.51526800	-3.97797300	-1.66800300
C	2.23584900	-6.35651500	-0.25370900
H	1.08130000	-5.19786100	1.14671400
C	3.11026700	-5.14415800	-2.13916300
H	2.62010500	-3.05056200	-2.22597500
C	2.97268500	-6.33869800	-1.43390700
H	2.13216900	-7.27897700	0.30978400
H	3.68578100	-5.12008400	-3.05959000
H	3.44143600	-7.24688600	-1.79996100
C	2.58345500	-0.85377300	-0.89487600
O	1.91519400	-0.64038100	-2.02189600
C	3.95955100	-0.28923900	-0.93964000
C	5.05067600	-0.98685600	-0.41546700
C	4.17131700	0.94097300	-1.57124700
C	6.32719700	-0.43605000	-0.47106900
H	4.89465900	-1.96860000	0.02355500
C	5.44431000	1.49418800	-1.61961300
H	3.32104500	1.45335100	-2.01156900
C	6.52447500	0.80863300	-1.06322100
H	7.16957300	-0.98305900	-0.05985100
H	5.59920400	2.45814500	-2.09431300
H	7.52035400	1.23878100	-1.10525300

TS6RR

C	1.03404400	0.46391500	0.39923000
O	0.26972500	0.81900200	1.45225400
C	1.35357500	-0.75314700	-0.06287800
C	0.75213500	-2.00793100	0.47758000
H	1.99315200	-0.80906500	-0.94036600
C	1.76389100	-3.14829100	0.58404000
H	-0.16147300	0.04884900	1.89482700
H	0.38554200	-1.79235400	1.47703200
H	2.54372900	-2.89988500	1.31070200
H	1.25822200	-4.05990100	0.91855800
H	2.23863100	-3.35835400	-0.37942300
C	-1.79221000	-0.79151900	-1.91103000
O	-1.32994300	0.26550900	-2.32156700
C	-1.50880300	-1.27632400	-0.52156000
C	-0.51760100	-2.43352400	-0.34514500

H	-1.02210300	-3.17394200	0.28695500
C	-2.63696000	-1.66294900	-2.78133000
C	-3.36766100	-2.71810000	-2.22463400
C	-2.69526600	-1.41047700	-4.15423900
C	-4.15266700	-3.51838300	-3.04955800
H	-3.32130300	-2.89841000	-1.15064100
C	-3.47414500	-2.21711500	-4.97328800
H	-2.11562600	-0.58588700	-4.55748200
C	-4.20253800	-3.27105900	-4.41959600
H	-4.72390200	-4.33561700	-2.62174500
H	-3.51539200	-2.03042600	-6.04159000
H	-4.81182100	-3.90114600	-5.06031200
C	-0.12496900	-3.11717900	-1.64344000
C	-0.39896500	-4.47703900	-1.80489200
C	0.53007200	-2.44673700	-2.68525600
C	-0.03907100	-5.15099100	-2.96933100
H	-0.91428800	-5.00638200	-1.00756500
C	0.89260900	-3.11676400	-3.84982500
H	0.72882700	-1.38175800	-2.60470700
C	0.60986200	-4.47261000	-3.99675500
H	-0.26958100	-6.20666000	-3.07393000
H	1.39300200	-2.57544100	-4.64731100
H	0.88872100	-4.99459200	-4.90657400
C	-2.10179000	-0.68543400	0.53520300
O	-1.74479800	-1.01765200	1.79745500
C	-3.07223300	0.44936600	0.48482400
C	-4.01689100	0.63203700	-0.53206300
C	-3.02386200	1.38492500	1.52911500
C	-4.86408600	1.73760900	-0.52032100
H	-4.11941900	-0.10480300	-1.32171300
C	-3.86465200	2.49212800	1.53600800
H	-2.31080500	1.23315700	2.33297300
C	-4.78566100	2.67632800	0.50711200
H	-5.59894100	1.85601500	-1.31077300
H	-3.78321900	3.22315200	2.33560000
H	-5.44277400	3.54097600	0.51003800
C	-2.34962000	-2.32932200	2.39168500
O	-2.90393800	-3.05477800	1.56505000
O	-0.99792200	-3.02858600	2.91197600
C	-0.07791500	-2.42591600	3.62833100
O	0.05770300	-1.21792800	3.77785900
C	0.88289700	-3.41895600	4.26594300
C	2.09068300	-2.75545800	4.91298600
H	0.31177900	-3.99801600	5.00285400

H	1.18679800	-4.13791300	3.49616100
C	3.02114700	-3.77109300	5.56903200
H	1.74122000	-2.02425200	5.64823400
H	2.63164300	-2.18014200	4.15292800
H	3.88189200	-3.28362800	6.03451700
H	3.39900200	-4.49120900	4.83596300
H	2.49673500	-4.33666400	6.34595800
C	-3.05674900	-1.89704100	3.67225800
C	-4.47066000	-1.40639600	3.38012700
H	-3.10156700	-2.77965400	4.32171200
H	-2.46281200	-1.13020600	4.17893100
C	-5.21160600	-0.99853300	4.65024100
H	-5.00816600	-2.20493400	2.85969600
H	-4.42578100	-0.55810600	2.68818100
H	-6.23033000	-0.66592300	4.43197700
H	-4.69361200	-0.17944800	5.16010300
H	-5.27535400	-1.83593700	5.35316000
C	-1.08184100	3.86855100	0.39387700
C	-1.98915300	4.80586300	-0.09192900
C	-2.44479800	5.82620700	0.73780600
C	-1.96997900	5.89305200	2.04590500
C	-1.05471300	4.95109900	2.52336600
C	-0.60324800	3.92303700	1.69892900
C	-0.79575800	2.81892800	-0.65369900
C	-1.41844600	3.39029700	-1.97715000
C	-2.38850500	4.49698200	-1.51150900
H	-3.15808200	6.55857200	0.37120800
H	-2.31436500	6.68562700	2.70268000
H	-0.69892000	5.01652300	3.54626400
H	0.08723100	3.16936700	2.06724200
H	-1.91974100	2.58314800	-2.51038900
H	-2.32786000	5.35809700	-2.18415500
H	-1.23510600	1.84616500	-0.42116900
H	-3.41779100	4.12329700	-1.53905700
C	1.40842500	3.45553900	-1.58272800
C	1.44087100	1.63105600	-0.38756200
N	2.64643400	3.06122400	-1.63417400
N	0.64347700	2.60831600	-0.82673100
N	2.65332200	1.92502500	-0.87242900
C	0.67071200	4.52380900	-2.32311200
H	0.38178200	5.33822800	-1.64474500
H	1.28799200	4.92124500	-3.12841400
C	3.87195100	1.24596900	-0.60318400
C	4.45527900	0.43286400	-1.57577100

C	4.50246800	1.40637500	0.63251900
C	5.65586500	-0.21747200	-1.32641800
C	5.70096100	0.75997600	0.90242800
C	6.26118700	-0.04212400	-0.08613900
H	6.10283000	-0.85244200	-2.08126300
H	6.18475800	0.88290200	1.86341700
Cl	3.65897800	0.21122600	-3.09399500
Cl	7.75729600	-0.85240300	0.23746500
Cl	3.78086700	2.41149200	1.83898600
O	-0.44721000	3.87972200	-2.89905100

TS6RS

C	1.11145000	-0.01011700	-0.92571900
O	1.49172300	-1.31407000	-0.92448900
C	-0.07939300	0.44453000	-1.35166600
C	-1.16054700	-0.44178200	-1.89934700
H	-0.33409600	1.49559900	-1.25478300
C	-1.26500300	-0.22402500	-3.41429400
H	0.72640800	-1.88682800	-0.67338900
H	-0.91798800	-1.48940100	-1.71389600
H	-0.30207400	-0.42642800	-3.89164200
H	-2.00568100	-0.89947200	-3.84938500
H	-1.55348000	0.80782700	-3.64763400
C	-2.80191600	1.53710800	0.71563500
O	-2.33935800	2.58216900	0.27763900
C	-2.21476300	0.21364200	0.32997200
C	-2.48723100	-0.10231400	-1.14336400
H	-2.83215900	0.84164200	-1.59124100
C	-4.07825300	1.55428500	1.50302300
C	-4.63179300	0.37759900	2.01890600
C	-4.73067100	2.77605900	1.70006900
C	-5.82824600	0.42983000	2.72922900
H	-4.11273600	-0.56754800	1.88001100
C	-5.92641700	2.82288900	2.40387800
H	-4.28208200	3.67410900	1.28801400
C	-6.47635200	1.64774400	2.91863900
H	-6.25323200	-0.48312900	3.13292100
H	-6.43272800	3.77124300	2.55352200
H	-7.41126100	1.68395600	3.46947300
C	-3.56585600	-1.13842600	-1.41374100
C	-4.31050000	-1.09299000	-2.59928200
C	-3.81369800	-2.17348700	-0.51130600
C	-5.24128800	-2.08476200	-2.89872100
H	-4.16327300	-0.26861500	-3.29298600

C	-4.75306500	-3.16027800	-0.80381200
H	-3.27779500	-2.21120900	0.43013500
C	-5.45983900	-3.13015900	-2.00289700
H	-5.80398100	-2.03450500	-3.82605000
H	-4.92431400	-3.95419200	-0.08216000
H	-6.18905400	-3.90179200	-2.23144100
C	-1.32960300	-0.49350100	1.08766800
O	-0.79066400	-1.61868600	0.66129600
C	-0.69849800	0.08486300	2.32257000
C	-1.34643200	0.82747600	3.31260300
C	0.69280900	-0.07429500	2.42021900
C	-0.61616400	1.43470000	4.33324500
H	-2.42528500	0.92536500	3.30364600
C	1.42771000	0.55145800	3.42074100
H	1.17661600	-0.70627100	1.68056900
C	0.77105300	1.32022600	4.38153200
H	-1.13965900	2.00164700	5.09696100
H	2.51140800	0.45633500	3.44574600
H	1.33308500	1.81102500	5.16981300
C	-1.34983200	-3.07285700	1.75051700
O	-2.36006400	-2.72711300	2.32948200
O	-1.62412600	-4.01464500	0.65015600
C	-1.06369400	-4.11330200	-0.54945500
O	-0.02437800	-3.60143800	-0.92192800
C	-1.88243200	-4.99268500	-1.47420600
C	-2.07205400	-4.32409300	-2.83839900
H	-1.34012300	-5.93860900	-1.59880900
H	-2.84592300	-5.21256200	-1.00990900
C	-2.91786900	-5.18003400	-3.77427800
H	-1.08571900	-4.12858500	-3.27186000
H	-2.55868400	-3.35187500	-2.69451700
H	-3.04821400	-4.69371800	-4.74474100
H	-3.91248800	-5.34322700	-3.34719100
H	-2.45687300	-6.15881400	-3.94398000
C	-0.07826600	-3.37535900	2.51772800
C	1.22502100	-3.61576800	1.77110800
H	0.03241700	-2.53534400	3.21079200
H	-0.32369200	-4.25339200	3.13045600
C	2.40514700	-3.62909100	2.73984300
H	1.35201200	-2.83042400	1.02423100
H	1.18296400	-4.55557400	1.21181400
H	3.35965900	-3.74705400	2.21400400
H	2.32151300	-4.44663600	3.46287100
H	2.43373400	-2.69369400	3.31288500

C	4.78250000	-1.34125100	-0.41221500
C	5.98976600	-1.72147400	0.16707500
C	7.03121300	-2.18102000	-0.63456400
C	6.84051600	-2.24630500	-2.01233700
C	5.62330400	-1.86835000	-2.58497700
C	4.57766100	-1.41406100	-1.78650400
C	3.80065100	-0.87765900	0.63936200
C	4.63763800	-0.81927800	1.97304500
C	5.94911100	-1.57997300	1.66681300
H	7.97718500	-2.48078700	-0.19347400
H	7.64561800	-2.59782200	-2.64950400
H	5.49026300	-1.93542900	-3.65955200
H	3.61896300	-1.14004700	-2.21726900
H	4.07385200	-1.29672500	2.77462200
H	6.80182000	-1.03002500	2.07793500
H	2.96190100	-1.56241100	0.74305100
H	5.93675500	-2.56182600	2.15168000
C	3.97336600	1.58032300	0.60889500
C	2.15128000	0.85299900	-0.37041500
N	3.38967900	2.65525800	0.18434400
N	3.25479000	0.45290100	0.30208500
N	2.26678000	2.19154700	-0.43830200
C	5.20072400	1.42618400	1.44230600
H	6.05007700	1.09133900	0.83042000
H	5.44901500	2.37515400	1.91706400
C	1.35045800	3.13547100	-0.97336500
C	1.34261200	3.41760200	-2.33997900
C	0.45041000	3.77587500	-0.11989900
C	0.43824400	4.32857200	-2.86373600
C	-0.46322000	4.69088800	-0.62891900
C	-0.45228700	4.95224700	-1.99257200
H	0.42532500	4.54400300	-3.92486100
H	-1.18940100	5.15408200	0.02654300
Cl	2.44081700	2.58830100	-3.39094600
Cl	-1.59363400	6.08443900	-2.64075200
Cl	0.44623500	3.38381600	1.55590600
O	4.87559000	0.49478200	2.45219000
TS6SR			
C	0.74420400	0.73427300	-1.17522400
O	1.46604300	-0.21502700	-1.82757200
C	-0.54932200	1.03051200	-1.36017800
C	-1.50160000	0.29683400	-2.26329100
H	-1.01081200	1.74599600	-0.68750900

C	-0.98039500	0.00648900	-3.67358800
H	0.99558000	-1.07763100	-1.81491500
H	-2.38139800	0.94417000	-2.34611600
H	-0.19333400	-0.75122800	-3.66782900
H	-1.80209600	-0.37208700	-4.28706200
H	-0.58553200	0.91197100	-4.14268000
C	-3.30045900	0.06360700	0.30141000
O	-3.28646500	1.28399400	0.20665300
C	-2.09202900	-0.75301900	-0.04273300
C	-1.92893000	-1.02247300	-1.53958900
H	-1.10630700	-1.73662600	-1.62223600
C	-4.56897100	-0.66024700	0.63752700
C	-4.60559100	-2.05809900	0.67985600
C	-5.73019100	0.08065100	0.87164300
C	-5.80820900	-2.70657100	0.94252100
H	-3.69690500	-2.62325600	0.48081200
C	-6.92640900	-0.57097700	1.14231200
H	-5.67090300	1.16350400	0.82803800
C	-6.96536400	-1.96555300	1.17327600
H	-5.84289200	-3.79081400	0.96142400
H	-7.83053700	0.00134200	1.32457800
H	-7.90239700	-2.47516000	1.37629400
C	-3.14157100	-1.64576800	-2.21297900
C	-3.11819400	-3.00569600	-2.53377200
C	-4.29470800	-0.90858300	-2.50575700
C	-4.22773500	-3.61616800	-3.11420100
H	-2.22836000	-3.57635700	-2.28837400
C	-5.40524300	-1.51865500	-3.08119300
H	-4.34554700	0.14925800	-2.25721000
C	-5.37589200	-2.87731100	-3.38619200
H	-4.19440000	-4.67524300	-3.35215000
H	-6.29540100	-0.93237200	-3.28808400
H	-6.24155800	-3.35462000	-3.83520000
C	-1.07450900	-1.00333400	0.82137000
O	0.03452100	-1.64002900	0.44446700
C	-1.05145800	-0.49424600	2.23294900
C	-2.18195800	-0.34462100	3.04349700
C	0.19014900	-0.12690600	2.76863800
C	-2.07343900	0.19470800	4.32382100
H	-3.15424600	-0.67077900	2.69067100
C	0.30511900	0.41155100	4.04421400
H	1.07610500	-0.28742000	2.16766000
C	-0.83412800	0.58511300	4.82772800
H	-2.96476700	0.29636700	4.93534800

H	1.28681600	0.68447100	4.42076500
H	-0.75631100	1.00245900	5.82666200
C	-0.23528100	-3.42427300	0.42867400
O	-1.13861900	-3.72381900	-0.33165400
O	1.16600000	-3.70067900	0.02308100
C	1.58532500	-3.38437300	-1.18925800
O	0.92520900	-2.84392500	-2.06087100
C	3.05013700	-3.72471200	-1.37920400
C	3.60464700	-3.20564400	-2.69886100
H	3.60217500	-3.29438300	-0.53098600
H	3.16630000	-4.81125900	-1.28632600
C	5.11326200	-3.40111500	-2.79021600
H	3.35637400	-2.14226300	-2.78729100
H	3.09481500	-3.70822000	-3.52669400
H	5.51090400	-2.99816900	-3.72544200
H	5.37868600	-4.46234000	-2.74001900
H	5.61842600	-2.88694400	-1.96535500
C	-0.33879800	-3.73675000	1.91350900
C	0.85641400	-3.38510400	2.78772300
H	-1.23462500	-3.20704700	2.25904400
H	-0.56932600	-4.80695600	1.98020000
C	0.48454000	-3.31619900	4.26607300
H	1.22427500	-2.41225200	2.45785700
H	1.66194300	-4.11038600	2.62454700
H	1.34920800	-3.06170400	4.88618200
H	0.08540700	-4.27274600	4.61960700
H	-0.28158600	-2.54939800	4.42797900
C	4.42936900	-0.41977800	-0.38215000
C	5.53504800	-0.91133000	0.30905300
C	6.79452100	-0.90404500	-0.28585300
C	6.92663900	-0.39805100	-1.57612300
C	5.81416400	0.08810100	-2.26741900
C	4.55379000	0.08318700	-1.67615700
C	3.18178000	-0.48056900	0.47637800
C	3.70006400	-0.93362200	1.89838000
C	5.15717200	-1.40131700	1.68090100
H	7.65975400	-1.28126400	0.25118400
H	7.90258300	-0.38205000	-2.05069700
H	5.93290400	0.47451100	-3.27424800
H	3.68246800	0.45032900	-2.20982200
H	3.06954600	-1.74207700	2.26708900
H	5.79882800	-1.00639900	2.47524700
H	2.41253300	-1.17122900	0.12227000
H	5.21489800	-2.49335400	1.73747600

C	2.95393900	1.77892000	1.47731000
C	1.50621600	1.37813000	-0.11245400
N	2.24415300	2.86237300	1.41329600
N	2.54172700	0.84527700	0.56168500
N	1.35427300	2.60770700	0.40772300
C	3.98840700	1.35910600	2.46602800
H	4.98993900	1.35918300	2.01361900
H	3.97806500	2.02694500	3.32692300
C	0.47040000	3.63633500	-0.01775100
C	0.75309900	4.35948000	-1.17773300
C	-0.67238200	3.93735400	0.72895400
C	-0.09614400	5.36928900	-1.60654000
C	-1.53155300	4.94741400	0.31377600
C	-1.22897000	5.64762200	-0.84848800
H	0.12331700	5.92566900	-2.50905900
H	-2.42400500	5.17193900	0.88434300
Cl	2.17031400	3.98970100	-2.09916300
Cl	-2.29840700	6.90703800	-1.37378000
Cl	-1.03259600	3.02452200	2.14284700
O	3.60058700	0.07018400	2.89820900

TS6SS

C	1.00959900	-0.01987700	-0.92904800
O	1.34473600	-1.33617200	-0.92122500
C	-0.13013100	0.52847800	-1.38945600
C	-1.27472500	-0.14686900	-2.09610600
H	-0.29329500	1.58320500	-1.19335700
C	-0.94257800	-1.50887800	-2.69857600
H	0.58431200	-1.89416300	-0.62884900
H	-1.48769400	0.52822300	-2.93699300
H	-1.68159300	-1.77382300	-3.45703200
H	0.04266100	-1.48505500	-3.17224400
H	-0.94731600	-2.29314000	-1.94509400
C	-2.68104900	1.65875200	0.56632200
O	-2.02000400	2.63137800	0.23431100
C	-2.23024800	0.25730500	0.26299100
C	-2.58509400	-0.09897300	-1.17961200
H	-3.13737600	0.77261300	-1.55357400
C	-4.05550900	1.82664200	1.13299600
C	-4.74492700	0.74275800	1.68697100
C	-4.64897000	3.09250800	1.09786000
C	-6.02426000	0.93250800	2.20347900
H	-4.26619100	-0.23312000	1.73362000
C	-5.92840700	3.27393000	1.60460100

H	-4.09026600	3.91568400	0.66389900
C	-6.61589800	2.19207200	2.15759600
H	-6.55689100	0.09512600	2.64165100
H	-6.39389800	4.25379400	1.57092800
H	-7.61558900	2.33427100	2.55641300
C	-3.52728000	-1.26934000	-1.41741800
C	-4.12980700	-1.39183100	-2.67799900
C	-3.84750300	-2.20054800	-0.43252800
C	-5.00598200	-2.43403000	-2.95784200
H	-3.90811700	-0.65587200	-3.44950800
C	-4.73069800	-3.24604600	-0.71140500
H	-3.42078800	-2.12283600	0.56233700
C	-5.30945300	-3.37135300	-1.96932600
H	-5.45865400	-2.51112900	-3.94181000
H	-4.95785800	-3.96181500	0.07349500
H	-5.99606800	-4.18540400	-2.18176200
C	-1.39445000	-0.43113000	1.06527700
O	-0.92316000	-1.64581600	0.71757800
C	-0.75277000	0.18389400	2.26540500
C	-1.41416900	0.97511000	3.20567800
C	0.63158900	0.00389400	2.39873900
C	-0.69967000	1.60545800	4.22266400
H	-2.49237000	1.08501400	3.15777800
C	1.35069100	0.64346100	3.40205100
H	1.12633400	-0.66526100	1.69981100
C	0.68238300	1.45632000	4.31763100
H	-1.23038400	2.21144400	4.95031800
H	2.42968200	0.51661500	3.46470800
H	1.23186800	1.95684400	5.10858600
C	-1.40887500	-2.75763700	1.82987900
O	-2.43451900	-2.38916800	2.41145300
O	-1.72476500	-3.92183100	0.88310500
C	-1.09997500	-4.25194100	-0.22332700
O	-0.04344300	-3.79241500	-0.63727200
C	-1.85210000	-5.31185700	-1.00856500
C	-2.07288600	-4.86175900	-2.45466700
H	-1.25350200	-6.23098600	-0.99488800
H	-2.80606000	-5.51668300	-0.51663100
C	-2.87232000	-5.88441800	-3.25357800
H	-1.09699500	-4.68014100	-2.91785500
H	-2.60860700	-3.90539800	-2.45107800
H	-3.02864300	-5.54832800	-4.28238000
H	-3.85680400	-6.04021400	-2.80031200
H	-2.36087400	-6.85225200	-3.28704200

C	-0.20521900	-3.13929100	2.68768500
C	1.12135600	-3.50394700	2.03610500
H	-0.06690200	-2.29529300	3.37147200
H	-0.56024800	-3.97496400	3.30297900
C	2.24520200	-3.51815900	3.06878000
H	1.33491400	-2.79068800	1.23485000
H	1.05336300	-4.47744900	1.54256100
H	3.21659200	-3.74291400	2.61330500
H	2.06131800	-4.27143300	3.84148200
H	2.31089300	-2.54781800	3.57713400
C	4.67909400	-1.42326200	-0.51010500
C	5.88109000	-1.85565100	0.04297400
C	6.90822800	-2.29638900	-0.78698300
C	6.70829300	-2.29043800	-2.16527100
C	5.49663800	-1.85928100	-2.71140600
C	4.46535000	-1.42299100	-1.88448400
C	3.71440600	-0.98975800	0.56927400
C	4.56656400	-0.98928700	1.89356300
C	5.84809500	-1.78365500	1.54830700
H	7.85049700	-2.63650900	-0.36799700
H	7.50235300	-2.62709000	-2.82392400
H	5.35704600	-1.86955500	-3.78710500
H	3.51256600	-1.10259600	-2.29670800
H	3.99897700	-1.46626900	2.69175600
H	6.72130000	-1.28781000	1.98388000
H	2.87074500	-1.66948600	0.65715900
H	5.79624100	-2.78698700	1.98432400
C	3.94784400	1.45503600	0.59608400
C	2.08215500	0.80672100	-0.36153900
N	3.39479400	2.55530100	0.19977400
N	3.18474000	0.35913500	0.28337400
N	2.24536400	2.14323800	-0.40998200
C	5.18533000	1.24971300	1.40265900
H	6.01491100	0.90762800	0.76852800
H	5.46643900	2.18169100	1.89270200
C	1.39387600	3.15330300	-0.93566200
C	1.40094600	3.44387100	-2.30110100
C	0.58936900	3.89090800	-0.06645600
C	0.59392900	4.44942900	-2.80955800
C	-0.22214600	4.90542700	-0.55949900
C	-0.20696000	5.16573200	-1.92277000
H	0.59073300	4.67071400	-3.86949500
H	-0.86896500	5.45782400	0.11010500
Cl	2.40411400	2.51820300	-3.36553600

Cl	-1.22793000	6.42090400	-2.55118500
Cl	0.57985900	3.50826300	1.61047800
O	4.85282600	0.30589800	2.39781500

M6RR

C	-1.33798500	-0.11010300	-0.74516500
O	-1.94666000	0.64864700	-1.57831000
C	-0.02196800	-0.46097600	-0.66700000
C	0.92984700	-0.03746600	-1.74287500
H	0.33187000	-1.11333200	0.12102200
C	0.92151200	-1.07815100	-2.87560300
H	0.53659700	0.88155900	-2.18175700
H	-0.08594100	-1.11622200	-3.29831200
H	1.62650000	-0.81695500	-3.67421800
H	1.17856700	-2.07507400	-2.50401700
C	3.82045200	1.07760500	0.68733400
O	3.83724900	0.82554300	1.87472800
C	2.53816000	1.23587500	-0.09560900
C	2.38028200	0.24295100	-1.25226500
H	2.90063400	0.68833300	-2.11297100
C	5.08753500	1.20673900	-0.10102700
C	5.13876900	1.99452200	-1.25489400
C	6.22817000	0.53577000	0.34416800
C	6.33309300	2.10630000	-1.96149000
H	4.24944200	2.53158700	-1.58122500
C	7.41279500	0.63496400	-0.37446300
H	6.15886800	-0.06691400	1.24436600
C	7.46481400	1.42037700	-1.52664400
H	6.37861000	2.72640300	-2.85070400
H	8.29748300	0.10207100	-0.04105200
H	8.39246600	1.49858700	-2.08511400
C	3.11168800	-1.05717900	-0.94135600
C	3.97601200	-1.61331500	-1.88863800
C	2.93627600	-1.72851200	0.27370300
C	4.63477600	-2.81398900	-1.64358600
H	4.14159300	-1.08760200	-2.82591300
C	3.60109100	-2.92644700	0.52498000
H	2.31179100	-1.28665400	1.04724200
C	4.44584700	-3.47791400	-0.43419400
H	5.30427500	-3.22500500	-2.39263800
H	3.47014900	-3.42516600	1.48089200
H	4.96161600	-4.41174600	-0.23403600
C	1.74225800	2.26313100	0.22160100
O	0.53859100	2.47389500	-0.44422200

C	1.97249500	3.29687600	1.26299100
C	3.20723900	3.93103400	1.41990000
C	0.89625500	3.69084500	2.06547900
C	3.37114000	4.91844900	2.38577900
H	4.03767500	3.66463300	0.77287100
C	1.06294600	4.67481800	3.03319800
H	-0.06907300	3.21375500	1.92679900
C	2.30243400	5.28938000	3.19768100
H	4.33447000	5.40555000	2.49629600
H	0.22416500	4.96367500	3.65848200
H	2.43268900	6.06044800	3.95016900
C	0.59847600	3.25499600	-1.56026000
O	1.64051400	3.65806300	-2.01313300
C	-0.77296700	3.45501600	-2.14061000
C	-1.83528600	3.83530100	-1.10719700
H	-0.68969500	4.19641200	-2.93852300
H	-1.06620200	2.48530200	-2.56423900
C	-3.23098500	3.78420800	-1.72089100
H	-1.62653900	4.83030000	-0.69677100
H	-1.76325200	3.12404200	-0.27877400
H	-4.00499300	4.02729500	-0.98415900
H	-3.42545300	2.77821000	-2.10853900
H	-3.32679000	4.49483900	-2.54765400
C	-5.12581100	0.78274300	-0.76448900
C	-6.35904100	1.31159100	-0.39505200
C	-7.45953300	1.16208400	-1.23481600
C	-7.29722500	0.48010700	-2.43835200
C	-6.05129100	-0.03512700	-2.80648500
C	-4.94627100	0.11450800	-1.97269600
C	-4.07918400	1.06066900	0.29088600
C	-4.88494100	1.66194000	1.50128300
C	-6.27402900	2.02841000	0.92826700
H	-8.42743800	1.56863100	-0.95649400
H	-8.14695300	0.35285900	-3.10178400
H	-5.94339300	-0.54954400	-3.75592100
H	-3.95425700	-0.23676000	-2.24488600
H	-4.36451300	2.53573900	1.89587300
H	-7.05571900	1.73725300	1.63723800
H	-3.30783000	1.73342400	-0.08093800
H	-6.35368500	3.11178900	0.78861600
C	-3.97137500	-1.03510100	1.59589400
C	-2.23159400	-0.70721500	0.29694100
N	-3.24142300	-2.09110900	1.77914200
N	-3.39621900	-0.17113700	0.70363400

N	-2.16642000	-1.88091500	0.95324400
C	-5.21314200	-0.56991300	2.28141900
H	-6.08938800	-0.69177500	1.62959300
H	-5.36908000	-1.12700300	3.20493600
C	-1.18609000	-2.89891100	0.82651200
C	-0.28947600	-3.13978000	1.86837800
C	-1.11272600	-3.67439300	-0.33332600
C	0.66567600	-4.14259400	1.76586400
C	-0.14732100	-4.66302300	-0.46507200
C	0.72780200	-4.88456800	0.59273800
H	1.35293900	-4.32809600	2.58215900
H	-0.08681300	-5.25128500	-1.37221000
Cl	-0.33283300	-2.15259500	3.28532200
Cl	1.93168100	-6.12229700	0.44674200
Cl	-2.22211700	-3.39635700	-1.62889200
O	-4.98456300	0.78517700	2.61651100

M6RS

C	1.21042200	-0.01150700	-1.24828200
O	1.86828900	-0.99737800	-1.73081400
C	-0.08709800	0.35839900	-1.46854100
C	-0.96649500	-0.53742400	-2.29314800
H	-0.53459500	1.20762900	-0.96261700
C	-1.08647800	-0.08012700	-3.75210200
H	-0.46618400	-1.51011900	-2.28845200
H	-0.09973800	-0.07702800	-4.22154900
H	-1.74252400	-0.74771800	-4.32237000
H	-1.49564500	0.93465700	-3.80705000
C	-3.17506600	0.63225700	0.35456900
O	-2.77786400	1.77447000	0.20792900
C	-2.36420000	-0.52914800	-0.15039500
C	-2.38934700	-0.67355000	-1.67416900
H	-2.96021400	0.19273400	-2.03586500
C	-4.54150300	0.34809000	0.89168800
C	-5.00075300	-0.96199900	1.07006000
C	-5.37229500	1.42971200	1.20374800
C	-6.28630200	-1.18224100	1.55697900
H	-4.35083300	-1.80100400	0.83603900
C	-6.65280900	1.20490000	1.68965600
H	-4.99040400	2.43429000	1.05467200
C	-7.11003400	-0.10236300	1.86499300
H	-6.64252600	-2.19737500	1.69620600
H	-7.29755000	2.04327300	1.93223300
H	-8.11171500	-0.27740600	2.24516000

C	-3.16916400	-1.91022100	-2.10233000
C	-4.56562100	-1.84102000	-2.15715200
C	-2.55604100	-3.12759000	-2.40622200
C	-5.32934700	-2.95697900	-2.48331600
H	-5.05868200	-0.89751000	-1.93346700
C	-3.31692100	-4.24707900	-2.73706000
H	-1.47369300	-3.20211700	-2.39609900
C	-4.70578100	-4.16847500	-2.77210400
H	-6.41155200	-2.87782000	-2.51678600
H	-2.81850000	-5.18318000	-2.97092700
H	-5.29695900	-5.04139800	-3.02936500
C	-1.55349300	-1.23728600	0.63696100
O	-0.79592200	-2.24511100	0.04093500
C	-1.12146600	-0.91221500	2.01619200
C	-1.98268800	-0.47879600	3.02533500
C	0.25806000	-0.95209500	2.26659300
C	-1.46714400	-0.06502900	4.25146500
H	-3.05485400	-0.47585800	2.86401600
C	0.77175200	-0.53005300	3.48723600
H	0.91997300	-1.30263500	1.47822300
C	-0.09385600	-0.07887200	4.48316600
H	-2.14628500	0.26587400	5.03073800
H	1.84589100	-0.54080900	3.65207200
H	0.29981000	0.25380100	5.43825800
C	-1.05327800	-3.50991800	0.47993600
O	-1.96362300	-3.76880000	1.22230000
C	-0.06041500	-4.49195500	-0.08998500
C	1.36598100	-3.94163000	-0.15522700
H	-0.12531500	-5.39661300	0.52045900
H	-0.40369300	-4.75893700	-1.09802300
C	2.35885600	-4.97877300	-0.67005800
H	1.65913200	-3.61826100	0.85424900
H	1.38062100	-3.05151300	-0.79578600
H	3.36861000	-4.56105300	-0.71946400
H	2.08882800	-5.30562500	-1.67885400
H	2.38655000	-5.86366500	-0.02630400
C	4.87078900	-0.99221500	-0.41903400
C	5.98766300	-1.47287000	0.25740100
C	7.22779500	-1.49283300	-0.37535500
C	7.31997100	-1.02625900	-1.68461600
C	6.18870700	-0.55967500	-2.36000300
C	4.94546000	-0.54298000	-1.73390000
C	3.63861800	-1.05194700	0.45352300
C	4.17446600	-1.46637100	1.87320900

C	5.62689800	-1.94817700	1.64167600
H	8.10809700	-1.86330300	0.14180700
H	8.28116700	-1.03067700	-2.18907500
H	6.28030300	-0.21418300	-3.38462200
H	4.03825800	-0.22640600	-2.24159000
H	3.54482600	-2.25518900	2.29022500
H	6.27817300	-1.55027700	2.42656500
H	2.90598900	-1.75481900	0.05843100
H	5.67949200	-3.04010000	1.70425700
C	3.40543000	1.23012400	1.37596300
C	1.95345900	0.76656200	-0.20639800
N	2.72734500	2.32639500	1.24270000
N	2.97137900	0.25653800	0.51768100
N	1.83561800	2.02815600	0.24499700
C	4.46018500	0.85383000	2.36127000
H	5.45313200	0.85414000	1.89016500
H	4.45865200	1.54664300	3.20231000
C	0.93257700	3.02803000	-0.19626500
C	-0.16167800	3.37714900	0.59704000
C	1.13107200	3.66760000	-1.42140800
C	-1.06406700	4.34169200	0.16690600
C	0.24125500	4.63365300	-1.86663000
C	-0.84741000	4.95283400	-1.06079600
H	-1.92999900	4.58411600	0.76932300
H	0.39298300	5.12272600	-2.82053700
Cl	-0.41100300	2.57748400	2.10403600
Cl	-1.97493100	6.15210100	-1.61469700
Cl	2.49380000	3.24939400	-2.40112200
O	4.11097400	-0.42924800	2.84585500

M6SR

C	-1.34675600	0.21795900	-1.34853000
O	-1.81803200	-0.91134500	-1.71095100
C	-0.09326000	0.74260200	-1.49368500
C	1.00324600	0.02465300	-2.21881600
H	0.12483700	1.75713900	-1.17926100
C	1.25567300	0.69889700	-3.57725300
H	0.67935300	-1.00237800	-2.40052700
H	0.32355000	0.73134600	-4.14615600
H	2.00776400	0.16586600	-4.16550400
H	1.60260300	1.73045000	-3.43807000
C	3.19579500	0.20034000	0.96326300
O	2.79113200	1.06365700	1.71961900
C	2.25209600	-0.52883300	0.03722400

C	2.32139700	0.03010400	-1.39048400
H	2.56279500	1.09753000	-1.25909400
C	4.65857000	-0.08048400	0.82631300
C	5.11906700	-1.31312000	0.35260800
C	5.56816500	0.92145400	1.17232800
C	6.48415200	-1.53439500	0.21108400
H	4.40468900	-2.08943400	0.09129900
C	6.93159900	0.70315100	1.01497500
H	5.18597600	1.86549400	1.54796100
C	7.38789000	-0.52311200	0.53140800
H	6.83993100	-2.48927800	-0.16110300
H	7.64022700	1.48580800	1.26600100
H	8.45309400	-0.69096400	0.40572900
C	3.48400400	-0.57914800	-2.16142200
C	4.54790300	0.21748100	-2.58635700
C	3.51223900	-1.94639700	-2.44635600
C	5.62958000	-0.33818300	-3.26490800
H	4.53703800	1.28177000	-2.36353000
C	4.59038500	-2.50549900	-3.12502100
H	2.70663200	-2.58717600	-2.09939500
C	5.65539100	-1.70386200	-3.53301200
H	6.45475200	0.29488000	-3.57593600
H	4.60200900	-3.57177600	-3.32865200
H	6.49946200	-2.14287800	-4.05557600
C	1.44711600	-1.48650900	0.51295300
O	0.47397500	-2.02453300	-0.31614600
C	1.35872400	-1.98054000	1.91020800
C	2.47362300	-2.10891600	2.74237000
C	0.09925300	-2.33786900	2.41065600
C	2.32882100	-2.55328300	4.05254800
H	3.46599100	-1.88740400	2.36539400
C	-0.04297400	-2.78049000	3.72069100
H	-0.76812200	-2.26401900	1.76080800
C	1.07182900	-2.88608400	4.54884300
H	3.20693000	-2.65076000	4.68269500
H	-1.02620900	-3.04798300	4.09520700
H	0.96290500	-3.23619900	5.57015800
C	-4.75754800	-1.20950900	-0.03992800
C	-6.08358200	-1.62972100	-0.08344200
C	-6.55595400	-2.52390700	0.87217400
C	-5.68559100	-2.96401000	1.86986300
C	-4.36704100	-2.50556100	1.92580300
C	-3.89134000	-1.61435100	0.96631700
C	-4.45722900	-0.28128000	-1.19082400

C	-5.86397200	0.15312900	-1.70827600
C	-6.80822300	-0.97872400	-1.23790400
H	-7.58688800	-2.86457500	0.85213400
H	-6.04297200	-3.65893800	2.62300800
H	-3.71103600	-2.84526400	2.72109900
H	-2.87085700	-1.23776600	0.99317900
H	-5.86090900	0.25441300	-2.79433500
H	-7.78365300	-0.56473300	-0.96647700
H	-3.85204700	-0.77059100	-1.95388700
H	-6.96959100	-1.69456200	-2.05157300
C	-4.32535500	1.85477800	-0.00877600
C	-2.36319900	1.11667700	-0.68744100
N	-3.48502900	2.72034100	0.46356800
N	-3.68993200	0.87398700	-0.71969100
N	-2.26760200	2.24605800	0.04507700
C	-5.81833400	1.80092200	0.04776000
H	-6.14392200	1.08968800	0.81923400
H	-6.22173100	2.78752900	0.27613600
C	-1.11044700	2.97862000	0.41694800
C	-0.82813200	4.18754400	-0.22152800
C	-0.26261700	2.51909700	1.42728400
C	0.28296900	4.93841600	0.13615900
C	0.85829000	3.25244000	1.79539700
C	1.10983500	4.45320600	1.14313100
H	0.49941400	5.87330700	-0.36550500
H	1.53261000	2.87000900	2.54953400
Cl	-1.84968800	4.73875600	-1.50560300
Cl	2.51247400	5.37223900	1.59090000
Cl	-0.57456100	1.00850000	2.19955300
O	-6.27392300	1.43438100	-1.23981100
C	0.61069700	-3.32552700	-0.69660600
O	1.58832600	-3.97967800	-0.43074400
C	-0.59805700	-3.76381400	-1.47379400
C	-1.84385500	-3.78598700	-0.58030500
H	-0.38534000	-4.74330500	-1.90816400
H	-0.77388900	-3.01971300	-2.25857500
C	-3.10945200	-4.08384600	-1.37385900
H	-1.71328700	-4.51147600	0.23237500
H	-1.93570900	-2.78928600	-0.14838000
H	-3.98801900	-4.08147400	-0.72060100
H	-3.24984500	-3.31174000	-2.13744400
H	-3.05459300	-5.05661100	-1.87374900

M6SS

C	-1.34736000	0.53549200	-1.47944700
O	-2.09429300	-0.36704300	-1.98895500
C	-0.00331600	0.73788900	-1.61555500
C	0.82369900	-0.20489100	-2.43070400
H	0.46567400	1.62550900	-1.21437600
C	1.21346800	0.40721600	-3.78425400
H	0.17955800	-1.05670500	-2.65401500
H	0.30513500	0.59795500	-4.36113600
H	1.85607900	-0.26913400	-4.36010900
H	1.74606000	1.35408500	-3.65913400
C	2.97772800	-0.92603700	0.73524200
O	2.79922900	-0.23815400	1.72259600
C	1.87351300	-1.23293000	-0.24601600
C	2.09536000	-0.73857500	-1.68314400
H	2.42804500	-1.61352100	-2.25994300
C	4.32640500	-1.48513800	0.40881700
C	4.45472000	-2.63126400	-0.38084000
C	5.46031600	-0.82887100	0.89075300
C	5.72238900	-3.11949700	-0.68351400
H	3.56256900	-3.13497600	-0.75022100
C	6.72359500	-1.30869700	0.56948700
H	5.32832600	0.06550400	1.49214000
C	6.85395000	-2.45440800	-0.21590800
H	5.82677700	-4.01453400	-1.28815900
H	7.60868500	-0.79184600	0.92624100
H	7.84205700	-2.82897000	-0.46474500
C	3.21920500	0.28494700	-1.74453200
C	4.31407500	0.06870800	-2.58339700
C	3.18520000	1.45855300	-0.98431300
C	5.35102800	0.99296000	-2.66257100
H	4.36001600	-0.84799600	-3.16610600
C	4.21775500	2.38911500	-1.06367200
H	2.35839200	1.62631100	-0.29987200
C	5.30519100	2.15906600	-1.90259400
H	6.19780000	0.79869700	-3.31344900
H	4.17608800	3.29296600	-0.46269400
H	6.11341800	2.88119200	-1.95971800
C	0.85395400	-1.98929700	0.18211000
O	-0.21726500	-2.28360200	-0.65152200
C	0.65945900	-2.60464700	1.51939400
C	1.70345300	-3.19467700	2.23537800
C	-0.63606600	-2.64857300	2.05235500
C	1.46301200	-3.78405900	3.47320000
H	2.70516900	-3.21611100	1.81717200

C	-0.87346700	-3.23047900	3.29154600
H	-1.45344600	-2.20581200	1.49061300
C	0.17829400	-3.79870300	4.00813200
H	2.28354500	-4.24372800	4.01444600
H	-1.88070300	-3.24106600	3.69696400
H	-0.00426800	-4.25907200	4.97378700
C	-4.78292600	-0.48877200	-0.23422500
C	-6.13787000	-0.54281700	0.07980000
C	-6.62711000	-1.56966000	0.88373800
C	-5.73914000	-2.52854800	1.36433700
C	-4.38226300	-2.47464800	1.03233400
C	-3.88913200	-1.45652600	0.21969700
C	-4.46836200	0.71226800	-1.09811800
C	-5.82360200	1.51211500	-1.18242600
C	-6.90030400	0.58155300	-0.57188500
H	-7.68280400	-1.62076500	1.13360800
H	-6.10513900	-3.33060700	1.99752700
H	-3.70881300	-3.24370700	1.40214700
H	-2.84896900	-1.41633600	-0.10211800
H	-6.04013100	1.74479800	-2.22511800
H	-7.52560700	1.14642600	0.12766500
H	-4.08465800	0.42045700	-2.07326500
H	-7.56409600	0.20156600	-1.35480200
C	-3.73250700	2.46924400	0.48339100
C	-2.07387700	1.48934400	-0.57463400
N	-2.67242900	3.02358600	0.98041400
N	-3.41925900	1.54036300	-0.47138400
N	-1.64453600	2.39920000	0.32328500
C	-5.17463300	2.76366200	0.72318300
H	-5.61861800	2.00772600	1.38679300
H	-5.28906700	3.74847900	1.17559700
C	-0.32548900	2.74311900	0.72827800
C	0.28388100	3.89202100	0.22247000
C	0.32666000	1.99473100	1.71054500
C	1.52569800	4.30259000	0.68995300
C	1.57069200	2.38627700	2.19148200
C	2.14272400	3.54476300	1.68031400
H	1.99296400	5.19591600	0.29411500
H	2.08356400	1.78065500	2.92690900
Cl	-0.51124100	4.80456300	-1.01318600
Cl	3.68763600	4.05486100	2.28850900
Cl	-0.40825200	0.56096100	2.31877800
O	-5.79202300	2.78117000	-0.54622600
C	-0.03259700	-3.19914000	-1.64420000

O	1.03786500	-3.69994800	-1.88297300
C	-1.33889000	-3.44826900	-2.34038300
C	-2.31186800	-4.21106800	-1.42848700
H	-1.13682000	-4.00650300	-3.25714700
H	-1.76021900	-2.46207800	-2.57342400
C	-3.72082100	-4.23407000	-2.00997700
H	-1.94485000	-5.23128700	-1.26969400
H	-2.32537600	-3.72391500	-0.44743100
H	-4.41118000	-4.77232900	-1.35456100
H	-4.09772800	-3.21330300	-2.12986700
H	-3.73333300	-4.72014000	-2.99076000

TS7RR

C	-1.37026400	-0.35265700	-1.21197400
O	-1.98015800	-0.07695000	-2.24498000
C	0.03682300	-0.32072200	-1.02055200
C	0.87385100	-0.55448200	-2.25854900
H	0.39827300	-0.80625200	-0.11357000
C	0.84470500	-1.99344200	-2.75826100
H	0.45151700	0.10659300	-3.02269300
H	-0.17338500	-2.25245300	-3.06389000
H	1.50489500	-2.12958300	-3.62183200
H	1.16597700	-2.69369400	-1.97882200
C	0.41661900	1.48821800	-0.86280100
O	-0.23503700	2.10583200	-1.76857600
C	1.93485200	1.28189100	-1.11394600
C	2.26586100	0.01094300	-1.88625600
H	2.80812000	0.28509000	-2.79974800
C	0.05200400	1.83386100	0.59396800
C	0.91654500	1.70860800	1.68450800
C	-1.22572400	2.35506300	0.81435800
C	0.49936600	2.08590400	2.96072600
H	1.93990100	1.37131500	1.54044800
C	-1.66253500	2.68514200	2.09365200
H	-1.83982700	2.53588500	-0.06365400
C	-0.79323400	2.55392000	3.17646500
H	1.19466800	2.00706400	3.79164100
H	-2.66926500	3.06418300	2.24760300
H	-1.11567900	2.83462800	4.17444800
C	3.11518500	-1.02924000	-1.17477200
C	3.98467400	-1.82308700	-1.93331100
C	3.01539100	-1.28992300	0.19585700
C	4.72524000	-2.84813800	-1.35136600
H	4.07578700	-1.63327700	-3.00054200

C	3.76140700	-2.30850700	0.78481200
H	2.38258200	-0.66354600	0.81915300
C	4.61465400	-3.09607100	0.01542000
H	5.38845300	-3.45065700	-1.96470600
H	3.68365600	-2.48097600	1.85451300
H	5.18998800	-3.89115800	0.47903600
C	2.87654600	2.17626500	-0.78274800
O	4.21053500	1.78276100	-1.03978600
C	2.72906500	3.55014000	-0.25437500
C	1.61393300	4.32601100	-0.60343200
C	3.71454700	4.11714400	0.56470900
C	1.47525200	5.61806500	-0.10844200
H	0.86116200	3.90592500	-1.26332700
C	3.57153800	5.41187500	1.05102200
H	4.58486400	3.53846300	0.84697200
C	2.44869200	6.16650000	0.72202900
H	0.60320900	6.20268000	-0.38458600
H	4.34026000	5.83009800	1.69346600
H	2.33790600	7.17631800	1.10499100
C	4.86828200	1.17777900	-0.02411600
O	4.47378900	1.17731800	1.11743300
C	6.12982200	0.48386200	-0.47454200
C	6.50922900	0.64026600	-1.94229800
H	6.93609300	0.81960200	0.18710800
H	5.96124300	-0.57544400	-0.23474500
C	7.70244200	-0.24130900	-2.29785700
H	6.72970400	1.69086400	-2.15816600
H	5.64851100	0.37181100	-2.56248100
H	7.98045400	-0.13068200	-3.34883100
H	7.46483100	-1.29539500	-2.11842500
H	8.57720300	0.01086000	-1.69000300
C	-5.21422900	0.46367000	-1.39505600
C	-6.41286200	1.14490300	-1.20255500
C	-7.57098300	0.70445000	-1.83712900
C	-7.50217100	-0.42064000	-2.65540900
C	-6.29305700	-1.09389400	-2.84756800
C	-5.13113800	-0.65325900	-2.22005600
C	-4.09465900	1.11281500	-0.61237100
C	-4.81704800	2.15610900	0.31665000
C	-6.22385100	2.33565600	-0.29740800
H	-8.51265800	1.22598100	-1.69472600
H	-8.39875900	-0.77745200	-3.15220900
H	-6.25939700	-1.96324800	-3.49568500
H	-4.17581800	-1.14520400	-2.37647600

H	-4.25373600	3.09029700	0.33764200
H	-6.97006300	2.40714400	0.49973600
H	-3.34918200	1.57347800	-1.26450000
H	-6.26987300	3.26793500	-0.86978500
C	-3.91745800	-0.33427700	1.38960600
C	-2.24546800	-0.53098100	0.00477300
N	-3.17175400	-1.25948800	1.91775100
N	-3.39386000	0.11878600	0.21009700
N	-2.13408700	-1.37671600	1.03556400
C	-5.12348900	0.38240300	1.90352400
H	-6.03165300	0.03464200	1.39261900
H	-5.22814100	0.22709700	2.97687700
C	-1.13852500	-2.37902500	1.20569300
C	-0.24217400	-2.30735000	2.27492100
C	-1.02822500	-3.42690200	0.28671300
C	0.77095900	-3.24849300	2.41003400
C	-0.01242500	-4.36599600	0.40006000
C	0.87876100	-4.25898700	1.46230500
H	1.46550300	-3.18288500	3.23862000
H	0.07689300	-5.16485300	-0.32557100
Cl	-0.35812800	-1.01912700	3.40901300
Cl	2.14930800	-5.42441100	1.61496000
Cl	-2.16086700	-3.57163700	-1.01381500
O	-4.87937900	1.75781600	1.68086000

TS7RS

C	-1.17672700	0.44676300	1.14696400
O	-1.39979100	0.13092900	2.30131800
C	0.10458600	0.80335100	0.57513700
C	1.13178700	1.20537200	1.61098500
H	0.04161300	1.47066400	-0.29130200
C	1.01091200	2.65245800	2.07002800
H	0.99421600	0.53299600	2.46632600
H	0.03302000	2.82926400	2.52883900
H	1.78255800	2.89986000	2.80527000
H	1.12027500	3.33624200	1.21950100
C	0.73524500	-0.76688100	0.02849800
O	0.25797800	-1.71847400	0.78051600
C	2.24499300	-0.43753300	0.22184500
C	2.48183200	0.86849200	0.95642800
H	2.67804900	1.63606700	0.18972800
C	0.38214100	-0.83544400	-1.47414100
C	1.07592400	-0.11378800	-2.45132400
C	-0.63755400	-1.69364100	-1.88117600

C	0.74926400	-0.25542700	-3.79713300
H	1.91115900	0.52184500	-2.16292800
C	-0.99682700	-1.80898800	-3.22149500
H	-1.09880600	-2.31566800	-1.12378800
C	-0.29726900	-1.09068200	-4.18870200
H	1.31542100	0.29047900	-4.54644700
H	-1.80144000	-2.48229500	-3.50407000
H	-0.55039000	-1.19425500	-5.23961400
C	3.61112700	0.91867000	1.96148800
C	4.47962800	2.01104800	1.98432400
C	3.76083200	-0.08054000	2.92924500
C	5.48034500	2.11145300	2.95072500
H	4.36888500	2.78855400	1.23104400
C	4.75546200	0.01805000	3.89683100
H	3.09433500	-0.93990700	2.90589500
C	5.61908900	1.11488100	3.91186600
H	6.14700000	2.96882100	2.95163000
H	4.86252900	-0.76522600	4.64092900
H	6.39634600	1.18778500	4.66610300
C	3.23023100	-1.18370600	-0.29553600
O	4.56849800	-0.79476500	-0.10027400
C	3.15929700	-2.42354700	-1.10080800
C	2.16141500	-3.38788700	-0.91174300
C	4.12967800	-2.63698300	-2.08961900
C	2.12994100	-4.52253100	-1.71725400
H	1.41538500	-3.22395500	-0.13922500
C	4.09221700	-3.77238100	-2.88955400
H	4.91478900	-1.90278100	-2.23879800
C	3.08847800	-4.72072400	-2.70758300
H	1.35056300	-5.26311400	-1.56341900
H	4.84729900	-3.91591100	-3.65616500
H	3.05871300	-5.61005800	-3.32958900
C	5.02734500	0.33316800	-0.67814000
O	4.37106800	1.03522800	-1.41049200
C	6.47064000	0.60151500	-0.31523700
C	7.04785800	-0.26954400	0.79582400
H	7.05215500	0.50275300	-1.24068100
H	6.51689900	1.66144400	-0.04190800
C	8.41416300	0.23556400	1.24742300
H	7.11696000	-1.30494400	0.44722600
H	6.35444800	-0.27245300	1.64166600
H	8.83562400	-0.40837900	2.02339500
H	8.33182600	1.24684300	1.65991500
H	9.12483800	0.26934800	0.41495800

C	-3.86725700	-2.29323800	1.95906500
C	-4.59163000	-3.48086500	1.88535900
C	-5.61724500	-3.72980600	2.79379300
C	-5.90447900	-2.77283600	3.76386900
C	-5.17279800	-1.58496500	3.83252900
C	-4.14254300	-1.33486900	2.93038500
C	-2.81348300	-2.22909000	0.87474300
C	-3.12466100	-3.46809500	-0.04698600
C	-4.09097500	-4.35792700	0.76708100
H	-6.18672300	-4.65312700	2.74436900
H	-6.70386100	-2.95215100	4.47577000
H	-5.40488200	-0.85344700	4.59965200
H	-3.54987400	-0.42721300	2.98428400
H	-2.19705000	-3.98863200	-0.28608200
H	-4.88634200	-4.73612500	0.11692000
H	-1.77282800	-2.23385300	1.22635700
H	-3.55806000	-5.22805700	1.16349200
C	-3.90580300	-0.84782700	-0.88703400
C	-2.31371700	0.17053800	0.18439400
N	-3.89884000	0.35340200	-1.38803500
N	-2.96446400	-0.98794300	0.09608000
N	-2.89737900	0.97893700	-0.70043900
C	-4.63497300	-2.08864400	-1.28859000
H	-5.44838100	-2.30711800	-0.58300600
H	-5.04429800	-1.97904000	-2.29236900
C	-2.67931700	2.37887600	-0.83139500
C	-2.11672900	2.89864800	-1.99927000
C	-3.04769900	3.24379800	0.20383500
C	-1.90471600	4.26566600	-2.12870800
C	-2.83231800	4.61044200	0.09329600
C	-2.26216300	5.10062300	-1.07658800
H	-1.46045700	4.66479000	-3.03207100
H	-3.11214700	5.27618800	0.90009300
Cl	-1.63934300	1.82745100	-3.25580000
Cl	-1.99396800	6.80609800	-1.22725200
Cl	-3.79673600	2.62208100	1.63566900
O	-3.66213700	-3.11399600	-1.31698000
TS7SR			
C	1.07081700	0.38883100	-1.10868300
O	1.14521500	0.08550800	-2.27919800
C	-0.07025500	0.88097000	-0.33341800
C	-1.21800200	1.51711100	-1.11286100
H	0.26826300	1.48886400	0.50844300

C	-0.80698600	2.40735900	-2.28421100
H	-1.77621600	2.12486500	-0.38754200
H	-1.67512700	2.92713800	-2.69742500
H	-0.08364700	3.16152500	-1.95494300
H	-0.34760900	1.81661400	-3.07944800
C	-0.69517900	-0.63504600	0.28703000
O	-0.09543300	-1.66930400	-0.27083400
C	-2.16171100	-0.46955600	-0.18740800
C	-2.11591100	0.31875600	-1.48538000
H	-1.50866600	-0.32375700	-2.14320200
C	-0.48381100	-0.50719200	1.80480000
C	-1.25296600	0.33970900	2.60991400
C	0.52683600	-1.26427700	2.39534700
C	-1.02254300	0.40801500	3.97979500
H	-2.07000900	0.90552700	2.16542000
C	0.76746000	-1.18884900	3.76597800
H	1.09184100	-1.94444000	1.76520700
C	-0.00941600	-0.35368500	4.56521600
H	-1.64347600	1.04968100	4.59808900
H	1.55342200	-1.79424300	4.20947100
H	0.16197600	-0.30397000	5.63632700
C	-3.35564700	0.69718500	-2.26543900
C	-3.70430200	-0.04105900	-3.40052800
C	-4.10800100	1.83863600	-1.96496800
C	-4.77081900	0.34088200	-4.21127500
H	-3.12068000	-0.92181500	-3.65473300
C	-5.17833800	2.22235400	-2.77025800
H	-3.85703500	2.43493800	-1.09199500
C	-5.51256700	1.47766000	-3.89972700
H	-5.01856400	-0.24747100	-5.08933400
H	-5.74631700	3.11342500	-2.51840800
H	-6.34176000	1.78214100	-4.53062200
C	-3.21664300	-1.00864200	0.42853000
O	-4.51787600	-0.77251600	-0.05948800
C	-3.22623500	-1.93456400	1.58514800
C	-2.26308500	-2.94393300	1.69826500
C	-4.23544700	-1.84596600	2.55132300
C	-2.29981500	-3.82610900	2.77380300
H	-1.48206700	-3.00558100	0.94356800
C	-4.26972900	-2.73208000	3.62133900
H	-4.98458800	-1.06397200	2.48286000
C	-3.30133800	-3.72677900	3.73620800
H	-1.54323600	-4.60066400	2.85701800
H	-5.05209400	-2.64324500	4.36871400

H	-3.32835000	-4.41983100	4.57144000
C	-5.13860300	0.34113600	0.37940100
O	-4.63150400	1.14534000	1.12559500
C	-6.55249300	0.44435200	-0.14196300
C	-6.90154400	-0.49339700	-1.29309300
H	-7.21505100	0.27592500	0.71720600
H	-6.69008900	1.49185600	-0.43025200
C	-8.23965300	-0.12408200	-1.92411000
H	-6.91974500	-1.52489900	-0.92775000
H	-6.10905900	-0.44442800	-2.04467600
H	-8.49738700	-0.80862500	-2.73624800
H	-8.19946300	0.88890300	-2.33907900
H	-9.05075300	-0.15296900	-1.18884600
C	3.52853100	-2.69785400	-1.95448100
C	4.07629200	-3.97329800	-1.83744000
C	5.00557600	-4.41862000	-2.77275300
C	5.37281600	-3.56869300	-3.81399800
C	4.81262800	-2.29399300	-3.92858400
C	3.87776200	-1.84691600	-2.99784200
C	2.54191600	-2.43573700	-0.84183200
C	2.74935000	-3.62319400	0.16105300
C	3.50622500	-4.70215300	-0.64569500
H	5.44072400	-5.41019800	-2.69056900
H	6.10038000	-3.90228900	-4.54705600
H	5.10428200	-1.65094100	-4.75236700
H	3.41587400	-0.86676000	-3.08407700
H	1.77878100	-3.96447900	0.52173400
H	4.26491600	-5.17771400	-0.01653900
H	1.49542100	-2.35722400	-1.15143200
H	2.81329400	-5.48624700	-0.96822100
C	3.88238200	-1.06175000	0.72707000
C	2.28097200	0.02822100	-0.25556200
N	4.01090600	0.15751800	1.16436900
N	2.84978600	-1.17020000	-0.16471500
N	3.00278200	0.82874400	0.53172100
C	4.52186400	-2.34477700	1.15070900
H	5.23668600	-2.69704700	0.39496600
H	5.03327600	-2.21441400	2.10402200
C	2.90799400	2.24635700	0.61590500
C	2.45162700	2.85536800	1.78773300
C	3.29760500	3.03687800	-0.46933200
C	2.38003600	4.23992700	1.87621700
C	3.22340100	4.42122900	-0.39843900
C	2.76707100	5.00209100	0.78000700

H	2.01787300	4.70898900	2.78261500
H	3.52207400	5.03004800	-1.24249500
Cl	1.92743500	1.87853600	3.10160600
Cl	2.67845200	6.72933900	0.88307300
Cl	3.89147500	2.29622900	-1.91716000
O	3.45381000	-3.25157400	1.34438300

TS7SS

C	-1.21452400	0.43075600	1.26484700
O	-1.59974100	0.07716300	2.36119200
C	0.13062400	0.76613200	0.81967200
C	1.18616100	1.12724200	1.86926800
H	0.11459500	1.47482700	-0.01639900
C	1.05493600	0.37496700	3.19607500
H	1.16689200	2.20613900	2.06942400
H	1.92492000	0.57611500	3.82388300
H	0.16354500	0.68855300	3.73616800
H	0.97564400	-0.69997400	3.00838400
C	0.70131400	-0.76059500	0.17552700
O	0.18802800	-1.75409300	0.85835300
C	2.22736800	-0.48299100	0.35201500
C	2.50629200	0.79719000	1.11545000
H	2.63102900	1.58227900	0.35310900
C	0.36315600	-0.74760300	-1.33965800
C	1.04768900	0.04070100	-2.27055800
C	-0.60644800	-1.63082900	-1.80804500
C	0.77224000	-0.07365000	-3.63036400
H	1.84801800	0.69968700	-1.94074500
C	-0.92352300	-1.71443400	-3.16145200
H	-1.04963600	-2.30173000	-1.08371400
C	-0.22384000	-0.93928300	-4.08253700
H	1.33804400	0.52123000	-4.34183900
H	-1.69052800	-2.41076600	-3.48934400
H	-0.43781800	-1.02080200	-5.14411700
C	3.73710200	0.83861400	1.99760200
C	4.51479000	1.99643400	2.04638000
C	4.09742300	-0.23998500	2.81514600
C	5.61683000	2.08810100	2.89817400
H	4.25666200	2.83430500	1.40191500
C	5.18150700	-0.14642200	3.67996800
H	3.51713700	-1.15707500	2.76167600
C	5.94711900	1.02016200	3.72566400
H	6.21152900	2.99662900	2.91534000
H	5.44057100	-0.99123300	4.31061000

H	6.80057000	1.08799300	4.39300200
C	3.18288000	-1.19602800	-0.26274000
O	4.52833000	-0.79037900	-0.16016400
C	3.06806600	-2.40637600	-1.10534200
C	2.06975500	-3.36785300	-0.90298900
C	3.99483700	-2.59843500	-2.13923400
C	1.99468400	-4.47772900	-1.73937700
H	1.35434700	-3.21609200	-0.09875600
C	3.91428200	-3.70955000	-2.96923300
H	4.78172400	-1.86848000	-2.29780500
C	2.91041400	-4.65483700	-2.77331800
H	1.21543400	-5.21640000	-1.57537300
H	4.63713300	-3.83744900	-3.76893600
H	2.84786600	-5.52606200	-3.41818000
C	4.91696600	0.36318200	-0.74114000
O	4.18838000	1.07554900	-1.39054100
C	6.38065600	0.65755300	-0.50369700
C	7.09593200	-0.25336800	0.48712400
H	6.86747800	0.63800400	-1.48700200
H	6.41966400	1.70017900	-0.16869000
C	8.48581700	0.27575900	0.82497800
H	7.15963200	-1.26489200	0.07281000
H	6.49541000	-0.32664600	1.39749000
H	9.00552000	-0.39195500	1.51680400
H	8.41457900	1.26039800	1.29938900
H	9.10497000	0.37901900	-0.07244200
C	-4.02896300	-2.24639800	1.78448700
C	-4.73717800	-3.43774200	1.63898800
C	-5.83398000	-3.70552500	2.45269100
C	-6.21347400	-2.76104900	3.40277100
C	-5.50243900	-1.56736100	3.54247000
C	-4.39942300	-1.29932800	2.73548600
C	-2.88733000	-2.17369900	0.78969700
C	-3.14779500	-3.38135500	-0.18561300
C	-4.14300800	-4.29846400	0.55558400
H	-6.38774400	-4.63331800	2.34353800
H	-7.07035500	-2.95407300	4.04039400
H	-5.81002100	-0.84321800	4.28985300
H	-3.82736400	-0.38398900	2.84699700
H	-2.20983800	-3.89330100	-0.40104300
H	-4.88259600	-4.69408800	-0.14719800
H	-1.87875800	-2.21646200	1.22227000
H	-3.61460100	-5.15504900	0.98687800
C	-3.83917100	-0.72298100	-0.98535700

C	-2.27287500	0.22860500	0.18491000
N	-3.78355900	0.49058800	-1.45069100
N	-2.95010200	-0.90985300	0.03660200
N	-2.80022000	1.07570000	-0.70108700
C	-4.57830900	-1.93469600	-1.45402300
H	-5.43158800	-2.14967300	-0.79619300
H	-4.93349200	-1.78826500	-2.47384600
C	-2.57643000	2.47930200	-0.77699300
C	-2.02213100	3.04552000	-1.92785200
C	-2.96647800	3.30950600	0.27962400
C	-1.81612000	4.41721700	-2.00827700
C	-2.75841100	4.68038400	0.21712900
C	-2.18018500	5.21366000	-0.92944600
H	-1.37555300	4.84944900	-2.89802800
H	-3.05334400	5.31662000	1.04207500
Cl	-1.56925100	2.03292200	-3.23934700
Cl	-1.91778500	6.92442000	-1.01933300
Cl	-3.75060900	2.64384100	1.67250700
O	-3.63291800	-2.98575400	-1.46484600

M7RR

C	1.11467200	0.16914600	-1.13048800
O	1.63055600	0.31732200	-2.28335400
C	-0.25205400	0.78972900	-0.69475000
C	-1.12402800	0.99560100	-1.93557400
H	-0.26299500	1.63882800	-0.00699200
C	-1.25345000	2.45648800	-2.34569500
H	-0.61242400	0.46767600	-2.74724700
H	-0.26341000	2.84199900	-2.60993400
H	-1.90737100	2.56975000	-3.21623300
H	-1.66101400	3.07162300	-1.53679200
C	-0.61960900	-0.60521000	-0.13158300
O	0.51437300	-1.19448800	-0.80824300
C	-1.98999900	-0.90676100	-0.72905500
C	-2.44005000	0.22288900	-1.65423300
H	-2.82255400	-0.21079400	-2.58567200
C	-0.53962700	-0.81405100	1.37554900
C	-1.60063700	-0.46041800	2.21755900
C	0.60403400	-1.36935700	1.95209000
C	-1.48427400	-0.59588500	3.59693800
H	-2.54284000	-0.12619600	1.79318600
C	0.72306900	-1.50719300	3.33266700
H	1.39451300	-1.72891300	1.30571900
C	-0.31593200	-1.10251900	4.16462800

H	-2.32027700	-0.31681800	4.23081300
H	1.62897000	-1.93723900	3.74999400
H	-0.23047600	-1.20759300	5.24174400
C	-3.54829400	1.09166300	-1.08884800
C	-4.74240700	1.24417200	-1.79380300
C	-3.40043500	1.78358900	0.11906800
C	-5.77952600	2.03174800	-1.29341500
H	-4.86038600	0.74125900	-2.75086200
C	-4.43068000	2.56732200	0.62397700
H	-2.46787700	1.70703300	0.67211800
C	-5.63036200	2.68775700	-0.07647500
H	-6.70265200	2.12923200	-1.85773100
H	-4.29876200	3.08583700	1.56855700
H	-6.43652000	3.29602500	0.32071900
C	-2.74887600	-1.96600000	-0.43152900
O	-4.05022500	-2.00898500	-0.95901700
C	-2.35990600	-3.16086900	0.34566300
C	-1.08187500	-3.70897900	0.18670700
C	-3.25754300	-3.76949500	1.23110100
C	-0.70228400	-4.82837600	0.92026600
H	-0.39323700	-3.25058300	-0.51674200
C	-2.87371300	-4.88916900	1.95972900
H	-4.24390500	-3.34492100	1.37790100
C	-1.59479300	-5.42120100	1.80885400
H	0.29158100	-5.24543400	0.78839500
H	-3.57402800	-5.34354800	2.65335500
H	-1.29883400	-6.29616500	2.37902800
C	-5.04486900	-1.48429300	-0.19704500
O	-4.86879600	-1.03099500	0.90531500
C	-6.39395600	-1.58462500	-0.86891600
C	-6.40016100	-2.02158500	-2.32990900
H	-6.98760800	-2.27728600	-0.25896800
H	-6.85813200	-0.60035100	-0.74514000
C	-7.81198100	-1.99682500	-2.90792500
H	-5.97217100	-3.02514300	-2.41234500
H	-5.74481000	-1.36308100	-2.90906200
H	-7.81864400	-2.31509800	-3.95301600
H	-8.23618300	-0.98859000	-2.85941600
H	-8.47679500	-2.66304700	-2.34901300
C	4.49801200	-1.80356700	-1.51658900
C	5.50062700	-2.74227200	-1.28930900
C	6.54949400	-2.86860600	-2.19581300
C	6.57065000	-2.03991900	-3.31575900
C	5.55654400	-1.10368400	-3.53396600

C	4.50002500	-0.97535900	-2.63507800
C	3.46597500	-1.83746900	-0.41083500
C	4.10845900	-2.75477600	0.69519700
C	5.24468500	-3.51891300	-0.02210400
H	7.33881900	-3.59616300	-2.03162900
H	7.38479000	-2.12440200	-4.02877500
H	5.58954000	-0.47339100	-4.41666800
H	3.68293500	-0.27107400	-2.78366900
H	3.35871200	-3.42974100	1.11137900
H	6.11682500	-3.58864200	0.63543000
H	2.49611800	-2.21202100	-0.74798100
H	4.92794000	-4.54238300	-0.24925900
C	4.13120400	0.08868600	0.98868500
C	2.24190800	0.37023800	-0.08611400
N	3.77357600	1.29732500	1.29546700
N	3.23280100	-0.50068100	0.13985500
N	2.59663000	1.46096700	0.60407100
C	5.21382000	-0.79419600	1.51693900
H	6.01946000	-0.91502800	0.78084200
H	5.62195200	-0.38652000	2.44119400
C	1.92498100	2.71228800	0.64177500
C	1.10887200	3.03949200	1.72802500
C	2.06020600	3.61369700	-0.41612700
C	0.40080300	4.23353100	1.74509700
C	1.35474600	4.81179400	-0.41693400
C	0.52950300	5.09850100	0.66366800
H	-0.24398700	4.47585700	2.58059300
H	1.45085900	5.50309000	-1.24499000
Cl	0.92478300	1.91893600	3.02499100
Cl	-0.36683600	6.58380400	0.66766000
Cl	3.11069400	3.24617800	-1.73361700
O	4.58173400	-2.02579000	1.82154700

M7RS

C	-0.87330400	0.29448100	0.94902900
O	-1.16311500	0.47740600	2.17111300
C	0.25313400	1.07552000	0.19362000
C	1.33327100	1.56792600	1.15318900
H	-0.02336600	1.82267700	-0.55534300
C	1.35040300	3.07814700	1.33220800
H	1.14101700	1.09778300	2.12568900
H	0.40240300	3.41552200	1.76307500
H	2.15989900	3.38855000	2.00000900
H	1.48842600	3.58251600	0.36801000

C	0.73260600	-0.29238200	-0.33321900
O	-0.13753800	-0.99182800	0.57354700
C	2.21817900	-0.35470600	-0.00127400
C	2.64524900	0.98443400	0.57136000
H	2.94487600	1.61528700	-0.28177400
C	0.43278800	-0.56720800	-1.79454800
C	1.18374800	0.07913300	-2.78247600
C	-0.60371900	-1.41318300	-2.18150900
C	0.87090100	-0.08894000	-4.12595000
H	2.03269300	0.69520000	-2.49364000
C	-0.92190300	-1.58080300	-3.52809700
H	-1.14452500	-1.96025300	-1.41829000
C	-0.19326300	-0.90895800	-4.50456600
H	1.45989100	0.41978500	-4.88301100
H	-1.73996900	-2.23830700	-3.80711700
H	-0.43807600	-1.03551800	-5.55450100
C	3.77810600	0.98985500	1.57130100
C	4.86240700	1.85281300	1.40380200
C	3.73007300	0.18557600	2.71595400
C	5.87686900	1.92227700	2.35846200
H	4.90998700	2.47161900	0.51061200
C	4.73694400	0.25659600	3.67314100
H	2.89476300	-0.49828800	2.84772200
C	5.81358200	1.12733100	3.49894800
H	6.71136800	2.60151600	2.21109800
H	4.68510800	-0.37078400	4.55756600
H	6.59901200	1.18088200	4.24636000
C	2.99496200	-1.38764000	-0.33872200
O	4.38028000	-1.35176900	-0.18943900
C	2.50783800	-2.67095500	-0.88856600
C	1.46995200	-3.36282800	-0.25841700
C	3.06260500	-3.18212700	-2.06641000
C	0.97279800	-4.53632000	-0.81808200
H	1.05404600	-2.96330400	0.66023000
C	2.55962300	-4.35139800	-2.62490500
H	3.86864700	-2.64216900	-2.55551100
C	1.51096400	-5.02901300	-2.00374900
H	0.16956700	-5.07206200	-0.32038500
H	2.98128700	-4.73381200	-3.54895100
H	1.12156000	-5.94308200	-2.44101500
C	5.09340400	-0.38511000	-0.82192900
O	4.61779000	0.38641500	-1.61720700
C	6.55132400	-0.42501600	-0.42968200
C	6.86227500	-1.17088300	0.86537500

H	7.09785700	-0.86137400	-1.27574900
H	6.86995500	0.62071000	-0.36711100
C	8.29226100	-0.91169100	1.32729400
H	6.69521100	-2.24208500	0.71662100
H	6.15911600	-0.85125700	1.63992600
H	8.51905300	-1.46883900	2.23975900
H	8.43944400	0.15257800	1.53970100
H	9.02002800	-1.20560300	0.56359400
C	-3.60111100	-2.39130100	1.87449400
C	-4.43668500	-3.50337000	1.82326300
C	-5.24315600	-3.81399900	2.91465200
C	-5.19404100	-2.99260700	4.03897600
C	-4.34712400	-1.88154700	4.07938800
C	-3.53319000	-1.56625700	2.99336500
C	-2.82559500	-2.23736800	0.58601600
C	-3.47388000	-3.28446400	-0.39363100
C	-4.29806200	-4.23161100	0.50965800
H	-5.90141700	-4.67738900	2.88951400
H	-5.82097100	-3.22031300	4.89540800
H	-4.32178100	-1.25952500	4.96816400
H	-2.85129700	-0.71570300	2.99866200
H	-2.69581300	-3.81738100	-0.94304700
H	-5.25541600	-4.46047100	0.03072100
H	-1.75287500	-2.40080400	0.71333900
H	-3.77021900	-5.18171200	0.64359400
C	-4.12994200	-0.51253000	-0.60899900
C	-2.19292800	0.19415200	0.13431400
N	-4.11650700	0.74708400	-0.91728100
N	-2.98219500	-0.88463700	0.04097500
N	-2.90526900	1.17404200	-0.43110300
C	-5.07669000	-1.60895000	-0.97247800
H	-5.70606800	-1.88718000	-0.11659800
H	-5.71021200	-1.30230700	-1.80428500
C	-2.55097400	2.54585700	-0.52367500
C	-2.01101400	3.05286200	-1.70840300
C	-2.74952300	3.39587500	0.56608900
C	-1.63134000	4.38493700	-1.79882000
C	-2.37112500	4.73184400	0.49376300
C	-1.81125700	5.20219400	-0.68773800
H	-1.19850700	4.77161400	-2.71288000
H	-2.51528100	5.38814600	1.34304900
Cl	-1.76012200	1.99445800	-3.04903800
Cl	-1.32533600	6.86535200	-0.78209800
Cl	-3.48824000	2.79788400	2.00444000

O	-4.26709200	-2.68559400	-1.41031500
M7SR			
C	0.45928800	0.38905700	-0.77522600
O	-0.47603500	1.18256500	-1.12997700
C	0.29784100	-1.11646400	-1.21477800
C	-0.81330100	-1.36615200	-2.22038300
H	1.22047300	-1.67564700	-1.37994500
C	-0.54088300	-2.50563000	-3.19449200
H	-0.97873600	-0.43023900	-2.76441200
H	0.31575600	-2.28090100	-3.83695100
H	-1.41031100	-2.67997500	-3.83717800
H	-0.32639100	-3.43487500	-2.65423700
C	-0.24077700	-1.28873800	0.21894600
O	0.43444900	-0.10171200	0.66738300
C	-1.74786400	-1.13573800	0.04141700
C	-2.09319700	-1.63630200	-1.35659500
H	-2.22161800	-2.72844100	-1.28152100
C	0.14453900	-2.56243600	0.94162200
C	-0.75335400	-3.62154700	1.10523600
C	1.44788100	-2.70161700	1.41766100
C	-0.32964000	-4.80884000	1.69997400
H	-1.79171400	-3.50934400	0.80257300
C	1.86866700	-3.88326500	2.01686900
H	2.10878500	-1.85023700	1.33474000
C	0.98043700	-4.94884800	2.14986900
H	-1.03595500	-5.62391000	1.82254600
H	2.88674500	-3.97187800	2.38777400
H	1.30318800	-5.87498300	2.61488500
C	-3.31431800	-1.08048800	-2.05290100
C	-4.17206600	-1.93017300	-2.75168500
C	-3.55504500	0.29878100	-2.07686800
C	-5.26350300	-1.42024500	-3.45684000
H	-3.99160100	-3.00233700	-2.73005400
C	-4.65456300	0.80515300	-2.76002400
H	-2.86258700	0.95102400	-1.54788200
C	-5.51457600	-0.05201900	-3.45108800
H	-5.92102300	-2.09450800	-3.99735600
H	-4.84326400	1.87468300	-2.75938700
H	-6.36995500	0.34893200	-3.98643100
C	-2.58630600	-0.65583100	0.96667900
O	-3.95281300	-0.56485200	0.67830000
C	-2.29595300	-0.04151700	2.28615700
C	-1.19052400	-0.38719400	3.07254700

C	-3.18224800	0.93045500	2.77637900
C	-0.97713100	0.22488700	4.30335300
H	-0.49669600	-1.14649000	2.73895400
C	-2.96544800	1.54134000	4.00635000
H	-4.04565200	1.20768400	2.18231300
C	-1.86157200	1.18923600	4.77959400
H	-0.11653900	-0.06594900	4.89744100
H	-3.66346300	2.29314400	4.36156600
H	-1.69473100	1.65850900	5.74438200
C	0.51197900	3.96567100	0.22949300
C	0.71348000	5.33564700	0.37820500
C	0.42590300	5.95464700	1.59232900
C	-0.05870300	5.18008200	2.64274400
C	-0.26475700	3.80693000	2.48310200
C	0.01405400	3.18250700	1.27004300
C	0.88441500	3.50747600	-1.16155100
C	1.42000600	4.79875700	-1.88688400
C	1.22048800	5.96877800	-0.89141700
H	0.57801700	7.02294100	1.71763700
H	-0.28272400	5.64987500	3.59565900
H	-0.65508200	3.21484100	3.30536300
H	-0.16521200	2.11807600	1.13430100
H	0.83590400	4.95131200	-2.79466900
H	2.16323700	6.51018600	-0.75304800
H	0.04540700	3.04842300	-1.67801100
H	0.50254200	6.69092000	-1.29138400
C	3.25988100	2.78199300	-1.13619500
C	1.83620100	1.12843800	-0.90063500
N	4.01220500	1.73562600	-0.99189800
N	1.93135900	2.45791000	-1.10459200
N	3.11200200	0.71751800	-0.83832300
C	3.64646900	4.20030900	-1.38465400
H	3.60060600	4.77336400	-0.44727500
H	4.65989100	4.24935600	-1.78299300
C	3.64745400	-0.56045100	-0.52774100
C	3.81007000	-1.53588300	-1.51265000
C	4.14960900	-0.79136600	0.75562100
C	4.38070800	-2.76430100	-1.20583900
C	4.75598400	-1.99935400	1.07298000
C	4.84250800	-2.97689800	0.08823900
H	4.47868500	-3.52940400	-1.96567100
H	5.12963900	-2.17829600	2.07390700
Cl	3.31128500	-1.20898000	-3.13596200
Cl	5.55205300	-4.50826500	0.48567600

Cl	3.95636900	0.40959000	1.97917100
O	2.75734000	4.70287800	-2.35462700
C	-4.66963200	-1.69154200	0.47373600
O	-4.20793200	-2.80492600	0.52968900
C	-6.10334500	-1.37223600	0.12530300
C	-6.58608700	0.03160400	0.47779100
H	-6.72191400	-2.14407500	0.59427900
H	-6.18107800	-1.52593100	-0.95893000
C	-8.01987600	0.25449900	0.00612500
H	-6.51216400	0.18817200	1.56022500
H	-5.92128500	0.76065600	0.00504000
H	-8.37258400	1.25581500	0.26525700
H	-8.08540100	0.14460600	-1.08150600
H	-8.70443200	-0.47099100	0.45698200

M7SS

C	0.64836300	0.37847900	-1.00622200
O	0.02150400	1.38995500	-1.45448600
C	0.02654600	-1.03106400	-1.29107300
C	-1.13343000	-1.09786800	-2.27309800
H	0.75834200	-1.83166400	-1.42154500
C	-1.39704700	-2.55288900	-2.66598800
H	-0.90095400	-0.51129800	-3.16805500
H	-0.51737900	-2.96872700	-3.16800700
H	-2.25388600	-2.64413300	-3.33811900
H	-1.60239900	-3.16776100	-1.78183900
C	-0.52334300	-0.91042900	0.14341700
O	0.50225300	0.03623600	0.50073800
C	-1.86781000	-0.23703300	-0.07131300
C	-2.32480300	-0.40084800	-1.52280900
H	-2.39377000	0.61873300	-1.91407600
C	-0.59794300	-2.15471200	1.01801800
C	-1.63762600	-2.36531000	1.93326700
C	0.39048800	-3.13578600	0.91031000
C	-1.66669100	-3.51094300	2.72591900
H	-2.43845900	-1.63678000	2.02500400
C	0.36524100	-4.28060900	1.69980900
H	1.18434100	-3.01306900	0.18403200
C	-0.66497500	-4.47074200	2.61661000
H	-2.48088500	-3.65018200	3.42978500
H	1.14415400	-5.03007700	1.58919300
H	-0.69175500	-5.36436100	3.23203500
C	-3.66889600	-1.06340300	-1.74118900
C	-4.45268600	-0.68322500	-2.83628300

C	-4.14302300	-2.07731000	-0.90498600
C	-5.67442800	-1.30026200	-3.09372100
H	-4.09591400	0.10708300	-3.49314700
C	-5.36853500	-2.69149500	-1.15260000
H	-3.55397800	-2.37282000	-0.04033000
C	-6.13798300	-2.30794700	-2.24902100
H	-6.26639100	-0.99126700	-3.95015500
H	-5.72403500	-3.46853900	-0.48327400
H	-7.09319500	-2.78635500	-2.44084700
C	-2.51354300	0.58919800	0.76349300
O	-3.71844200	1.09392400	0.23776900
C	-2.15863900	1.16809700	2.07996400
C	-1.07187600	0.74078200	2.85951000
C	-2.93451600	2.23225700	2.56625600
C	-0.79150500	1.34941500	4.07886500
H	-0.42776400	-0.05752100	2.52050000
C	-2.64808300	2.84028200	3.78226900
H	-3.76566900	2.59905500	1.97600500
C	-1.57667700	2.39806900	4.55222400
H	0.05270600	0.99522800	4.66258500
H	-3.26833500	3.66160500	4.12713800
H	-1.35466300	2.86510100	5.50670600
C	1.78972000	3.81788200	-0.20228600
C	2.37432500	5.07963400	-0.13124200
C	2.20999100	5.85922100	1.01130600
C	1.45614300	5.35306200	2.06708800
C	0.86893700	4.08711400	1.98554400
C	1.02898800	3.30323300	0.84629800
C	2.08176000	3.15740500	-1.53033900
C	3.06052000	4.14270400	-2.27043800
C	3.11169400	5.42347800	-1.40043500
H	2.66077400	6.84534000	1.07750800
H	1.32017700	5.95096100	2.96323600
H	0.27259800	3.70745800	2.81066500
H	0.56351500	2.32346200	0.77354300
H	2.66526300	4.35325500	-3.26437000
H	4.15330100	5.71748400	-1.22950200
H	1.17295000	2.95761700	-2.09211800
H	2.63179100	6.25677600	-1.92275400
C	4.07839700	1.73678100	-1.16125000
C	2.18914100	0.62832400	-1.07091400
N	4.43502700	0.52962400	-0.84859500
N	2.72318900	1.83845100	-1.32148500
N	3.24493500	-0.14385300	-0.78573300

C	4.91298500	2.94710800	-1.41221400
H	4.92805700	3.58720300	-0.51815000
H	5.93406400	2.65683300	-1.66001200
C	3.29943100	-1.49166700	-0.34353300
C	3.39242500	-2.53654200	-1.26425500
C	3.42010500	-1.76183300	1.02228000
C	3.58091700	-3.84507600	-0.83800300
C	3.62122000	-3.06286900	1.46694500
C	3.70448300	-4.08344100	0.52703500
H	3.64566800	-4.65357800	-1.55548000
H	3.70256300	-3.27203100	2.52643600
Cl	3.27170800	-2.19857200	-2.95629800
Cl	3.96263000	-5.71035400	1.07382600
Cl	3.31187900	-0.47807500	2.16528400
O	4.35181600	3.60673500	-2.52421400
C	-4.84826800	0.49885400	0.69795600
O	-4.85519800	-0.27806200	1.61947300
C	-6.06619100	0.88862400	-0.10069400
C	-5.90839200	2.07055500	-1.05077000
H	-6.88045600	1.04787300	0.61387000
H	-6.32704500	-0.01558800	-0.66872800
C	-7.17586100	2.28621200	-1.87166500
H	-5.66231900	2.97510400	-0.48339500
H	-5.06043600	1.88027600	-1.71514600
H	-7.06860500	3.13039900	-2.55726700
H	-7.40163400	1.39385100	-2.46523600
H	-8.03783200	2.48342900	-1.22629200

TS8RR

C	1.02846300	-0.02210000	-1.46588700
O	1.69219300	0.05846200	-2.48748100
C	-0.25622500	0.67755200	-1.01253000
C	-1.23141600	0.79492000	-2.19417400
H	-0.18362000	1.58320400	-0.41266900
C	-1.39753700	2.22197800	-2.70004200
H	-0.81403700	0.19533800	-3.01159000
H	-0.43811800	2.59014900	-3.07671600
H	-2.12637100	2.26958300	-3.51505600
H	-1.73851000	2.89188100	-1.90431900
C	-0.58447300	-0.66784600	-0.29859200
O	0.55234700	-1.28341100	-0.98437700
C	-1.96899700	-1.03528100	-0.82230200
C	-2.51563700	0.06483400	-1.72915400
H	-3.01912400	-0.39337700	-2.58790400

C	-0.44951000	-0.82900900	1.21003300
C	-1.50845400	-0.51752900	2.07113600
C	0.70673100	-1.38874400	1.75861700
C	-1.38795600	-0.72027200	3.44271300
H	-2.45927500	-0.18093500	1.66987500
C	0.82696000	-1.59517800	3.12972700
H	1.50061300	-1.70618400	1.09440100
C	-0.21904400	-1.25303700	3.98098300
H	-2.22595500	-0.47992200	4.08958200
H	1.73831000	-2.03332400	3.52625000
H	-0.13371900	-1.41959000	5.05031200
C	-3.52313300	0.98841300	-1.06632100
C	-4.80163900	1.12011400	-1.60894900
C	-3.20080500	1.75685200	0.05953400
C	-5.74705900	1.96742400	-1.03166300
H	-5.06098300	0.54919100	-2.49795900
C	-4.13885500	2.60359800	0.63841800
H	-2.20690800	1.69324600	0.49478400
C	-5.42014300	2.70775700	0.09883800
H	-6.73715700	2.04939500	-1.47058300
H	-3.86769300	3.18726400	1.51299800
H	-6.15248400	3.36768900	0.55224600
C	-2.67275500	-2.11748600	-0.47486500
O	-3.99602900	-2.20536000	-0.93532600
C	-2.21739000	-3.28756700	0.30251500
C	-0.93629900	-3.81277200	0.10023900
C	-3.06576200	-3.89543300	1.23592000
C	-0.50529000	-4.91112500	0.83739100
H	-0.28483900	-3.35777600	-0.63915100
C	-2.63091600	-4.99390300	1.96737700
H	-4.05383000	-3.48660900	1.41452300
C	-1.34907100	-5.50421700	1.77192100
H	0.49028100	-5.31119500	0.67215200
H	-3.29331400	-5.44942800	2.69648600
H	-1.01307300	-6.36362100	2.34360400
C	-4.96380000	-1.66077500	-0.15118900
O	-4.74524600	-1.16733600	0.92532700
C	-6.33639400	-1.78802900	-0.76892800
C	-6.39435300	-2.28733400	-2.20890600
H	-6.90895000	-2.45192300	-0.10921500
H	-6.79545400	-0.79819200	-0.67007300
C	-7.82746700	-2.29943500	-2.73254700
H	-5.96054200	-3.29022000	-2.26403000
H	-5.76718900	-1.65093100	-2.84230900

H	-7.87022700	-2.66129900	-3.76237100
H	-8.26103300	-1.29439200	-2.70971700
H	-8.46257600	-2.94808900	-2.12121100
C	4.85265600	-1.38033800	-1.43895800
C	5.92242300	-2.24053500	-1.20443700
C	6.98448600	-2.29300200	-2.10181500
C	6.95372600	-1.46982800	-3.22563900
C	5.87496900	-0.61241600	-3.45397000
C	4.80588000	-0.55991500	-2.56166600
C	3.82284200	-1.49124900	-0.33341100
C	4.55454300	-2.31570500	0.78715200
C	5.71791500	-3.02855000	0.06485400
H	7.82474500	-2.95840800	-1.92640200
H	7.77769800	-1.49536200	-3.93187600
H	5.86767700	0.01635000	-4.33832500
H	3.94533700	0.08176700	-2.73196200
H	3.86621300	-3.02219300	1.25522600
H	6.59818800	-3.05672200	0.71375000
H	2.90818100	-1.98654700	-0.67479000
H	5.44580800	-4.06531600	-0.16212700
C	4.27802200	0.52001700	1.00908000
C	2.30799900	0.51667900	-0.02295200
N	3.76891300	1.67013700	1.32381200
N	3.43462100	-0.18858400	0.19036800
N	2.55942500	1.64683100	0.65913000
C	5.47826200	-0.21309500	1.51205300
H	6.26929900	-0.25378500	0.75180900
H	5.86616100	0.25682300	2.41544200
C	1.66653500	2.74455400	0.73709500
C	0.85574300	2.91787300	1.86154800
C	1.50014500	3.59751000	-0.35730500
C	-0.12923600	3.89853300	1.88687100
C	0.51955400	4.58189000	-0.35443800
C	-0.28879400	4.70898600	0.76923900
H	-0.76485600	4.01299300	2.75643600
H	0.38343300	5.22427100	-1.21568700
Cl	1.03603800	1.86334800	3.21327800
Cl	-1.53894700	5.91514700	0.77490800
Cl	2.48481300	3.39267500	-1.76386300
O	5.01525300	-1.50849000	1.86483500
TS8RS			
C	0.64919600	-0.02704400	-1.35353300
O	1.04433400	-0.17382900	-2.49677600

C	-0.32359300	0.98392400	-0.72185500
C	-1.50594600	1.29476200	-1.64704800
H	0.09034000	1.86461500	-0.22786200
C	-1.59364900	2.75841500	-2.05498600
H	-1.39673300	0.68414400	-2.55199100
H	-0.70546900	3.05368700	-2.62175600
H	-2.47405600	2.93720800	-2.67998300
H	-1.66482000	3.40131400	-1.16977100
C	-0.74348800	-0.20469700	0.17936000
O	0.07214500	-1.11152100	-0.61273700
C	-2.24296000	-0.35871800	-0.03451000
C	-2.75454200	0.79611100	-0.87531700
H	-3.06191000	1.59102000	-0.17693600
C	-0.34504300	-0.18320900	1.63982500
C	-1.01947100	0.66541700	2.52279100
C	0.63460400	-1.04065000	2.13673400
C	-0.71659100	0.65084500	3.87981500
H	-1.81734300	1.30437400	2.15041200
C	0.93977700	-1.05477800	3.49589600
H	1.12354600	-1.72714700	1.45391600
C	0.26385700	-0.21084400	4.37153500
H	-1.25403100	1.30726600	4.55722700
H	1.70020900	-1.73576800	3.86631800
H	0.49370200	-0.22611600	5.43240300
C	-3.91433400	0.50964800	-1.80239800
C	-5.02145800	1.35824900	-1.84374300
C	-3.86188300	-0.57201500	-2.68872000
C	-6.05508400	1.13930700	-2.75549000
H	-5.07253500	2.19511900	-1.15049000
C	-4.88737200	-0.79053500	-3.60161000
H	-3.00606500	-1.24269300	-2.65554500
C	-5.98817900	0.06688100	-3.63945700
H	-6.90907200	1.80977500	-2.77473000
H	-4.83099500	-1.63249800	-4.28435600
H	-6.78893800	-0.10476200	-4.35173800
C	-2.97543200	-1.29339900	0.57800000
O	-4.36587300	-1.30652400	0.49083100
C	-2.45065700	-2.40973000	1.39405400
C	-1.48747400	-3.28487600	0.88710900
C	-2.92102600	-2.57820100	2.70023800
C	-0.98945900	-4.30929000	1.68816700
H	-1.12856700	-3.14625900	-0.12759300
C	-2.41436500	-3.59513200	3.49951700
H	-3.66349000	-1.88778400	3.09089800

C	-1.44772600	-4.46397000	2.99352700
H	-0.24597800	-4.99248900	1.28871600
H	-2.77057800	-3.71046700	4.51809500
H	-1.05672600	-5.26175000	3.61718900
C	-5.07303200	-0.23030000	0.92397700
O	-4.57837300	0.70260500	1.50526500
C	-6.54452100	-0.36830500	0.61298800
C	-6.90407400	-1.43176700	-0.42044400
H	-7.05548100	-0.55382300	1.56625600
H	-6.86965500	0.62369700	0.28126900
C	-8.35750800	-1.30454300	-0.86430300
H	-6.71642500	-2.42514600	-0.00108400
H	-6.24118500	-1.32830100	-1.28456300
H	-8.61809100	-2.08084800	-1.58803900
H	-8.52939300	-0.33261200	-1.33882400
H	-9.04470900	-1.38993900	-0.01611000
C	3.85508200	-2.42003000	-1.76169400
C	4.70292200	-3.51416300	-1.61366800
C	5.54282900	-3.88976400	-2.65861700
C	5.51448700	-3.15255400	-3.84061100
C	4.65482500	-2.06044100	-3.98137900
C	3.81055800	-1.68196200	-2.94033300
C	3.04921600	-2.17915900	-0.50311000
C	3.69869900	-3.13927300	0.56153900
C	4.53772600	-4.14913400	-0.25565400
H	6.21244700	-4.73846100	-2.55385700
H	6.16692400	-3.43076600	-4.66233800
H	4.64260500	-1.50324700	-4.91244900
H	3.11689600	-0.85054700	-3.03681000
H	2.92298100	-3.63471300	1.14867600
H	5.48498700	-4.34454800	0.25656400
H	1.98485200	-2.38749200	-0.64434100
H	4.00989800	-5.10561500	-0.33530100
C	4.28509100	-0.34534200	0.58106800
C	2.29803000	0.23136700	-0.23446400
N	4.21857700	0.92688800	0.81621800
N	3.15568300	-0.79304800	-0.05736800
N	2.98570000	1.25931700	0.29020900
C	5.26282200	-1.38493900	1.02048700
H	5.90518100	-1.70613300	0.18933200
H	5.88429500	-1.00832200	1.83261600
C	2.52894400	2.59802900	0.35977900
C	2.17652800	3.16186200	1.58916700
C	2.38005500	3.36107600	-0.80205700

C	1.68902500	4.46083900	1.66618700
C	1.88164700	4.65733300	-0.74765100
C	1.54686400	5.18888800	0.49147500
H	1.41350300	4.88575900	2.62329600
H	1.76274500	5.23606100	-1.65533400
Cl	2.28928600	2.21684300	3.02768700
Cl	0.92656800	6.80914600	0.57485100
Cl	2.78764500	2.68426900	-2.33943800
O	4.48331900	-2.45540900	1.52954500

TS8SR

C	0.62058300	0.00159200	-1.26519500
O	0.88472500	-0.16172200	-2.44888200
C	-0.22224800	1.07769300	-0.54022600
C	-1.41008600	1.66958300	-1.29635800
H	0.35003800	1.83276200	-0.00030900
C	-1.07518700	2.29210900	-2.64529500
H	-1.83551700	2.44409900	-0.64128500
H	-1.98149900	2.68196100	-3.11907200
H	-0.36978500	3.12050800	-2.52406900
H	-0.61348600	1.54834800	-3.29837000
C	-0.75102100	-0.11439700	0.29759000
O	0.02810500	-1.05704900	-0.48193800
C	-2.20647000	-0.28097600	-0.10598800
C	-2.45983500	0.53088300	-1.36919100
H	-2.19589400	-0.11170400	-2.22279800
C	-0.42006200	-0.11804900	1.76659100
C	-1.01081600	0.83424900	2.60119800
C	0.46435000	-1.04755000	2.30902800
C	-0.73520500	0.84308700	3.96331700
H	-1.70909500	1.55473900	2.17987500
C	0.73961700	-1.04054200	3.67477800
H	0.91364000	-1.78957000	1.65642900
C	0.13887400	-0.09896400	4.50546700
H	-1.20449900	1.58255200	4.60493600
H	1.42224000	-1.77715400	4.08752500
H	0.34919100	-0.09707800	5.57041300
C	-3.85417200	1.07474900	-1.58326300
C	-4.51354200	0.88991200	-2.79988300
C	-4.48027100	1.84024800	-0.59334500
C	-5.76644600	1.45776900	-3.02864700
H	-4.03689900	0.29646100	-3.57614900
C	-5.72823900	2.41272300	-0.81824100
H	-3.99393800	1.96620200	0.37108400

C	-6.37482500	2.22733000	-2.04044700
H	-6.26149700	1.30316900	-3.98255200
H	-6.20077100	2.99735400	-0.03517100
H	-7.34779700	2.67512200	-2.21661000
C	-3.02635800	-1.16958200	0.45212600
O	-4.26272600	-1.39889700	-0.16363300
C	-2.66254900	-2.10832500	1.54939500
C	-1.90294400	-3.23601900	1.22534700
C	-3.01102000	-1.86711100	2.88067300
C	-1.49473500	-4.11640200	2.22356500
H	-1.61812100	-3.40140500	0.19044700
C	-2.58692900	-2.74041300	3.87670600
H	-3.59487400	-0.98608000	3.12068900
C	-1.83128800	-3.86551300	3.55097000
H	-0.90564000	-4.99122100	1.96561800
H	-2.84132300	-2.53828800	4.91242100
H	-1.50265900	-4.54367000	4.33255800
C	-5.37044800	-0.92894800	0.45517100
O	-5.34493800	-0.38827300	1.53275900
C	-6.60864600	-1.10464700	-0.38679500
C	-6.48885800	-2.01318300	-1.60614700
H	-7.40729900	-1.43381300	0.28628500
H	-6.87683200	-0.08823200	-0.70516600
C	-7.76975100	-1.98291800	-2.43461700
H	-6.26267700	-3.03624800	-1.28690100
H	-5.64410400	-1.67971000	-2.21597900
H	-7.69632700	-2.63790900	-3.30614600
H	-7.96798700	-0.96623300	-2.79090700
H	-8.63363800	-2.30374700	-1.84383700
C	3.52630600	-2.69332800	-1.85408800
C	4.29761500	-3.84755400	-1.75365000
C	5.06593700	-4.26638900	-2.83691500
C	5.04316600	-3.51141800	-4.00762400
C	4.25805300	-2.35941600	-4.10083300
C	3.48538800	-1.93723000	-3.02178000
C	2.78774700	-2.41290200	-0.56370600
C	3.37753100	-3.45513000	0.45829500
C	4.13826100	-4.49346100	-0.40051500
H	5.67482900	-5.16337700	-2.77101100
H	5.64080900	-3.82294700	-4.85859100
H	4.24740100	-1.79051200	-5.02480400
H	2.84683500	-1.05845800	-3.07975200
H	2.57108800	-3.91579600	1.03127600
H	5.08885800	-4.74640200	0.07998700

H	1.70518800	-2.51709500	-0.66926500
H	3.56016800	-5.42040500	-0.47675700
C	4.21192700	-0.72811600	0.54131500
C	2.30922100	0.06770000	-0.28044600
N	4.28656800	0.54360300	0.77801600
N	3.03974100	-1.04943200	-0.09622900
N	3.10170700	1.01253000	0.24891000
C	5.08590400	-1.86253200	0.96261600
H	5.69985500	-2.22156900	0.12500300
H	5.73707300	-1.55946200	1.78225000
C	2.81374400	2.39819000	0.31048000
C	2.50781100	2.99978700	1.53459800
C	2.80458200	3.17620800	-0.85073100
C	2.21115000	4.35515700	1.60882600
C	2.49888500	4.53104400	-0.79837800
C	2.21221600	5.10072100	0.43602600
H	1.97260600	4.81225200	2.56108400
H	2.49037700	5.12583900	-1.70323200
Cl	2.43575100	2.03761400	2.96471400
Cl	1.83622600	6.79419300	0.51383100
Cl	3.15607600	2.45143400	-2.37964700
O	4.21201600	-2.86700900	1.44720300

TS8SS

C	0.73753200	-0.11207700	-1.42034700
O	1.24954600	-0.38072100	-2.50014300
C	-0.32642500	0.92437200	-0.97076900
C	-1.53188000	1.14102400	-1.91961400
H	0.05326100	1.85830800	-0.55332300
C	-1.40911200	0.43444700	-3.26996100
H	-1.63704000	2.21229700	-2.11940700
H	-2.29031400	0.63920800	-3.88239000
H	-0.51689400	0.78149100	-3.79254500
H	-1.30600500	-0.64780400	-3.15106800
C	-0.72893100	-0.17483600	0.04936900
O	0.10775300	-1.14140900	-0.62892600
C	-2.22382900	-0.37775600	-0.13174900
C	-2.76324700	0.68944500	-1.06040800
H	-3.02916800	1.54177900	-0.41639600
C	-0.35138400	0.00857200	1.50649800
C	-1.02946600	0.96157300	2.27288500
C	0.57003500	-0.83056700	2.12954500
C	-0.79859300	1.05726700	3.64056900
H	-1.78609500	1.58862300	1.80670300

C	0.80355600	-0.73454500	3.49954300
H	1.05961600	-1.59770500	1.53910600
C	0.11526500	0.20568000	4.26034600
H	-1.34277900	1.79153900	4.22657300
H	1.51386200	-1.40890900	3.96884700
H	0.28624000	0.27477300	5.33021200
C	-3.99984100	0.33007200	-1.85623500
C	-5.04461500	1.24827100	-1.97335400
C	-4.11379100	-0.89725700	-2.52120600
C	-6.16729200	0.96421900	-2.75206100
H	-4.97748900	2.19614600	-1.44387900
C	-5.22094900	-1.17666900	-3.31410700
H	-3.32652100	-1.63718100	-2.40761600
C	-6.25301100	-0.24513700	-3.43432500
H	-6.96931100	1.69228600	-2.82818700
H	-5.28686800	-2.12989200	-3.82934900
H	-7.12176200	-0.46871400	-4.04540500
C	-2.93234300	-1.23127800	0.61416400
O	-4.32615700	-1.22258300	0.62158000
C	-2.35298000	-2.25195400	1.51344100
C	-1.44532100	-3.19554700	1.02742500
C	-2.67878900	-2.23793400	2.87337500
C	-0.85489000	-4.10697700	1.89936600
H	-1.19609800	-3.19339500	-0.02875100
C	-2.07721100	-3.13956500	3.74233100
H	-3.37507000	-1.49182400	3.24645900
C	-1.16337800	-4.07518100	3.25645700
H	-0.15432100	-4.84316100	1.51659700
H	-2.31444700	-3.11082300	4.80100000
H	-0.69836900	-4.78142600	3.93727100
C	-4.96839100	-0.08685400	1.00463500
O	-4.40354900	0.87817300	1.45489700
C	-6.46387700	-0.19174900	0.82517000
C	-6.95372700	-1.35910700	-0.02471400
H	-6.90227300	-0.22035600	1.83077200
H	-6.77206900	0.76375700	0.38622300
C	-8.43865000	-1.22630300	-0.34612200
H	-6.75620500	-2.30025500	0.49805700
H	-6.37503100	-1.38926800	-0.95163700
H	-8.79143600	-2.07499700	-0.93741800
H	-8.62564000	-0.31451900	-0.92329400
H	-9.04317500	-1.17633800	0.56546300
C	3.90002100	-2.52361500	-1.53643100
C	4.65911000	-3.65494300	-1.24408300

C	5.54720400	-4.16270100	-2.18704500
C	5.66185300	-3.51626600	-3.41616000
C	4.89504500	-2.38444700	-3.70173800
C	3.99870400	-1.87556900	-2.76305200
C	3.01777300	-2.15515700	-0.36039300
C	3.59555300	-3.00955800	0.82399600
C	4.35135100	-4.16762700	0.14064900
H	6.14585400	-5.04144700	-1.96576300
H	6.35590800	-3.89616900	-4.15932400
H	4.99625200	-1.89814700	-4.66659900
H	3.37485000	-1.01117000	-2.97250300
H	2.79136200	-3.36783400	1.47054800
H	5.23822500	-4.43210000	0.72344200
H	1.96553800	-2.38488300	-0.54540500
H	3.71332400	-5.05733400	0.09085900
C	4.22744400	-0.23866000	0.57586200
C	2.23524500	0.26926000	-0.26436800
N	4.15020800	1.04463500	0.73165000
N	3.10276200	-0.73560400	-0.03202500
N	2.91221300	1.33580200	0.19183000
C	5.21150200	-1.24061000	1.08402500
H	5.84385800	-1.62655400	0.27394000
H	5.84112700	-0.79776100	1.85552900
C	2.45918100	2.67840400	0.19837100
C	2.16560800	3.31780900	1.40654400
C	2.29392300	3.38300600	-0.99797300
C	1.71945700	4.63368100	1.42793300
C	1.83908800	4.69599800	-0.99750000
C	1.56257400	5.30328600	0.22098400
H	1.49177800	5.11828400	2.36916900
H	1.70931900	5.22968900	-1.93063600
Cl	2.31163400	2.45567900	2.89310700
Cl	0.99933800	6.94645400	0.23476000
Cl	2.62132100	2.60730000	-2.50621300
O	4.44217100	-2.26571300	1.69349200

M8RR

C	-2.25589600	-2.32270700	-1.94684500
O	-2.84686200	-3.01493400	-2.71700300
C	-1.19581000	-2.47672000	-0.87837700
C	0.21291600	-2.57138000	-1.51203000
H	-1.38869000	-3.18335200	-0.06952700
C	0.90749900	-3.90244900	-1.25693700
H	0.10027700	-2.45124100	-2.59635200

H	0.33900300	-4.71775600	-1.71202400
H	1.91279700	-3.90267200	-1.68843700
H	1.00188300	-4.09892900	-0.18566400
C	-1.47206200	-0.96738100	-0.62145200
O	-2.34128600	-0.96570400	-1.82622600
C	-0.14166100	-0.27594000	-0.80430600
C	0.96556800	-1.30394900	-1.01282400
H	1.64302700	-0.95214800	-1.79865600
C	-2.28976100	-0.61553800	0.60500100
C	-1.72798900	0.03949400	1.70545600
C	-3.63171900	-1.00679300	0.65921500
C	-2.49770200	0.28691900	2.83934500
H	-0.69380700	0.37214600	1.67866500
C	-4.39547300	-0.75678000	1.79427500
H	-4.09182800	-1.49389400	-0.19465900
C	-3.83017100	-0.10990100	2.89015300
H	-2.04882600	0.80199800	3.68247800
H	-5.43645500	-1.06292600	1.81755500
H	-4.42695300	0.09068600	3.77415900
C	1.80842000	-1.54963000	0.22509300
C	3.19979800	-1.51820100	0.13152200
C	1.22716800	-1.82700400	1.46674300
C	3.99882200	-1.73042100	1.25479000
H	3.66457000	-1.32555400	-0.83293300
C	2.01948300	-2.04000000	2.58833900
H	0.14473800	-1.85801700	1.56600400
C	3.40938900	-1.98544100	2.48793400
H	5.08016500	-1.69440500	1.16213700
H	1.55120700	-2.24156100	3.54648500
H	4.02594600	-2.14475600	3.36662500
C	0.09237900	1.04087400	-0.72992800
O	1.43263400	1.44317900	-0.79922600
C	-0.87950400	2.14806700	-0.62738500
C	-2.11289500	2.07712600	-1.28547100
C	-0.57260500	3.29186800	0.12137300
C	-3.03007400	3.11619400	-1.17186000
H	-2.34875500	1.21654300	-1.90050500
C	-1.49258300	4.32737900	0.23057100
H	0.37336100	3.36126500	0.64526500
C	-2.72530200	4.24227900	-0.41274700
H	-3.98197200	3.04685100	-1.68804800
H	-1.24602900	5.20255500	0.82284300
H	-3.44211300	5.05253400	-0.32656500
C	2.11491200	1.53202700	0.37648400

O	1.59707800	1.36847100	1.45113900
C	3.56206000	1.90689000	0.17097500
C	4.07863100	1.87543700	-1.26360200
H	3.68164500	2.90962000	0.60044800
H	4.13543500	1.23257500	0.81616100
C	5.56543200	2.21346300	-1.32158300
H	3.50407500	2.57903100	-1.87331000
H	3.90208400	0.88358200	-1.69348100
H	5.93478500	2.19967600	-2.34946500
H	6.15321300	1.49466100	-0.74180800
H	5.75708000	3.20870800	-0.90840300

M8RS

C	1.75319400	2.98549800	-1.14788000
O	2.02558400	3.93460800	-1.81546200
C	1.14330500	2.69844800	0.20793800
C	-0.39351800	2.82877500	0.19253200
H	1.63340100	3.13283400	1.08022400
C	-0.93767000	3.86655700	1.16343700
H	-0.71477000	3.09674100	-0.82223700
H	-0.57884300	4.86725200	0.91006400
H	-2.03111500	3.87727500	1.13540100
H	-0.62272800	3.63598900	2.18662300
C	1.47692600	1.22260700	-0.14495600
O	1.88393000	1.67030900	-1.49501000
C	0.16263000	0.47463900	-0.09171700
C	-0.90241600	1.39395000	0.48436900
H	-0.88244900	1.25214700	1.57673000
C	2.63651600	0.60576200	0.60104100
C	2.39955600	-0.09222500	1.78920700
C	3.94711000	0.79063500	0.16148700
C	3.46632700	-0.59212800	2.52765600
H	1.37853800	-0.26438500	2.12252100
C	5.01151500	0.28214700	0.90246800
H	4.13344600	1.31444100	-0.76983600
C	4.77542800	-0.40623100	2.08795000
H	3.27233600	-1.13551600	3.44696400
H	6.02710000	0.42247100	0.54625000
H	5.60581200	-0.80255800	2.66356900
C	-2.32652700	1.20467400	0.01183500
C	-3.37317500	1.14463800	0.93299600
C	-2.62700000	1.16392100	-1.35422800
C	-4.69726500	1.05332900	0.50323500
H	-3.14433600	1.16551500	1.99625100

C	-3.94602300	1.07875900	-1.78604200
H	-1.81551800	1.19566100	-2.07801700
C	-4.98659700	1.02532500	-0.85756700
H	-5.49983600	1.00771500	1.23320100
H	-4.16433200	1.04990700	-2.84884200
H	-6.01548000	0.95666200	-1.19600200
C	0.03686100	-0.83961700	-0.32436300
O	-1.16674200	-1.49276700	-0.07603500
C	1.06995800	-1.75911500	-0.84142600
C	1.93639700	-1.38104100	-1.87047400
C	1.18756900	-3.03475500	-0.27674800
C	2.92260300	-2.25872000	-2.30945100
H	1.83093500	-0.40454200	-2.32980400
C	2.17606200	-3.90649600	-0.71571300
H	0.51107300	-3.33319200	0.51848000
C	3.04679500	-3.51955800	-1.73300100
H	3.58925400	-1.95746000	-3.11085100
H	2.26902400	-4.88873700	-0.26384100
H	3.81603000	-4.20272900	-2.07856200
C	-1.66468900	-1.51811600	1.18897200
O	-1.07145800	-1.08420800	2.14441100
C	-3.01909800	-2.18099400	1.24294900
C	-3.73512600	-2.32920500	-0.09662800
H	-2.87522000	-3.15666600	1.72439800
H	-3.61354400	-1.58214700	1.94107000
C	-5.18871300	-2.74802000	0.09551300
H	-3.20344300	-3.05939400	-0.71448900
H	-3.69053400	-1.37635500	-0.63179800
H	-5.68940500	-2.88372300	-0.86620300
H	-5.73745000	-1.98275300	0.65450800
H	-5.26406500	-3.68864500	0.65066700

M8SR

C	1.41470500	2.96576100	-1.55683600
O	1.40420000	3.80648200	-2.40302100
C	1.03029700	2.84114800	-0.09025100
C	-0.46170400	2.88653200	0.24037800
H	1.66416500	3.43293500	0.57253200
C	-1.18470900	4.13647300	-0.24107100
H	-0.54559800	2.81473300	1.33295200
H	-2.25107300	4.06910200	-0.00680200
H	-0.78459300	5.03373200	0.23791200
H	-1.07112400	4.25250600	-1.32314200
C	1.43520700	1.36001900	-0.29685500

O	1.81083400	1.66715200	-1.69156500
C	0.12916900	0.59194900	-0.30073900
C	-1.03677400	1.57130200	-0.35118000
H	-1.26891900	1.75312300	-1.41239800
C	2.58089700	0.81390500	0.50427700
C	2.42292900	0.67057900	1.88445700
C	3.77954300	0.44111200	-0.09747100
C	3.45193300	0.14336500	2.65546400
H	1.48360700	0.95833100	2.35220600
C	4.80646700	-0.09446000	0.67644800
H	3.89235700	0.54800500	-1.17094900
C	4.64586300	-0.24616000	2.05035400
H	3.32087100	0.03111400	3.72702300
H	5.73241300	-0.40013400	0.19956900
H	5.44737800	-0.66602200	2.64965100
C	-2.31753600	1.16961700	0.34744100
C	-3.55016800	1.30885200	-0.29300400
C	-2.29635700	0.72683600	1.67400900
C	-4.73907200	1.01988300	0.37593300
H	-3.57776000	1.64964600	-1.32508100
C	-3.48008900	0.43690600	2.34531300
H	-1.34131300	0.57836200	2.17216800
C	-4.70722100	0.58885500	1.69967400
H	-5.68862100	1.13645600	-0.13709400
H	-3.44383000	0.08535900	3.37144900
H	-5.63078700	0.36565800	2.22411200
C	0.05408100	-0.73396100	-0.41773000
O	-1.20868100	-1.28984000	-0.62742400
C	1.21222400	-1.65972700	-0.55299900
C	1.83182800	-1.76146400	-1.80123000
C	1.71494900	-2.37997700	0.53376000
C	2.94577400	-2.58062400	-1.96405300
H	1.44897700	-1.18004900	-2.63487700
C	2.83669200	-3.18502000	0.36912600
H	1.22971700	-2.28722700	1.49827300
C	3.45123100	-3.28886800	-0.87771900
H	3.42339400	-2.65603900	-2.93573700
H	3.23686900	-3.72813500	1.21940800
H	4.32641000	-3.91954500	-1.00028300
C	-1.76553900	-2.00485400	0.38214100
O	-1.19884600	-2.22153500	1.42294200
C	-3.17984100	-2.41656700	0.06549300
C	-3.61783900	-2.29833800	-1.39086300
H	-3.30752900	-3.43432400	0.44800100

H	-3.80669700	-1.77034300	0.69511200
C	-5.08963600	-2.66804300	-1.54870300
H	-2.99321000	-2.94065700	-2.02059200
H	-3.45219600	-1.27057900	-1.72772400
H	-5.40993400	-2.58967700	-2.59030500
H	-5.71904200	-2.00140600	-0.94977100
H	-5.27781500	-3.69316200	-1.21444700

M8SS

C	-1.75071200	3.10874700	0.75433300
O	-2.03818500	4.12790300	1.30147300
C	-1.16143900	2.66755900	-0.57281400
C	0.37719700	2.82266500	-0.67217300
H	-1.71212600	2.98775500	-1.45715300
C	0.95796300	3.70726500	0.43135600
H	0.62664500	3.28263600	-1.63196600
H	2.03675200	3.82049700	0.30683900
H	0.49348900	4.69588100	0.40093600
H	0.77796500	3.28654200	1.42640700
C	-1.47681100	1.24336000	-0.03490300
O	-1.87297900	1.84515900	1.25613300
C	-0.16009600	0.50533300	-0.00504100
C	0.90420200	1.34696300	-0.69105400
H	0.89371900	1.03039900	-1.74435100
C	-2.64230300	0.53865000	-0.68961500
C	-2.41865000	-0.29721400	-1.78778100
C	-3.94807200	0.77653400	-0.26095400
C	-3.49401100	-0.88285000	-2.44696100
H	-1.40126100	-0.50947500	-2.10895500
C	-5.02087300	0.18367800	-0.92284800
H	-4.12515000	1.40881700	0.60256000
C	-4.79811200	-0.64434100	-2.01817700
H	-3.30992600	-1.53529500	-3.29465600
H	-6.03240200	0.36729800	-0.57469300
H	-5.63438400	-1.10830200	-2.53120900
C	2.32697900	1.19954500	-0.19540700
C	3.37402600	1.14961300	-1.11700900
C	2.63415800	1.17033300	1.17015400
C	4.70119500	1.09059100	-0.69155100
H	3.14447200	1.15401200	-2.18033000
C	3.95640500	1.12762500	1.59842400
H	1.82667600	1.17419400	1.89768900
C	4.99587300	1.08981900	0.66839300
H	5.50169000	1.04930200	-1.42396700

H	4.17722600	1.11257800	2.66101600
H	6.02709000	1.04913900	1.00427200
C	-0.02714600	-0.78114200	0.35281300
O	1.18079400	-1.44487000	0.14849600
C	-1.04804100	-1.65845100	0.95753700
C	-1.95241900	-1.18637700	1.91361200
C	-1.11965400	-2.99473100	0.54573500
C	-2.93074700	-2.03270500	2.42528300
H	-1.88351600	-0.16150900	2.26171500
C	-2.09946900	-3.83538000	1.05786100
H	-0.41366800	-3.36787300	-0.18958300
C	-3.00997100	-3.35496900	1.99748600
H	-3.62861000	-1.65690400	3.16634300
H	-2.15443200	-4.86606600	0.72285300
H	-3.77390100	-4.01293500	2.39903700
C	1.62986700	-1.61726600	-1.12311400
O	0.98904200	-1.31301000	-2.09835800
C	2.99831900	-2.25130300	-1.16292800
C	3.74252100	-2.31575600	0.16658700
H	2.87023600	-3.25020200	-1.59838800
H	3.56691500	-1.67151200	-1.89858200
C	5.19562500	-2.73339400	-0.03172300
H	3.23055800	-3.01198500	0.83850000
H	3.70002800	-1.33307100	0.64394000
H	5.71936100	-2.80276700	0.92482000
H	5.72352900	-2.00021200	-0.65068300
H	5.26883500	-3.70679400	-0.52749800

PRR

C	0.94624800	2.99540000	-0.17376900
C	-0.55193800	3.11636700	-0.16572800
H	1.60578000	3.85864200	-0.14955000
C	-1.10519100	4.19019000	-1.09758300
H	-0.89104300	3.33872100	0.85683500
H	-2.19963300	4.17748500	-1.08694100
H	-0.77492100	5.18704900	-0.79245700
H	-0.76795100	4.01739500	-2.12449300
C	1.37725800	1.72392700	-0.23429100
C	0.21340600	0.81163000	-0.30599400
C	-1.02273300	1.67700000	-0.53933100
H	-1.24007900	1.66911900	-1.61742000
C	2.80383300	1.33121800	-0.29924500
C	3.71707300	1.84457000	0.62497200
C	3.25993100	0.44623500	-1.28286200

C	5.05603100	1.46367900	0.58337200
H	3.36343400	2.52342600	1.39594500
C	4.59428700	0.06372200	-1.32328300
H	2.55370900	0.04297900	-2.00253700
C	5.49587600	0.56680700	-0.38526300
H	5.75304100	1.86052200	1.31483200
H	4.93181800	-0.63469200	-2.08254800
H	6.53647900	0.25922000	-0.41106000
C	-2.28571700	1.29544200	0.20056600
C	-3.52725700	1.36141700	-0.43592200
C	-2.24706500	0.95466200	1.55680800
C	-4.70540400	1.09870500	0.26251900
H	-3.56974800	1.62371600	-1.49061300
C	-3.41923700	0.68369200	2.25570600
H	-1.28575900	0.87574300	2.05851800
C	-4.65437200	0.76100000	1.61261300
H	-5.66101000	1.15976500	-0.24946500
H	-3.36774300	0.40720500	3.30400200
H	-5.56858600	0.55307200	2.15926600
C	0.18904200	-0.53021400	-0.22985900
O	-1.01526400	-1.13989100	-0.59074900
C	1.29991300	-1.43592300	0.12057900
C	1.58667900	-2.55128100	-0.67107600
C	2.09605600	-1.16411200	1.23642100
C	2.68907200	-3.34917700	-0.37970500
H	0.95580100	-2.77473900	-1.52694900
C	3.20028600	-1.95590500	1.52203800
H	1.84521900	-0.31692600	1.86740900
C	3.50416000	-3.04627300	0.70891200
H	2.91641900	-4.20560100	-1.00677400
H	3.82239000	-1.72404900	2.38048800
H	4.36784200	-3.66535800	0.93005800
C	-1.68200600	-1.83684500	0.37144800
O	-1.22617300	-2.05480400	1.46258900
C	-3.07017300	-2.21915400	-0.07662700
C	-3.37861000	-2.07619100	-1.56328700
H	-3.25696800	-3.23660600	0.28176500
H	-3.73388700	-1.56287900	0.50395800
C	-4.85217700	-2.35341600	-1.84570100
H	-2.74334300	-2.75427400	-2.14369500
H	-3.12569000	-1.06044400	-1.88098400
H	-5.08018600	-2.24970500	-2.90936700
H	-5.48369400	-1.64898000	-1.29371400
H	-5.13381700	-3.36527300	-1.53779400

PRS

C	-0.62041200	-2.74960400	-1.03675100
C	0.75899900	-2.59497100	-1.61997900
H	-1.12267600	-3.71143300	-0.97501700
C	1.70445100	-3.73394700	-1.24426900
H	0.67797100	-2.57242900	-2.71644400
H	1.31949600	-4.68131400	-1.63253300
H	2.70254600	-3.57565900	-1.66203700
H	1.80495000	-3.82080800	-0.15905000
C	-1.13850700	-1.59778700	-0.57521800
C	-0.14725600	-0.51808800	-0.74652800
C	1.17964300	-1.15655500	-1.14605500
H	1.59832800	-0.59837100	-1.99037500
C	-2.43603700	-1.46850900	0.12334300
C	-2.54144200	-0.68666800	1.28061400
C	-3.56896600	-2.13428000	-0.35081600
C	-3.75810000	-0.56929000	1.94065100
H	-1.66771200	-0.15135100	1.64427700
C	-4.78768300	-2.01652600	0.31210700
H	-3.49529000	-2.72661300	-1.25883500
C	-4.88609900	-1.23063200	1.45662500
H	-3.82731100	0.04687500	2.83145200
H	-5.66288700	-2.53085200	-0.07254100
H	-5.83840400	-1.12972100	1.96747100
C	2.23319300	-1.15749600	-0.05424200
C	3.58676200	-1.10738600	-0.40457500
C	1.89634200	-1.23091600	1.29922100
C	4.58101900	-1.12145800	0.56966600
H	3.86125100	-1.05218100	-1.45602400
C	2.88745400	-1.23634600	2.27777800
H	0.84959300	-1.25444800	1.58984900
C	4.23205000	-1.18146000	1.91777600
H	5.62574700	-1.07989300	0.27674600
H	2.60598700	-1.27611700	3.32516400
H	5.00258800	-1.18257900	2.68221500
C	-0.31203100	0.81099900	-0.62124100
O	0.87180100	1.57071000	-0.63856500
C	-1.57327000	1.57179000	-0.57475100
C	-2.64843200	1.17130300	-1.37901800
C	-1.72500500	2.69557900	0.24624900
C	-3.86429900	1.84096700	-1.32265500
H	-2.52324600	0.32492900	-2.04756100
C	-2.94071700	3.36926900	0.29426200

H	-0.90249900	3.01554400	0.87446700
C	-4.01580900	2.93973200	-0.48010600
H	-4.69122900	1.50934400	-1.94229100
H	-3.05028500	4.22966300	0.94690300
H	-4.96474100	3.46466800	-0.43396900
C	1.44925900	1.80213400	0.57097300
O	0.86325500	1.66571200	1.61574000
C	2.89431600	2.21770900	0.46122400
C	3.45594800	2.37502800	-0.94682200
H	3.01180100	3.13690900	1.04567800
H	3.44380000	1.43788400	1.00746200
C	4.96035700	2.62545800	-0.91196800
H	2.94181000	3.19282800	-1.46235000
H	3.24267500	1.46583400	-1.51779500
H	5.36794300	2.74675800	-1.91840600
H	5.47560600	1.78453000	-0.43565700
H	5.19937400	3.52833300	-0.34116600

PSR

C	-0.98485800	-2.92482900	0.56299400
C	0.50984900	-3.08345000	0.53227300
H	-1.66253400	-3.76080900	0.71122600
C	0.95602000	-3.81490900	-0.73879800
H	0.85894300	-3.66536000	1.39338100
H	2.04394500	-3.90829900	-0.78600400
H	0.52136100	-4.81867700	-0.75848000
H	0.61666500	-3.28566900	-1.63417300
C	-1.39189400	-1.65710300	0.38240700
C	-0.21215100	-0.76737300	0.27959400
C	0.99799400	-1.60066000	0.68168100
H	1.13543200	-1.42611400	1.75649100
C	-2.80923900	-1.22956800	0.41852200
C	-3.21373700	-0.19220300	1.26663200
C	-3.76048700	-1.85739500	-0.38763800
C	-4.53824300	0.22460700	1.28535800
H	-2.47220500	0.29849800	1.89130800
C	-5.08960300	-1.44097800	-0.36743400
H	-3.44550600	-2.65790000	-1.05149000
C	-5.47948800	-0.39467400	0.46290500
H	-4.83697000	1.03993400	1.93658700
H	-5.81790000	-1.92873100	-1.00793400
H	-6.51251800	-0.06161300	0.47091600
C	2.31216700	-1.29808100	-0.00152500
C	3.48710400	-1.26594900	0.75263800

C	2.40451100	-1.10065200	-1.38456400
C	4.72662000	-1.06254500	0.14579000
H	3.42714800	-1.40000200	1.83049900
C	3.63928500	-0.91370800	-1.99656700
H	1.49593400	-1.08343100	-1.98031300
C	4.80723300	-0.89628600	-1.23310600
H	5.62695800	-1.03989600	0.75230200
H	3.69068200	-0.76817800	-3.07109000
H	5.76992300	-0.74287000	-1.71027900
C	-0.19211500	0.54688900	-0.00950900
O	0.99013300	1.28034600	0.11533500
C	-1.30433500	1.38151800	-0.50278700
C	-2.13658600	0.94271500	-1.53607100
C	-1.54791000	2.62474000	0.09033600
C	-3.22995200	1.70589600	-1.92965400
H	-1.93052500	-0.01121500	-2.01227400
C	-2.63846100	3.38970700	-0.30633600
H	-0.89448000	2.97208600	0.88573100
C	-3.48756400	2.92664500	-1.31002000
H	-3.88123700	1.34712800	-2.72009000
H	-2.83055900	4.34501400	0.17174100
H	-4.34349300	3.52072700	-1.61407500
C	1.59404800	1.36743400	1.32929600
O	1.11649300	0.92932600	2.34502500
C	2.91530500	2.09597600	1.25131000
C	3.46179100	2.34005600	-0.15096600
H	2.78940800	3.03823600	1.79946500
H	3.61599500	1.49506500	1.84179400
C	4.89585800	2.85676800	-0.10528900
H	2.81403500	3.04857800	-0.67695500
H	3.42146900	1.40403400	-0.71422300
H	5.27713500	3.05403500	-1.11033100
H	5.55435800	2.11769500	0.36339600
H	4.96858000	3.78482800	0.47115600
PSS			
C	1.01879900	2.92081300	-0.08407400
C	-0.47678200	3.06035800	-0.14982800
H	1.69276100	3.77277400	-0.10153200
C	-1.04420200	4.21478500	0.66887300
H	-0.78650300	3.19087900	-1.19763800
H	-0.70568300	5.17951000	0.28073000
H	-2.13820700	4.20108100	0.63984000
H	-0.72687500	4.13525000	1.71331100

C	1.42084900	1.64414000	0.04203600
C	0.23294000	0.75903300	0.10531200
C	-0.96581900	1.66650900	0.34546700
H	-1.09620100	1.73604700	1.43501400
C	2.83042500	1.23082500	0.22519200
C	3.17777800	0.31846300	1.22834600
C	3.83778300	1.76853300	-0.57955000
C	4.50289100	-0.05544400	1.41092200
H	2.39607500	-0.10261100	1.85484900
C	5.16651300	1.39561500	-0.39467000
H	3.56927000	2.46521200	-1.36901600
C	5.50162100	0.47924000	0.59770900
H	4.75792500	-0.76828800	2.18882800
H	5.93806600	1.81443000	-1.03318600
H	6.53564500	0.18040600	0.73751000
C	-2.28877400	1.27071300	-0.26827100
C	-3.45272500	1.27918000	0.50241200
C	-2.39006000	0.96317300	-1.62993100
C	-4.69288000	0.99476200	-0.07048700
H	-3.38210100	1.50820100	1.56350500
C	-3.62425500	0.68555000	-2.20638900
H	-1.48738900	0.93935300	-2.23614500
C	-4.78278400	0.70273200	-1.42751500
H	-5.58718000	1.00697200	0.54531400
H	-3.68458300	0.45022600	-3.26442800
H	-5.74613900	0.48499600	-1.87767000
C	0.20196900	-0.58244600	0.00682300
O	-0.97746000	-1.28899700	0.24376600
C	1.29604000	-1.47635700	-0.41846800
C	2.10837500	-1.14061700	-1.50561600
C	1.52922400	-2.67614100	0.26207900
C	3.16608100	-1.96310700	-1.87496600
H	1.90726200	-0.22492800	-2.05361100
C	2.58552900	-3.50022000	-0.10978200
H	0.88970100	-2.94837800	1.09683000
C	3.41100300	-3.14169100	-1.17409100
H	3.79614100	-1.68623100	-2.71397900
H	2.76819100	-4.42203600	0.43328400
H	4.23754300	-3.78366900	-1.46132000
C	-1.61328100	-1.15907000	1.43756100
O	-1.17134600	-0.53226700	2.36628800
C	-2.92216200	-1.91314300	1.45572000
C	-3.44786300	-2.36115000	0.09533500
H	-2.78903500	-2.76808900	2.13055900

H	-3.63800900	-1.24652800	1.94876800
C	-4.88242200	-2.86895200	0.19445200
H	-2.79190300	-3.13713600	-0.31135600
H	-3.39998000	-1.51779000	-0.59962100
H	-5.24773800	-3.21304100	-0.77629500
H	-5.54842700	-2.07081500	0.53935600
H	-4.96504900	-3.70219200	0.90007300

Coordinates for the decarboxylation process

CO2

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16277000
O	0.00000000	0.00000000	-1.16277000

TS9RR-Direct

C	-1.58138400	-2.45807000	-2.10438700
O	-1.18674600	-3.24093000	-2.95155000
C	-1.13977100	-2.62707000	-0.60290500
C	0.36035800	-2.87880400	-0.44960300
H	-1.77087300	-3.37523000	-0.11597700
C	0.66846000	-3.58447400	0.86914100
H	0.68459000	-3.51161700	-1.28133100
H	0.17296000	-4.55948100	0.87400900
H	1.73994000	-3.74421200	1.00832900
H	0.29537600	-3.01951500	1.73072600
C	-1.38261300	-1.23516900	-0.14045400
O	-2.31446400	-1.42422500	-2.20804100
C	-0.17010900	-0.48900600	-0.31545200
C	0.98692600	-1.44917800	-0.62183500
H	1.22459400	-1.31694700	-1.68549400
C	-2.52181500	-0.82607800	0.66849500
C	-2.32854400	0.05370900	1.74636800
C	-3.79104000	-1.37953200	0.43940400
C	-3.39473800	0.37920700	2.57423600
H	-1.34156700	0.46519200	1.93787900
C	-4.85308400	-1.03485200	1.26146200
H	-3.93167100	-2.02042400	-0.42453800
C	-4.65639000	-0.15847600	2.33000600
H	-3.24014200	1.05417300	3.40901400
H	-5.83880700	-1.44473100	1.06906100
H	-5.49018100	0.10434000	2.97311400
C	2.26784800	-1.25842900	0.16047000
C	3.49794800	-1.41059300	-0.48512400
C	2.26167900	-1.02850900	1.54058100

C	4.69348700	-1.34753200	0.22839500
H	3.51617100	-1.59151400	-1.55697100
C	3.45281800	-0.96377700	2.25732400
H	1.31524000	-0.88325100	2.05478500
C	4.67370000	-1.12937400	1.60439500
H	5.63857900	-1.47359600	-0.29052500
H	3.42680000	-0.78047300	3.32656300
H	5.60248700	-1.08306400	2.16374100
C	-0.08676200	0.87282800	-0.41313900
O	1.18293100	1.38881600	-0.56357000
C	-1.16876900	1.85665200	-0.55229900
C	-2.31304400	1.54192500	-1.30026900
C	-1.03590000	3.13370100	0.01546400
C	-3.32259100	2.48613700	-1.44252900
H	-2.39687700	0.57263900	-1.78275800
C	-2.05947900	4.06108500	-0.11913700
H	-0.15512400	3.38453900	0.59367100
C	-3.20552600	3.73886600	-0.84549800
H	-4.20153700	2.24004200	-2.02859000
H	-1.96172300	5.03881900	0.34067500
H	-4.00043800	4.46985200	-0.95430800
C	1.86690600	1.78777300	0.55661200
O	1.33345500	1.86941800	1.63155600
C	3.31153300	2.07825100	0.26159400
C	3.71172900	2.13938200	-1.20865200
H	3.55844900	3.00496100	0.79024400
H	3.86742100	1.27907600	0.77039100
C	5.21924100	2.32484800	-1.35093600
H	3.17631000	2.95351500	-1.70817800
H	3.40255600	1.21167000	-1.69940700
H	5.51367600	2.37823200	-2.40141600
H	5.75226500	1.48609000	-0.89100000
H	5.55367200	3.24363800	-0.85923900

TS9RS-Direct

C	-1.76786800	2.90063400	1.18251000
O	-1.89011800	4.06372700	1.53056100
C	-1.24393800	2.56666700	-0.25929100
C	0.28077800	2.80918000	-0.30115800
H	-1.80561600	3.09564600	-1.03370600
C	0.70439100	3.90935400	-1.26170900
H	0.61073700	3.08794400	0.70596300
H	0.26017100	4.86215000	-0.96195600
H	1.79305000	4.02365600	-1.26483500

H	0.37819800	3.68062900	-2.28199500
C	-1.43314600	1.09163300	-0.28874300
O	-1.94168900	1.82191300	1.83413400
C	-0.17490900	0.43148700	-0.26066900
C	0.91364900	1.43001900	-0.64189300
H	1.04766200	1.37070300	-1.73091200
C	-2.69490000	0.46885800	-0.69820400
C	-2.65962600	-0.53341000	-1.68152000
C	-3.93314800	0.92452900	-0.22152400
C	-3.84239200	-1.07710600	-2.16737700
H	-1.70375100	-0.85492400	-2.08445100
C	-5.10800900	0.36439700	-0.70275200
H	-3.95561000	1.66803600	0.56653700
C	-5.06723300	-0.63483000	-1.67525600
H	-3.80481700	-1.84405500	-2.93379400
H	-6.06132000	0.70540700	-0.31313500
H	-5.99039300	-1.06463800	-2.05056300
C	2.26284200	1.24581200	0.01331300
C	3.43031200	1.29648700	-0.74948000
C	2.36538800	1.09696900	1.40132700
C	4.68278900	1.20726600	-0.14114900
H	3.35379200	1.41115000	-1.82887200
C	3.61232400	1.00913700	2.01016400
H	1.45714500	1.06581200	2.00093200
C	4.77557200	1.06400800	1.23963400
H	5.58260800	1.25293500	-0.74706900
H	3.67913500	0.89905000	3.08777600
H	5.74800400	0.99361200	1.71639300
C	0.00152000	-0.90529800	0.01813100
O	1.19151600	-1.51274700	-0.23358700
C	-0.93135500	-1.80067200	0.70509700
C	-1.83658300	-1.31105100	1.65815100
C	-0.89478300	-3.17186800	0.40752700
C	-2.71749400	-2.19050800	2.27493100
H	-1.83939200	-0.25487300	1.91378900
C	-1.78702800	-4.03761600	1.02169100
H	-0.17845500	-3.54657300	-0.31584800
C	-2.70194600	-3.54639400	1.95377300
H	-3.41626300	-1.81300100	3.01352500
H	-1.77096200	-5.09438400	0.77744500
H	-3.39785600	-4.22575100	2.43582500
C	1.82426700	-1.37850100	-1.45669900
O	1.27400300	-0.90313100	-2.40950400
C	3.21163400	-1.96236200	-1.42268500

C	3.79184200	-2.20913600	-0.03248100
H	3.17509600	-2.88926600	-2.00924200
H	3.83638800	-1.26695900	-1.99331800
C	5.28028200	-2.53179700	-0.10678800
H	3.24650300	-3.02566900	0.45110000
H	3.63558400	-1.31952400	0.58451400
H	5.68860200	-2.72606400	0.88766500
H	5.83373300	-1.69118200	-0.53801100
H	5.46894500	-3.41329000	-0.72781300

TS9SR-Direct

C	1.72436300	2.80731800	-1.57477700
O	1.62066000	3.88675800	-2.13687600
C	1.16560300	2.65522100	-0.09526700
C	-0.35208900	2.85361600	0.05220100
H	1.75463600	3.29392400	0.56683300
C	-0.95380900	4.06132700	-0.65051200
H	-0.56076800	2.93805500	1.12716100
H	-0.78836100	4.01003700	-1.72767700
H	-2.02874500	4.10361100	-0.44808000
H	-0.49737300	4.98742900	-0.29277300
C	1.37555500	1.20330400	0.12132300
O	2.24044400	1.72058100	-1.96974900
C	0.17361200	0.50075200	-0.19132200
C	-0.96109000	1.50515700	-0.41870900
H	-1.12272400	1.55502100	-1.50511100
C	2.52485500	0.65945300	0.83250800
C	2.33975700	-0.35940000	1.78193500
C	3.80007600	1.21323000	0.64293600
C	3.42100800	-0.81917900	2.52175000
H	1.34699800	-0.76978300	1.94607000
C	4.87686600	0.73260600	1.37281600
H	3.93626800	1.96961200	-0.12229700
C	4.68919200	-0.28024800	2.31444000
H	3.27332800	-1.59842800	3.26156600
H	5.86630500	1.14526200	1.20732200
H	5.53381100	-0.64729500	2.88882600
C	-2.29380100	1.24699600	0.24750000
C	-3.47580800	1.31444200	-0.49363700
C	-2.37899400	1.04518400	1.62979600
C	-4.71747200	1.19595000	0.12904100
H	-3.42096300	1.47602900	-1.56726800
C	-3.61599300	0.92194000	2.25504800
H	-1.46593300	0.97577000	2.21681900

C	-4.79075600	1.00368500	1.50664100
H	-5.62554900	1.25994500	-0.46237700
H	-3.66340800	0.76267300	3.32744600
H	-5.75574500	0.91377900	1.99494500
C	0.08351800	-0.84399800	-0.43920600
O	-1.18475000	-1.35908800	-0.58048400
C	1.15742700	-1.79582300	-0.72461000
C	2.29443900	-1.38123500	-1.43515400
C	1.02111200	-3.13743500	-0.33562900
C	3.29623000	-2.30093500	-1.71742100
H	2.37301600	-0.35143500	-1.77359800
C	2.03695100	-4.04154500	-0.60838000
H	0.14214900	-3.45904000	0.21149500
C	3.17588200	-3.62389600	-1.29752300
H	4.17155800	-1.98300500	-2.27353300
H	1.94170500	-5.07313700	-0.28690800
H	3.96594100	-4.33591600	-1.51467100
C	-1.82099600	-1.79481500	0.55805300
O	-1.24432700	-1.88078400	1.60948900
C	-3.26328100	-2.12894900	0.30600800
C	-3.69920100	-2.22283900	-1.15256700
H	-3.46736500	-3.05584500	0.85215000
H	-3.82998400	-1.34034000	0.81862900
C	-5.19887300	-2.48465100	-1.25147800
H	-3.13859900	-3.01515300	-1.65980300
H	-3.44940500	-1.28578500	-1.65909900
H	-5.52141700	-2.54664100	-2.29319000
H	-5.76083700	-1.67788400	-0.76943700
H	-5.47044900	-3.42260000	-0.75730300

TS9SS-Direct

C	-0.84635700	2.90330600	1.00769000
O	-0.49266100	4.00521700	1.39349400
C	-0.91297500	2.59081400	-0.53362300
C	0.43783800	2.59860100	-1.27417100
H	-1.65364000	3.24977900	-0.99328900
C	1.37534400	3.74231800	-0.91061900
H	0.20513100	2.67971900	-2.34249200
H	2.27906700	3.69704500	-1.52618400
H	0.88178600	4.70180600	-1.08354500
H	1.66311200	3.70680100	0.14072900
C	-1.32750800	1.16055200	-0.49604300
O	-1.21188800	1.88273500	1.67698000
C	-0.17726500	0.33084700	-0.62362000

C	1.02461800	1.15827800	-1.06915900
H	1.36024900	0.80463000	-2.04815000
C	-2.71898100	0.73662300	-0.62316200
C	-3.04287700	-0.32119300	-1.48620100
C	-3.74092300	1.42520500	0.04662000
C	-4.36853900	-0.69622100	-1.65921900
H	-2.25193200	-0.83047800	-2.02808000
C	-5.06102400	1.03228300	-0.11825700
H	-3.47451400	2.21513500	0.74043600
C	-5.37718400	-0.02688200	-0.96969000
H	-4.61413600	-1.51176600	-2.33087200
H	-5.84740100	1.54895200	0.42150200
H	-6.41190100	-0.32836500	-1.09747900
C	2.21160400	1.06084900	-0.12917400
C	3.50141900	1.04376100	-0.66567700
C	2.05400400	1.02356200	1.26017500
C	4.61980800	0.98732600	0.16379900
H	3.62804800	1.08007800	-1.74609400
C	3.17156800	0.96784400	2.08952000
H	1.05350200	1.05383200	1.68905200
C	4.45558500	0.94618900	1.54568400
H	5.61554800	0.97562100	-0.26920700
H	3.03727800	0.94486000	3.16619800
H	5.32284100	0.90084100	2.19661900
C	-0.12464300	-0.98672800	-0.22865800
O	1.01703700	-1.70670500	-0.36943100
C	-1.13702300	-1.75403300	0.51162700
C	-1.88351500	-1.17017500	1.54206300
C	-1.32182500	-3.10357400	0.18170000
C	-2.83797300	-1.93160100	2.20552300
H	-1.70863500	-0.13299000	1.81375200
C	-2.29055800	-3.84930500	0.83913700
H	-0.72066000	-3.55250900	-0.60298500
C	-3.05149000	-3.26167300	1.84933500
H	-3.41609100	-1.48195400	3.00572900
H	-2.45066500	-4.88764500	0.56886200
H	-3.80616700	-3.84613600	2.36603500
C	1.75545500	-1.74367900	-1.53748800
O	1.28367100	-1.43211900	-2.59355400
C	3.14555600	-2.27031300	-1.29424800
C	3.56503200	-2.40042000	0.16753900
H	3.21460400	-3.23129400	-1.81881700
H	3.81225100	-1.58541000	-1.83072000
C	5.05220400	-2.71595600	0.28543800

H	2.96870000	-3.18123400	0.65009100
H	3.34233100	-1.46541600	0.69062300
H	5.34731600	-2.81901600	1.33220600
H	5.65103900	-1.91105500	-0.15309000
H	5.30740000	-3.64649100	-0.23178000

TS9RR-NHC·H+

C	0.35696800	-0.92235000	-0.68948400
O	1.39638500	-1.49763900	-1.03145800
C	-1.01933100	-1.26589700	-1.21880700
C	-1.55998700	-2.51618200	-0.48660000
H	-1.09345900	-1.33193200	-2.30838200
C	-1.57384700	-3.75946900	-1.36370600
H	-0.90412100	-2.70599900	0.37135000
H	-1.94091700	-4.62974400	-0.81271300
H	-2.21506400	-3.61733200	-2.23805100
H	-0.55826700	-3.97390000	-1.70786400
C	-1.75377100	-0.07811000	-0.62643400
O	0.22442400	0.00785100	0.17921000
C	-2.74217500	-0.56283800	0.28385400
C	-2.92877400	-2.07114200	0.10808300
H	-3.06925200	-2.53695400	1.08922700
C	-1.81152500	1.20248200	-1.34604700
C	-3.02575300	1.90364800	-1.44371400
C	-0.70311500	1.65857600	-2.08299500
C	-3.11905200	3.03918100	-2.24123300
H	-3.91234600	1.54178600	-0.93221700
C	-0.81074900	2.78241500	-2.88581400
H	0.25039000	1.14665300	-2.00909700
C	-2.01578100	3.48221100	-2.96253100
H	-4.06494700	3.56536400	-2.30896900
H	0.05029300	3.11872300	-3.45470600
H	-2.09040700	4.36410800	-3.59046900
C	-4.12392000	-2.45291200	-0.74547200
C	-4.78446500	-3.65986500	-0.48850300
C	-4.56265200	-1.66308200	-1.81092100
C	-5.86216400	-4.06508200	-1.27050000
H	-4.45015200	-4.28644500	0.33544300
C	-5.64710700	-2.06101600	-2.59002700
H	-4.07623200	-0.71391600	-2.02345700
C	-6.30046000	-3.26123000	-2.32195100
H	-6.36216800	-5.00432800	-1.05620900
H	-5.98329300	-1.42808100	-3.40453400
H	-7.14661700	-3.56823100	-2.92756000

C	-3.52044900	0.15090200	1.15886300
O	-4.64333300	-0.51395300	1.59953300
C	-3.27595300	1.45138200	1.76310200
C	-1.97210400	1.97054700	1.84665700
C	-4.35227300	2.17166700	2.30778200
C	-1.76913300	3.20372500	2.45068800
H	-1.13070700	1.39368900	1.46897000
C	-4.13663100	3.41012100	2.89274200
H	-5.35657300	1.76973600	2.25687400
C	-2.84489900	3.92755000	2.96400900
H	-0.76346800	3.59471900	2.55354600
H	-4.97263700	3.96784400	3.29996100
H	-2.67340800	4.89008600	3.43482700
C	-5.77687900	-0.35149200	0.82043900
O	-5.85300400	0.53738500	0.01704700
C	-6.83344400	-1.37971000	1.10179700
C	-6.55451500	-2.36063100	2.23520600
H	-7.76926600	-0.83341400	1.26251300
H	-6.95584400	-1.91349300	0.14848000
C	-7.63940300	-3.43049000	2.30394800
H	-6.48750600	-1.82023700	3.18522600
H	-5.57913200	-2.83012400	2.07286200
H	-7.45032600	-4.13352500	3.11788900
H	-7.67761700	-3.99650800	1.36738700
H	-8.62529000	-2.98452200	2.46516900
C	4.92896800	-3.05516500	0.07336000
C	6.30294700	-3.24626800	-0.09402300
C	6.78023600	-3.86925900	-1.24083400
C	5.86631500	-4.27927600	-2.21072300
C	4.49620000	-4.07239600	-2.04099200
C	4.00938700	-3.45770000	-0.88884400
C	4.65953300	-2.36839400	1.38629200
C	5.98931300	-2.55928000	2.16025600
C	7.07793000	-2.68497800	1.07264700
H	7.84405100	-4.03394800	-1.38073100
H	6.22538500	-4.76727500	-3.11105500
H	3.80358000	-4.39826800	-2.80945000
H	2.94418800	-3.28452500	-0.75991700
H	5.91043700	-3.51067200	2.69069100
H	7.50301900	-1.70935400	0.80712600
H	3.79182000	-2.74422300	1.93190500
H	7.90379400	-3.31951800	1.40017700
C	5.18346400	0.07898400	1.80657600
C	3.52618300	-0.31397700	0.44661100

N	4.75970600	1.25785700	1.44852400
N	4.44915000	-0.91064400	1.20318400
N	3.72689900	0.98638200	0.60140700
C	6.32092900	-0.26490600	2.72016900
H	7.27236400	-0.09390500	2.20131200
H	6.29188800	0.38028600	3.59911500
C	2.99255700	2.04044700	-0.00961500
C	3.32826100	2.47727700	-1.29115300
C	1.97173900	2.67614900	0.69854100
C	2.66330500	3.55408400	-1.86428700
C	1.28891900	3.74586400	0.13716300
C	1.66154500	4.18168500	-1.13099700
H	2.93824900	3.90639700	-2.85116500
H	0.49276300	4.24193900	0.67827400
Cl	4.59670100	1.69159900	-2.16225500
Cl	0.86473000	5.56127300	-1.80997700
Cl	1.59599200	2.14506900	2.29673000
O	6.19036600	-1.59334600	3.16987000
H	2.73530400	-0.78829100	-0.16915600

TS9RS-NHC·H+

C	0.32546400	-0.66011600	-1.09369500
O	1.40188100	-1.22107900	-1.32541300
C	-0.92659800	-0.84086800	-1.92339100
C	-1.60848300	-2.18202400	-1.57816000
H	-0.79382900	-0.68339400	-2.99770600
C	-1.53071200	-3.22082400	-2.68521000
H	-1.13008700	-2.58891200	-0.67815800
H	-2.04243900	-4.14043700	-2.38719100
H	-2.00036200	-2.84601000	-3.60039300
H	-0.48843800	-3.46357000	-2.90842600
C	-1.76255700	0.23373200	-1.24935000
O	0.03814800	0.11622300	-0.11763800
C	-2.90360700	-0.37493300	-0.64867100
C	-3.05705000	-1.79475100	-1.18912300
H	-3.65625300	-1.74136300	-2.10863600
C	-1.72786000	1.62837000	-1.71896800
C	-2.93807200	2.23535000	-2.09390500
C	-0.52122200	2.29957800	-1.97851900
C	-2.94086300	3.49036400	-2.69316500
H	-3.87180600	1.69611500	-1.97119700
C	-0.53455400	3.54534100	-2.58689700
H	0.41854700	1.85367700	-1.67155200
C	-1.74180800	4.14897300	-2.94026800

H	-3.88329100	3.94250000	-2.98275800
H	0.40318600	4.05462400	-2.78547000
H	-1.74209300	5.12480700	-3.41482200
C	-3.68632900	-2.81021700	-0.26265000
C	-4.64788700	-3.70077900	-0.74281400
C	-3.26367900	-2.92183300	1.06642600
C	-5.17373900	-4.69324900	0.08493700
H	-4.98232200	-3.61752300	-1.77482600
C	-3.78423300	-3.91101500	1.89299500
H	-2.51980800	-2.22587100	1.45041300
C	-4.74127400	-4.80141600	1.40304700
H	-5.91713700	-5.38216600	-0.30359300
H	-3.44717200	-3.98770300	2.92166000
H	-5.14850400	-5.57190300	2.04939000
C	-3.78886800	0.26399000	0.18793300
O	-5.01801100	-0.25609600	0.42473200
C	-3.52941200	1.43078000	1.03489000
C	-2.26898300	1.63538100	1.61342200
C	-4.59660800	2.28661200	1.34914800
C	-2.10161700	2.67943700	2.51698700
H	-1.44785800	0.96034800	1.38371600
C	-4.40248800	3.35319300	2.21305600
H	-5.57190000	2.11149100	0.90762000
C	-3.15600900	3.54186800	2.80947800
H	-1.15097300	2.80169900	3.02482900
H	-5.22419300	4.02345600	2.43987700
H	-3.01142300	4.35242200	3.51625800
C	-5.83526600	-0.67972200	-0.61727400
O	-5.58930800	-0.40939400	-1.75810800
C	-7.04048500	-1.42036100	-0.10720400
C	-6.97077100	-1.88325500	1.34555600
H	-7.90383200	-0.76445300	-0.27679600
H	-7.16967500	-2.26985200	-0.78658800
C	-8.11505900	-2.83610400	1.67351900
H	-6.99681400	-1.01216100	2.00764600
H	-6.01181500	-2.38043500	1.51820200
H	-8.07282200	-3.15225100	2.71818300
H	-8.06045800	-3.73353300	1.04874300
H	-9.08845300	-2.36580000	1.50303000
C	4.86536700	-2.96408100	-0.40186200
C	6.24589500	-3.12188600	-0.55077900
C	6.77065000	-3.50719400	-1.77835600
C	5.89707000	-3.71651900	-2.84474200
C	4.52055300	-3.54371700	-2.69060500

C	3.98607600	-3.16723700	-1.45981100
C	4.54165100	-2.55679000	1.01161300
C	5.84204000	-2.90559200	1.78103300
C	6.97223100	-2.80797500	0.73403100
H	7.83989800	-3.64469500	-1.90583200
H	6.29297200	-4.02070800	-3.80824800
H	3.85918000	-3.71042900	-3.53399700
H	2.91600200	-3.02104100	-1.34192700
H	5.74805500	-3.94503400	2.10281500
H	7.39795700	-1.79813100	0.68838800
H	3.65630900	-3.03423700	1.43610400
H	7.78990100	-3.49550000	0.95864400
C	5.04563800	-0.24925200	1.93707900
C	3.42523800	-0.34855500	0.48246200
N	4.62851200	0.97921400	1.81888400
N	4.33041300	-1.09132000	1.12363500
N	3.62041600	0.89208200	0.90609100
C	6.14880400	-0.77561400	2.80428100
H	7.11935700	-0.51007200	2.36695400
H	6.08295500	-0.31853200	3.79260800
C	2.87488400	2.04863600	0.54351600
C	3.30102800	2.85981300	-0.50848300
C	1.75002200	2.40637600	1.28853000
C	2.62081700	4.03247400	-0.81320400
C	1.05004300	3.56597700	0.98761900
C	1.50963900	4.37290400	-0.04811600
H	2.96584500	4.67290300	-1.61606300
H	0.17212900	3.84745400	1.55415000
Cl	4.69507700	2.41410500	-1.42439400
Cl	0.68098900	5.85535500	-0.38039900
Cl	1.26578800	1.42007900	2.61924600
O	6.00173000	-2.16597000	2.97332100
H	2.64694400	-0.68686400	-0.23419300

TS9SR-NHC·H+

C	0.60562400	0.46656100	-2.14739600
O	0.98364700	-0.49804900	-2.80935800
C	-0.45151500	1.49237700	-2.60742700
C	-1.78806600	0.90425000	-3.07866000
H	-0.01699600	2.20781800	-3.31000500
C	-1.72273800	-0.12361600	-4.19790600
H	-2.40626400	1.74925900	-3.41070900
H	-1.13623600	-0.99464500	-3.90055100
H	-2.73466700	-0.44516600	-4.45958600

H	-1.25926400	0.30368800	-5.09055300
C	-0.78254800	2.07735800	-1.25230700
O	0.97397400	0.76898900	-0.95825000
C	-1.84839200	1.30243300	-0.69019200
C	-2.42572200	0.37244400	-1.77091400
H	-2.02388800	-0.63666700	-1.57815700
C	-0.33472500	3.37472300	-0.79247300
C	-1.18131600	4.18652500	-0.01585900
C	0.93471600	3.84716800	-1.16941100
C	-0.75373200	5.44502200	0.38333200
H	-2.17505200	3.83510700	0.24738800
C	1.36116800	5.09545100	-0.74703900
H	1.59356400	3.20156700	-1.74115900
C	0.51590800	5.89563700	0.02615800
H	-1.41073000	6.07611100	0.97114800
H	2.34936500	5.45034600	-1.01827700
H	0.84879400	6.87741300	0.34658700
C	-3.92460400	0.24961300	-1.90372600
C	-4.50437700	-1.01147800	-2.06291400
C	-4.73688900	1.38497700	-1.98265400
C	-5.87091300	-1.13842300	-2.30536700
H	-3.87435600	-1.89726100	-2.01139900
C	-6.10350600	1.26075000	-2.21534100
H	-4.29608600	2.37014800	-1.84656400
C	-6.67307400	-0.00161200	-2.38348300
H	-6.30676100	-2.12358100	-2.43782900
H	-6.72379500	2.14937900	-2.26660100
H	-7.73705800	-0.09745500	-2.57301400
C	-2.13567600	1.16766400	0.64498400
O	-3.20606600	0.34894500	0.92616200
C	-1.37195300	1.55193100	1.83847900
C	0.03120400	1.64224700	1.81334700
C	-2.04788800	1.69865700	3.06055900
C	0.73110100	1.88663200	2.98725100
H	0.57203400	1.48957800	0.88616300
C	-1.34029400	1.96018800	4.22507300
H	-3.12867700	1.63279100	3.09826300
C	0.04994300	2.05055100	4.19273100
H	1.81563100	1.93709700	2.96108500
H	-1.87323700	2.08903000	5.16061400
H	0.60094800	2.24803900	5.10688200
C	-4.45385600	0.93661500	1.04622700
O	-4.57767400	2.12923700	1.05821500
C	-5.54157300	-0.09189900	1.15288700

C	-5.09450900	-1.52299300	1.43833300
H	-6.24394200	0.27328900	1.90872800
H	-6.07375700	-0.04555000	0.19304600
C	-6.28530100	-2.47647800	1.41661600
H	-4.58974800	-1.56576600	2.41118300
H	-4.36059500	-1.82640100	0.68349500
H	-5.97436000	-3.50293200	1.62282100
H	-6.76938500	-2.45888900	0.43493300
H	-7.03234400	-2.19286500	2.16382700
C	-0.64423700	-2.94508300	-0.10614700
C	-1.12437800	-3.93331000	0.75742100
C	-1.54152800	-5.15602000	0.24416500
C	-1.46056000	-5.37062600	-1.13146900
C	-0.96976100	-4.38175700	-1.98631500
C	-0.55602200	-3.15029200	-1.47974400
C	-0.29019000	-1.70356200	0.66731700
C	-0.99809400	-1.93045200	2.03141000
C	-1.09675500	-3.46266200	2.19043100
H	-1.92471300	-5.93047700	0.90129000
H	-1.78627500	-6.32003700	-1.54394800
H	-0.91446100	-4.57053700	-3.05308400
H	-0.16739700	-2.37449800	-2.13731300
H	-2.00609700	-1.52045800	1.92073500
H	-0.22134200	-3.87143900	2.70970800
H	-0.58640600	-0.77188800	0.17981500
H	-1.97996000	-3.75035600	2.76487300
C	1.73132600	-1.32287800	2.12800200
C	2.11137900	-1.34570300	-0.01449800
N	2.98784900	-1.00706300	2.01199600
N	1.16201800	-1.55206600	0.90011700
N	3.20662100	-1.03478500	0.66336300
C	0.92149000	-1.48020500	3.37684600
H	1.07160900	-2.48837800	3.78488300
H	1.25534700	-0.75168200	4.11731400
C	4.47128400	-0.66559700	0.12791600
C	5.38287000	-1.64330900	-0.27281900
C	4.81237000	0.68538000	0.02707200
C	6.62385900	-1.28472400	-0.78112100
C	6.05125600	1.06101600	-0.47284800
C	6.93933500	0.06684600	-0.87207800
H	7.32824800	-2.04463700	-1.09599400
H	6.31692200	2.10804900	-0.54948500
Cl	4.96419700	-3.31566800	-0.14024600
Cl	8.48386500	0.52852200	-1.50159300

Cl	3.68435100	1.90031000	0.51841400
O	-0.43474800	-1.21363800	3.10767600
H	2.00102400	-1.38943500	-1.09491400

TS9SS-NHC·H+

C	0.28774100	0.53345300	-1.67933100
O	1.06758300	-0.22868300	-2.24702700
C	-0.64291100	1.53126900	-2.36249500
C	-1.79222700	0.94667200	-3.20763600
H	-0.05974700	2.27403900	-2.91298100
C	-1.40828200	-0.26833500	-4.04378300
H	-2.10477400	1.74223000	-3.89121800
H	-2.25128400	-0.57769400	-4.66721600
H	-0.56237800	-0.02816000	-4.69237000
H	-1.11925400	-1.11467200	-3.41659200
C	-1.29076100	2.08035200	-1.10366500
O	0.12297000	0.65617000	-0.40883300
C	-2.57191100	1.47344900	-0.94032700
C	-2.98491500	0.72982500	-2.20823100
H	-3.85251100	1.23568400	-2.64206300
C	-0.86308000	3.33918200	-0.49395300
C	-1.82372500	4.28310500	-0.10024200
C	0.49977200	3.66163200	-0.40096300
C	-1.42447400	5.51396100	0.40605200
H	-2.87845900	4.06182400	-0.22822600
C	0.89098800	4.88600000	0.11788100
H	1.24336400	2.93067600	-0.70109000
C	-0.07033500	5.81291900	0.52571400
H	-2.17256100	6.24204600	0.69996800
H	1.94617500	5.12499100	0.20096900
H	0.23998400	6.77314000	0.92450000
C	-3.39071300	-0.71344600	-1.96706800
C	-4.42452100	-1.26792600	-2.72587600
C	-2.74775300	-1.51471800	-1.02037700
C	-4.81638100	-2.59186800	-2.53860700
H	-4.92625700	-0.65418100	-3.47134400
C	-3.13925200	-2.83712100	-0.82596500
H	-1.93116300	-1.09350600	-0.43517800
C	-4.17765500	-3.37760900	-1.58238300
H	-5.62159900	-3.00680800	-3.13681900
H	-2.62514300	-3.44899600	-0.08935700
H	-4.48460100	-4.40695500	-1.42857000
C	-3.29779500	1.45319900	0.22980600
O	-4.53763400	0.89816500	0.23744000

C	-2.87325000	1.79681200	1.59459000
C	-1.55571600	1.59694300	2.02876100
C	-3.83848100	2.26777500	2.49742100
C	-1.21369200	1.86851900	3.34728400
H	-0.81055900	1.22494300	1.33670300
C	-3.48080900	2.56558500	3.80531100
H	-4.86195300	2.40804700	2.16628800
C	-2.17024600	2.36023200	4.23376400
H	-0.19931400	1.68643000	3.68588800
H	-4.22565000	2.94810500	4.49449800
H	-1.89767200	2.57831600	5.26119400
C	-5.52230100	1.27640300	-0.66138000
O	-5.43755900	2.28940500	-1.29418000
C	-6.66302400	0.29493600	-0.67863400
C	-6.48871100	-0.95891300	0.17358300
H	-7.56130200	0.85556900	-0.39452600
H	-6.79962000	0.02946900	-1.73392000
C	-7.61181000	-1.95728200	-0.08612600
H	-6.46369700	-0.67987400	1.23202700
H	-5.52215200	-1.41947700	-0.05448500
H	-7.49578600	-2.84701700	0.53680500
H	-7.60780300	-2.27831100	-1.13281300
H	-8.59224300	-1.52055000	0.12746100
C	0.16047700	-3.03151900	0.59333200
C	-0.06540100	-4.11740100	1.44168100
C	-0.33561700	-5.37069300	0.90107000
C	-0.34726000	-5.51652800	-0.48593200
C	-0.09111800	-4.43065800	-1.32557700
C	0.16190700	-3.16905800	-0.79151500
C	0.38260900	-1.77376500	1.38984300
C	-0.01221200	-2.17870700	2.83842200
C	0.06381600	-3.72032600	2.89209800
H	-0.52659700	-6.22271600	1.54625400
H	-0.55510000	-6.48960300	-0.91916300
H	-0.10696400	-4.56584400	-2.40167400
H	0.34129200	-2.31443000	-1.44187500
H	-1.05130600	-1.86966400	2.97211900
H	1.02249000	-4.06870300	3.29339300
H	-0.17601000	-0.91329400	1.01989100
H	-0.71858100	-4.13479500	3.53126300
C	2.61833600	-1.26651000	2.46287600
C	2.50830000	-0.93619300	0.31566900
N	3.80134100	-0.83126900	2.13404700
N	1.79998600	-1.34884900	1.36733700

N	3.71215200	-0.63812300	0.78850400
C	2.09718200	-1.64448200	3.81454100
H	2.39499600	-2.67303200	4.05263800
H	2.52319700	-0.98133600	4.56823800
C	4.82186700	-0.13475600	0.05320700
C	5.76495900	-1.01308300	-0.48292700
C	4.98299600	1.24195700	-0.11047300
C	6.85717100	-0.52668800	-1.18783000
C	6.06767900	1.74661100	-0.81258200
C	6.99087700	0.84950000	-1.34273700
H	7.58789200	-1.20861900	-1.60461700
H	6.19254400	2.81474300	-0.94079900
Cl	5.56808400	-2.71595700	-0.26884400
Cl	8.34898200	1.46580100	-2.21979800
Cl	3.81761700	2.32311800	0.57088600
O	0.69858700	-1.47173100	3.83707000
H	2.15252900	-0.82752200	-0.71406800

TS9RR-DMAP·H+

C	1.21429300	0.06177100	-2.09927800
O	1.97801800	-0.72454400	-2.67064100
C	-0.19618400	0.37785300	-2.55450200
C	-1.12674500	-0.83559700	-2.66167500
H	-0.18860300	0.99858400	-3.45454000
C	-2.27029100	-0.53806900	-3.62991600
H	-0.55658500	-1.69010300	-3.03906100
H	-1.85686900	-0.34909800	-4.62421100
H	-2.96910400	-1.37318900	-3.69999200
H	-2.83434000	0.35050300	-3.32627900
C	-0.60849400	1.12455800	-1.29717700
O	1.43497000	0.71846500	-1.02471200
C	-1.28094300	0.19746100	-0.42962200
C	-1.55022700	-1.11921300	-1.17587800
H	-0.85161600	-1.85841500	-0.76172000
C	-0.74506700	2.57648200	-1.25922600
C	-1.87120500	3.15728000	-0.65285300
C	0.19054300	3.39181400	-1.91455400
C	-2.04673200	4.53410500	-0.69688300
H	-2.61178900	2.52781800	-0.16816800
C	0.01716200	4.76690300	-1.93695200
H	1.07096400	2.93994100	-2.36018400
C	-1.10299000	5.33883900	-1.33084300
H	-2.92259500	4.97848300	-0.23739500
H	0.75181200	5.39666700	-2.42672700

H	-1.24123400	6.41470000	-1.35830300
C	-2.94093100	-1.70943500	-1.07267400
C	-3.08825700	-3.09460800	-0.96515600
C	-4.08994400	-0.92037200	-1.18928400
C	-4.35120000	-3.68322800	-0.98411600
H	-2.20275300	-3.71943800	-0.87667000
C	-5.35346900	-1.50361300	-1.20628800
H	-3.99690200	0.16099900	-1.24841500
C	-5.48811300	-2.88804300	-1.11046600
H	-4.44509300	-4.76158400	-0.90398600
H	-6.23369400	-0.87484500	-1.29076200
H	-6.47332600	-3.34234100	-1.12826700
C	-1.46816100	0.35807900	0.91807700
O	-2.14057700	-0.66398900	1.54834900
C	-0.93625900	1.38379100	1.82760600
C	0.29918900	2.00527600	1.58621000
C	-1.65392800	1.71719700	2.98810000
C	0.77903300	2.96691400	2.46480200
H	0.88710300	1.72119500	0.72333700
C	-1.17160100	2.68839000	3.85464600
H	-2.60567300	1.24717300	3.19833300
C	0.04267800	3.31934200	3.59401400
H	1.73542000	3.44022100	2.26931800
H	-1.74556500	2.95244300	4.73602500
H	0.41833500	4.07623800	4.27480500
C	-3.50487100	-0.54540100	1.71047600
O	-4.07690900	0.48428300	1.47599200
C	-4.13006800	-1.82482300	2.18717200
C	-3.17948400	-2.93250400	2.62853100
H	-4.83301400	-1.55189600	2.98126800
H	-4.74478200	-2.16648700	1.34337400
C	-3.95141800	-4.20657800	2.95804800
H	-2.59817700	-2.60157900	3.49567100
H	-2.46365100	-3.12859300	1.82431000
H	-3.27891000	-5.00357100	3.28259200
H	-4.49765500	-4.56023100	2.07742200
H	-4.67968900	-4.03417200	3.75614700
C	5.23306700	-1.74285100	-1.69793600
C	6.37054700	-1.88728100	-0.95019300
C	6.48684800	-1.21166900	0.29846200
C	5.37911200	-0.41152500	0.69816100
C	4.27637300	-0.31855900	-0.10899300
N	4.20989300	-0.97313000	-1.28335200
H	5.10351600	-2.23705000	-2.65331800

H	7.16299800	-2.51666800	-1.32908700
H	5.38426500	0.13168100	1.63228600
H	3.40090100	0.27465000	0.13393800
N	7.58720900	-1.32276800	1.05984500
C	7.67317800	-0.60777800	2.32760300
H	8.64372600	-0.80307600	2.77823900
H	7.57563200	0.47157500	2.17514200
H	6.89565800	-0.94242600	3.02177200
C	8.70153100	-2.15569900	0.62212600
H	9.48609600	-2.11733000	1.37450900
H	8.38957700	-3.19794200	0.50195800
H	9.11392600	-1.79423400	-0.32512400
H	3.32610100	-0.87630500	-1.87301200

TS9RS-DMAP·H+

C	1.32360000	0.28017900	-2.01595300
O	2.27815000	-0.14353500	-2.67781900
C	-0.09651200	0.41406900	-2.51472700
C	-0.77832400	-0.97567800	-2.51768800
H	-0.20996600	0.96653500	-3.45090800
C	-1.19293800	-1.45702300	-3.89989600
H	-0.07676200	-1.70311900	-2.09242000
H	-0.32049400	-1.56002900	-4.55014500
H	-1.68655000	-2.43091500	-3.83192400
H	-1.88812100	-0.74990600	-4.36374100
C	-0.63463000	1.14381200	-1.29419200
O	1.32372800	0.61377500	-0.77888900
C	-1.58799300	0.31780200	-0.62790200
C	-1.97229800	-0.84880800	-1.53327500
H	-2.85780700	-0.54449000	-2.10741000
C	-0.62321600	2.61554100	-1.21826300
C	-1.84840600	3.27694100	-1.03700000
C	0.53602000	3.37055200	-1.44535200
C	-1.90437500	4.66542500	-1.06171700
H	-2.75949900	2.69989600	-0.91185500
C	0.47236600	4.75697800	-1.45589100
H	1.48943400	2.87018700	-1.56372900
C	-0.74560300	5.40849600	-1.26318000
H	-2.85797900	5.16410400	-0.92645400
H	1.37836700	5.33283300	-1.61198800
H	-0.78966300	6.49244400	-1.27597800
C	-2.27587900	-2.16111000	-0.84532000
C	-3.38735100	-2.91704100	-1.22009600
C	-1.40899900	-2.66686000	0.12953900

C	-3.62886500	-4.16154800	-0.63666300
H	-4.06640700	-2.52733500	-1.97536300
C	-1.64669900	-3.90655200	0.71172200
H	-0.54116600	-2.07970000	0.42557900
C	-2.75879900	-4.65851200	0.32880000
H	-4.49552100	-4.74072400	-0.93948300
H	-0.96643600	-4.28902000	1.46576600
H	-2.94470900	-5.62548800	0.78457400
C	-2.12751900	0.59796100	0.60696800
O	-3.20843800	-0.08482700	1.06042400
C	-1.60877900	1.52482700	1.61681600
C	-0.23757600	1.79117900	1.73010300
C	-2.51535000	2.14521700	2.48968900
C	0.21046500	2.69332900	2.68529100
H	0.46503300	1.28509900	1.07787700
C	-2.05893000	3.05295700	3.43463000
H	-3.57470800	1.92572900	2.41122900
C	-0.69584600	3.32995500	3.53148700
H	1.27189000	2.89848600	2.77435800
H	-2.76363100	3.54328400	4.09722800
H	-0.33907500	4.03734700	4.27300700
C	-4.34924200	-0.22997400	0.28256100
O	-4.50787800	0.39656000	-0.72598600
C	-5.32504000	-1.18433900	0.91385900
C	-4.75619000	-2.08615800	2.00640500
H	-6.15576500	-0.57536200	1.29281100
H	-5.73608000	-1.77353800	0.08708400
C	-5.74147500	-3.18864800	2.37838000
H	-4.50784700	-1.48186900	2.88436100
H	-3.81958300	-2.52852100	1.65475400
H	-5.33786100	-3.82236000	3.17123100
H	-5.95067200	-3.82589500	1.51307200
H	-6.69202200	-2.77460500	2.72857800
C	4.18995800	-0.27865100	0.20348600
C	5.19420700	-0.50831100	1.10621900
C	6.44343400	-1.02626000	0.66200200
C	6.57252300	-1.27663600	-0.73390300
C	5.51912200	-1.02154100	-1.57068500
N	4.35370600	-0.53215400	-1.10835700
H	3.21516400	0.11425600	0.47402000
H	5.01404600	-0.28847800	2.14880800
H	7.48617200	-1.67064000	-1.15555700
H	5.57262000	-1.20190200	-2.63766600
N	7.45037500	-1.26816600	1.51702600

C	8.72086100	-1.78824800	1.02485800
H	9.40522700	-1.89839300	1.86305500
H	8.58932000	-2.76788800	0.55483900
H	9.17075300	-1.10172000	0.30098800
C	7.27647600	-1.01282800	2.94180700
H	8.18978900	-1.28906200	3.46379600
H	7.07752200	0.04687900	3.13074400
H	6.45349100	-1.60867900	3.34898900
H	3.53325400	-0.35396800	-1.77215100

TS9SR-DMAP·H+

C	1.28937000	-0.20463200	-2.03131200
O	2.10795500	-0.98726300	-2.53308000
C	-0.12139100	0.01747100	-2.54775800
C	-1.07138000	-1.18690300	-2.49027600
H	-0.10145100	0.50134200	-3.52773200
C	-0.52757200	-2.49183300	-3.05353900
H	-1.96587500	-0.90343900	-3.05774700
H	-1.29056400	-3.27141100	-2.97345000
H	-0.25689600	-2.38234700	-4.10645400
H	0.36448400	-2.81041500	-2.50980900
C	-0.58050800	0.92639500	-1.41827900
O	1.46646700	0.54587400	-1.01358800
C	-1.29182100	0.13370900	-0.45805700
C	-1.49602500	-1.28714900	-1.00012000
H	-0.78695300	-1.94083800	-0.47082600
C	-0.70141700	2.37171700	-1.58328200
C	-1.86377300	3.02953400	-1.14781500
C	0.29017600	3.09208000	-2.26684000
C	-2.01601500	4.38995200	-1.38128200
H	-2.65106300	2.46949300	-0.65133300
C	0.13821800	4.45373400	-2.47818900
H	1.19412800	2.58280000	-2.58461000
C	-1.01547600	5.10389200	-2.03670200
H	-2.91945600	4.89234800	-1.05346100
H	0.91654600	5.01075400	-2.98819200
H	-1.13646800	6.16795100	-2.21149500
C	-2.87453200	-1.90418100	-0.89473000
C	-3.02664200	-3.21215200	-0.42971300
C	-3.99973600	-1.22294900	-1.37098700
C	-4.27469100	-3.83331000	-0.44620700
H	-2.15643100	-3.75277000	-0.06550900
C	-5.24799900	-1.83640800	-1.38226800
H	-3.89798500	-0.19809000	-1.72124500

C	-5.38780400	-3.14762400	-0.92613100
H	-4.37392700	-4.85349900	-0.08934200
H	-6.11231500	-1.29180700	-1.74788400
H	-6.35998000	-3.62921100	-0.94298400
C	-1.59963000	0.52052700	0.81990200
O	-2.37716900	-0.35029500	1.54510900
C	-1.11761500	1.67610900	1.58312600
C	0.16715200	2.19882000	1.36947100
C	-1.93885000	2.24087000	2.57161800
C	0.60029100	3.29168000	2.10755100
H	0.82146200	1.73517800	0.64068100
C	-1.50167700	3.34144500	3.29478500
H	-2.93106500	1.84493400	2.74904500
C	-0.23372100	3.87124500	3.06198400
H	1.59480700	3.69176000	1.94120300
H	-2.15077300	3.78591300	4.04125200
H	0.10635400	4.73025800	3.63132400
C	-3.74575500	-0.17924200	1.48257700
O	-4.23178200	0.77791400	0.94382900
C	-4.48667700	-1.29845000	2.15435800
C	-3.65191500	-2.27606100	2.97491900
H	-5.27308300	-0.83118500	2.75649100
H	-5.00222700	-1.82626000	1.34087300
C	-4.52174200	-3.40738300	3.51386200
H	-3.15964600	-1.74632700	3.79725900
H	-2.85772500	-2.68349900	2.34207600
H	-3.93129300	-4.11543200	4.09929600
H	-4.99146000	-3.95489400	2.69019700
H	-5.31900000	-3.02140200	4.15601800
C	4.39448100	-0.13933500	-0.05953100
C	5.48210900	-0.12744600	0.77347700
C	6.51433000	-1.09308900	0.60719600
C	6.34527800	-2.03535400	-0.44673000
C	5.23015800	-1.97699500	-1.23872900
N	4.27631900	-1.04712600	-1.04647400
H	3.56747300	0.55834000	0.02045500
H	5.52920500	0.62044000	1.55232100
H	7.08094100	-2.80225900	-0.64331700
H	5.06369500	-2.67353700	-2.05179300
N	7.59421000	-1.11742900	1.40591400
C	8.61994700	-2.13737200	1.22081000
H	9.38961500	-2.00446400	1.97778100
H	8.19828500	-3.14114300	1.33158700
H	9.08718000	-2.05205000	0.23462400

C	7.74223900	-0.12783900	2.46608000
H	8.68810800	-0.29635300	2.97589200
H	7.74926900	0.88680400	2.05597600
H	6.93385900	-0.21166100	3.19948900
H	3.40644000	-1.02281400	-1.67033200

TS9SS-DMAP·H+

C	0.16643900	-1.39573700	-2.25929200
O	-0.84228300	-1.48920900	-2.96823600
C	1.44057000	-0.65817800	-2.63547400
C	1.29256700	0.83667900	-2.95931000
H	2.00719900	-1.20714500	-3.39190600
C	0.24569600	1.17209700	-4.01237000
H	2.27187300	1.16141800	-3.32926200
H	0.25922400	2.24358500	-4.23055300
H	0.45857100	0.63359500	-4.93947700
H	-0.75664400	0.89630800	-3.68222900
C	2.06323900	-0.69363800	-1.24861400
O	0.31177600	-1.85214800	-1.07142400
C	1.74041700	0.53466900	-0.58980000
C	1.10798300	1.52414200	-1.56547100
H	1.69348800	2.44922100	-1.58537200
C	3.16821400	-1.58663900	-0.90607800
C	4.31076700	-1.06060400	-0.28398100
C	3.14059500	-2.93711900	-1.28376900
C	5.40175600	-1.88227500	-0.03089700
H	4.34706800	-0.00587300	-0.02926600
C	4.22614000	-3.75505300	-1.00857400
H	2.24521800	-3.34218900	-1.74331600
C	5.35764500	-3.22881500	-0.38338900
H	6.28746400	-1.46940600	0.43924500
H	4.19394000	-4.80434300	-1.28116400
H	6.20834300	-3.86979900	-0.17637200
C	-0.32086500	1.90590200	-1.20625400
C	-0.80661200	3.15579700	-1.60345500
C	-1.16998300	1.05459700	-0.49473000
C	-2.10694800	3.54871100	-1.29839000
H	-0.15563900	3.83085100	-2.15522600
C	-2.47149200	1.44550500	-0.18679300
H	-0.80630400	0.08437300	-0.16447300
C	-2.94414100	2.69349200	-0.58478200
H	-2.46355000	4.52446900	-1.61258400
H	-3.11318700	0.77102900	0.37522800
H	-3.95486900	3.00107500	-0.33731100

C	1.82226400	0.75569000	0.76228500
O	1.45566300	1.97458700	1.24253800
C	2.12719200	-0.19162200	1.83965000
C	1.71310000	-1.52922200	1.78772700
C	2.83773000	0.28072600	2.95207400
C	2.03920100	-2.38787800	2.82905900
H	1.13590600	-1.88270200	0.94028700
C	3.17495000	-0.58983700	3.97941600
H	3.14132500	1.32186400	2.99287700
C	2.77746000	-1.92458300	3.91725200
H	1.71766100	-3.42322300	2.79266900
H	3.74431300	-0.22930500	4.82915500
H	3.03786900	-2.60303100	4.72314300
C	2.06021700	3.13505500	0.78770200
O	3.14098900	3.11188900	0.27299400
C	1.20198700	4.34709300	1.03080300
C	-0.13106600	4.11218900	1.73732600
H	1.82423000	5.07454000	1.56369300
H	1.03390500	4.77615500	0.03387600
C	-0.96682800	5.38800200	1.75754800
H	0.05265900	3.75877100	2.75725500
H	-0.68068500	3.31868800	1.22055400
H	-1.92027800	5.22228100	2.26403800
H	-1.18333300	5.72045100	0.73695600
H	-0.44626000	6.20056900	2.27319500
C	-2.61327900	-2.20050000	-0.02883400
C	-3.60348800	-2.20062200	0.91867900
C	-4.91534400	-1.76449100	0.57476900
C	-5.11181500	-1.32199200	-0.76496600
C	-4.06757600	-1.34914000	-1.65043300
N	-2.84907400	-1.78936400	-1.28871800
H	-1.59296200	-2.51196000	0.16825200
H	-3.36513100	-2.54103900	1.91635200
H	-6.07124500	-0.96065800	-1.10659100
H	-4.16892600	-1.01667600	-2.67665800
N	-5.91636400	-1.76534700	1.46904100
C	-7.24880000	-1.32068500	1.07688500
H	-7.91940400	-1.42229200	1.92712400
H	-7.23919500	-0.27038500	0.76862100
H	-7.63870100	-1.93037000	0.25601800
C	-5.67678600	-2.21494400	2.83570600
H	-6.60261700	-2.13407300	3.40067400
H	-5.35113900	-3.25971800	2.85411600
H	-4.91860300	-1.59526700	3.32463300

H	-2.04930100	-1.76838300	-1.99277600
TS9RR-nPrCOOH			
C	-1.86649700	-1.23463400	-0.71806000
O	-2.36198700	-2.24969500	-1.22898500
C	-1.14508500	-1.29915900	0.63303600
C	0.00512400	-2.30650700	0.69208500
H	-1.89509300	-1.42771100	1.41839000
C	0.28905500	-2.71692800	2.13577600
H	-0.27595000	-3.19273600	0.11532100
H	-0.59964300	-3.20075300	2.54986600
H	1.12642800	-3.41426700	2.20618500
H	0.51796900	-1.84919600	2.76478200
C	-0.50334500	0.06108500	0.61137900
O	-1.85538600	-0.05095800	-1.16073300
C	0.80979800	-0.07762000	0.04875000
C	1.17829800	-1.56581200	-0.04111100
H	1.12890400	-1.83136900	-1.10549100
C	-0.99871300	1.19046300	1.37498600
C	-0.09914800	2.07646500	1.99488700
C	-2.38264300	1.34385300	1.56741900
C	-0.58217700	3.11134200	2.78166800
H	0.97094900	1.93347100	1.87522500
C	-2.85283500	2.39495800	2.34050300
H	-3.07192900	0.66052500	1.07726600
C	-1.95706100	3.27666000	2.94693900
H	0.11211500	3.78798800	3.26780400
H	-3.92119200	2.52630800	2.47413800
H	-2.33151400	4.09172300	3.55839900
C	2.54264700	-1.97671800	0.46727500
C	3.25152200	-2.97429600	-0.20772100
C	3.07731400	-1.46229400	1.65317900
C	4.45947900	-3.45713100	0.29168600
H	2.84544800	-3.38267300	-1.12988600
C	4.28543400	-1.93892900	2.15416100
H	2.55135300	-0.67039200	2.18007000
C	4.97818400	-2.94256800	1.47824600
H	4.99139300	-4.23687800	-0.24432000
H	4.68629500	-1.52397400	3.07321300
H	5.91773000	-3.31706000	1.87139300
C	1.53451500	0.91932100	-0.54539900
O	2.76823500	0.54579000	-1.03685500
C	1.12908300	2.28780300	-0.89758100
C	-0.18571100	2.55599200	-1.30638600

C	2.07649800	3.32375100	-0.88204300
C	-0.54811300	3.85024500	-1.65786700
H	-0.90751000	1.74910200	-1.37096300
C	1.69801000	4.61546700	-1.22021700
H	3.09484200	3.12840100	-0.56971700
C	0.38530300	4.88236500	-1.60600600
H	-1.56446900	4.04864400	-1.98086300
H	2.42986800	5.41552000	-1.18511400
H	0.09478000	5.89281400	-1.87562600
C	3.87421800	0.71565800	-0.24229500
O	3.82985300	1.34520200	0.78126500
C	5.08444900	0.02292800	-0.80246200
C	4.96494000	-0.53512000	-2.21681000
H	5.91807800	0.72743300	-0.71233400
H	5.29450900	-0.78890600	-0.09278700
C	6.21422200	-1.32662800	-2.59208300
H	4.79999800	0.28077100	-2.92813900
H	4.08446200	-1.18231200	-2.27085000
H	6.13579700	-1.73269000	-3.60299000
H	6.35733600	-2.16312500	-1.90002900
H	7.10992700	-0.69938800	-2.54864500
O	-4.47288700	-0.91510100	0.49010500
C	-5.22161900	-1.11417100	-0.45199900
O	-4.85178000	-1.66857700	-1.59101200
C	-6.68412700	-0.72547100	-0.43407200
C	-7.61532100	-1.78891500	-1.01789800
H	-6.78024600	0.20090700	-1.01538500
H	-6.94605600	-0.48995100	0.60074800
C	-9.07745400	-1.35939500	-0.94491200
H	-7.32514700	-1.98228200	-2.05422500
H	-7.47567100	-2.73038100	-0.47454900
H	-9.73805300	-2.12123500	-1.36625700
H	-9.38415700	-1.18422000	0.09116500
H	-9.23944900	-0.42982100	-1.50007100
H	-3.86994800	-1.90193700	-1.54831300

TS9RS-nPrCOOH

C	-1.85052000	-1.51331900	0.56381700
O	-2.71149900	-2.38647500	0.73617800
C	-0.74352200	-1.24080100	1.57966700
C	0.44307100	-2.19868600	1.33138200
H	-1.08181700	-1.21604400	2.61929400
C	0.66392900	-3.21391800	2.44121500
H	0.25467300	-2.73627000	0.39456200

H	-0.21637200	-3.85203400	2.55353400
H	1.52441800	-3.85070800	2.21467200
H	0.84886000	-2.70976400	3.39555600
C	-0.29373800	0.10469300	1.06138000
O	-1.69122000	-0.74513700	-0.43268400
C	1.04270600	0.01785600	0.58173800
C	1.67003400	-1.27701200	1.09056700
H	2.13966200	-1.06490600	2.06091200
C	-0.96678900	1.34470500	1.45171800
C	-0.19116600	2.42844000	1.90002400
C	-2.36758000	1.43500200	1.48651100
C	-0.80729600	3.59022900	2.34490400
H	0.89007700	2.33654200	1.93657300
C	-2.97111800	2.60745900	1.91913300
H	-2.99304200	0.62239400	1.13125500
C	-2.19723700	3.68660300	2.34481000
H	-0.20126200	4.41824600	2.69697700
H	-4.05407600	2.67111000	1.91372300
H	-2.67641800	4.59932800	2.68508400
C	2.69477600	-1.93356500	0.19386700
C	3.89921900	-2.40162300	0.72042700
C	2.41633400	-2.15202500	-1.16048100
C	4.81112500	-3.08332300	-0.08640200
H	4.11916000	-2.23349100	1.77260300
C	3.32156200	-2.83365300	-1.96574200
H	1.47683800	-1.79059400	-1.57546200
C	4.52254100	-3.30244500	-1.42981500
H	5.74182700	-3.44726900	0.33802900
H	3.09179700	-3.00170600	-3.01296000
H	5.22812600	-3.83500800	-2.05931800
C	1.66215700	0.97490600	-0.18976500
O	3.00846300	0.94958800	-0.37199700
C	1.02343700	2.01769200	-0.99573800
C	-0.25571300	1.83127800	-1.53931200
C	1.72215900	3.21090400	-1.23508600
C	-0.83396400	2.84892400	-2.28707800
H	-0.78386500	0.89593800	-1.38247300
C	1.13015100	4.22403300	-1.97440900
H	2.71808900	3.34143800	-0.82518100
C	-0.15016700	4.04434900	-2.49873500
H	-1.82227600	2.70419700	-2.70947900
H	1.66364400	5.15298900	-2.14454900
H	-0.61157500	4.83644500	-3.07986900
C	3.87572400	0.81330500	0.69995700

O	3.50406900	0.90827300	1.83507700
C	5.29390600	0.61482900	0.23586400
C	5.46418900	0.22201900	-1.22915900
H	5.82908700	1.54578900	0.46288100
H	5.71599100	-0.14599500	0.90091000
C	6.89547600	-0.21684000	-1.51871800
H	5.18637100	1.06677600	-1.86721500
H	4.77214400	-0.59111800	-1.46605500
H	7.02058800	-0.47110800	-2.57376900
H	7.15301100	-1.10182000	-0.92779400
H	7.61380600	0.57228300	-1.27450900
O	-4.92773800	-0.10106100	0.49162500
C	-5.36866500	-0.86198900	-0.35160700
O	-4.79104900	-1.98917500	-0.71743000
C	-6.65761600	-0.59813000	-1.10217700
C	-7.60199800	-1.80183100	-1.12450900
H	-6.39139500	-0.32830600	-2.13218900
H	-7.13438400	0.27185900	-0.64345800
C	-8.89692000	-1.49300800	-1.87015300
H	-7.08529200	-2.64589900	-1.58951900
H	-7.82849000	-2.10214500	-0.09496700
H	-9.56610000	-2.35718500	-1.88052300
H	-9.43024900	-0.65994100	-1.40148800
H	-8.69187700	-1.21409500	-2.90875400
H	-3.93881600	-2.13837700	-0.18174900

TS9SR-nPrCOOH

C	-1.86468400	-1.53150100	-0.28798700
O	-2.51185200	-2.56023800	-0.54302500
C	-0.94357100	-1.46580800	0.94179400
C	0.30309400	-2.36503300	0.90693300
H	-1.54510500	-1.59823000	1.84456500
C	0.07755000	-3.80220400	0.46048400
H	0.71908300	-2.37341000	1.92267600
H	-0.33294400	-3.83755300	-0.55088800
H	1.02635300	-4.34721800	0.48382500
H	-0.63002100	-4.30964000	1.12043000
C	-0.40205100	-0.07058400	0.77184400
O	-1.86343900	-0.43387800	-0.91014700
C	0.85939600	-0.13966400	0.10671200
C	1.31687000	-1.59920100	0.01209000
H	1.17507300	-1.91230400	-1.03217100
C	-0.92795100	1.06843500	1.50200400
C	-0.05091800	2.02121600	2.05209400

C	-2.30986800	1.16507000	1.73602400
C	-0.55738800	3.06492900	2.81229400
H	1.02069900	1.92014300	1.90424000
C	-2.80388900	2.22670200	2.47976400
H	-2.98850700	0.43962400	1.29425500
C	-1.93245900	3.17401600	3.01863400
H	0.12032900	3.79165200	3.24693900
H	-3.87321100	2.31281800	2.64003800
H	-2.32519900	3.99626500	3.60871600
C	2.73635700	-1.92187200	0.42106700
C	3.53310700	-2.74864200	-0.37431800
C	3.23712000	-1.48889100	1.65386900
C	4.79918400	-3.14556600	0.05473700
H	3.15085700	-3.09535900	-1.33118400
C	4.50234800	-1.87680700	2.08261900
H	2.63147500	-0.83241600	2.27491000
C	5.28528100	-2.71351900	1.28648600
H	5.40110600	-3.79655100	-0.57157700
H	4.87725400	-1.52688200	3.03888000
H	6.26875300	-3.02364200	1.62424200
C	1.48139700	0.90501100	-0.52624200
O	2.74927000	0.65951300	-1.00278400
C	0.93261500	2.20714600	-0.91071900
C	-0.41583900	2.32543400	-1.28103600
C	1.77454200	3.32921100	-0.96217200
C	-0.91490000	3.56327800	-1.66479000
H	-1.05333400	1.44694300	-1.28516200
C	1.25955000	4.56352000	-1.33008100
H	2.81678600	3.24202500	-0.67830200
C	-0.08535900	4.68265000	-1.67990700
H	-1.95518400	3.65070600	-1.95893000
H	1.90643300	5.43399500	-1.34714800
H	-0.48319100	5.64855300	-1.97476700
C	3.80763900	0.91528400	-0.16193500
O	3.65862400	1.48954600	0.88343400
C	5.10529900	0.40035500	-0.71571400
C	5.09778000	-0.03439300	-2.17759400
H	5.85373200	1.17694700	-0.52691800
H	5.37372300	-0.44636900	-0.06985400
C	6.45340500	-0.60715900	-2.57899100
H	4.83710900	0.81579600	-2.81681800
H	4.31683100	-0.78695300	-2.32125300
H	6.45495000	-0.92145400	-3.62504100
H	6.69977700	-1.47814100	-1.96276800

H	7.25009600	0.13143700	-2.44746100
O	-4.66245500	-0.73827300	0.67570500
C	-5.29527000	-1.02516900	-0.32596500
O	-4.84789200	-1.80164200	-1.29311100
C	-6.69119800	-0.50130600	-0.59115800
C	-7.66311300	-1.56551700	-1.10265500
H	-6.60126700	0.29733500	-1.33909000
H	-7.05154700	-0.04519600	0.33452700
C	-9.05570300	-0.99041100	-1.34357200
H	-7.26221700	-1.99479500	-2.02483300
H	-7.71913200	-2.38379500	-0.37562300
H	-9.74520700	-1.75544900	-1.70939500
H	-9.47368600	-0.57419400	-0.42147700
H	-9.02212300	-0.18595100	-2.08544600
H	-3.90681900	-2.11301000	-1.07039100

TS9SS-nPrCOOH

C	1.44566400	-1.36572500	-0.80418100
O	1.97298600	-2.48125100	-0.91128400
C	0.72639000	-0.69565300	-1.98349700
C	-0.56915100	-1.36250900	-2.47911700
H	1.44783700	-0.52040100	-2.78584300
C	-0.49528500	-2.87552300	-2.63682900
H	-0.78199700	-0.92657500	-3.46208400
H	-1.44121800	-3.26033000	-3.02938900
H	0.30454500	-3.14210900	-3.33227000
H	-0.28566300	-3.36739000	-1.68572000
C	0.27286700	0.56713200	-1.29534000
O	1.42507700	-0.60646100	0.21077000
C	-1.07911700	0.39976000	-0.87159700
C	-1.69382400	-0.83698000	-1.52075500
H	-2.53466400	-0.53007800	-2.14913300
C	1.00230000	1.82255300	-1.40327300
C	0.30097200	3.01803500	-1.63135400
C	2.40572000	1.82980400	-1.35748300
C	0.99438900	4.20945900	-1.78653600
H	-0.78152000	2.99812800	-1.71015700
C	3.08678400	3.03112500	-1.49444800
H	2.94862300	0.90878400	-1.16056200
C	2.38632100	4.21873200	-1.70695900
H	0.45143000	5.12988000	-1.97224400
H	4.16975400	3.03795700	-1.43350400
H	2.92638300	5.15362800	-1.81922300
C	-2.22773600	-1.84965700	-0.52390500

C	-3.39439100	-2.55491800	-0.83066900
C	-1.56653700	-2.12571800	0.67737200
C	-3.89419600	-3.52255500	0.03892700
H	-3.91178100	-2.34575500	-1.76516600
C	-2.06466400	-3.09349500	1.54597000
H	-0.65468400	-1.58737900	0.92857500
C	-3.22893000	-3.79321600	1.23179800
H	-4.80064400	-4.06302500	-0.21610200
H	-1.53870200	-3.30216400	2.47199800
H	-3.61481700	-4.54425600	1.91351300
C	-1.67738800	1.14307100	0.11908700
O	-2.95971400	0.89247900	0.48918700
C	-1.06525300	2.14177200	1.00862400
C	0.22331800	1.97313200	1.52949200
C	-1.82190200	3.27140900	1.34935500
C	0.75682900	2.95478300	2.35543800
H	0.79109400	1.07987200	1.28960400
C	-1.27162100	4.25480700	2.15950500
H	-2.82830400	3.38179300	0.95764700
C	0.02003200	4.09749700	2.66098900
H	1.75296800	2.82438700	2.76428000
H	-1.84901900	5.13961100	2.40511200
H	0.44819200	4.86323300	3.30000000
C	-4.00238800	0.77378500	-0.41014500
O	-3.92389700	1.19648900	-1.52840400
C	-5.20509600	0.12612400	0.22449000
C	-4.97573300	-0.52189900	1.58779400
H	-5.98690800	0.89425500	0.27278100
H	-5.55462500	-0.61270900	-0.50539400
C	-6.18536400	-1.34883600	2.01100200
H	-4.76447200	0.25467000	2.32968000
H	-4.08911000	-1.16151000	1.54019400
H	-6.02394100	-1.80347200	2.99108100
H	-6.36732700	-2.15549600	1.29348000
H	-7.09102100	-0.73634000	2.06664400
O	4.42297200	-0.61963600	-0.78203700
C	4.74264100	-1.30088100	0.17643200
O	4.06206000	-2.34540900	0.60896000
C	5.97124400	-1.01193500	1.01313200
C	6.76789000	-2.25649700	1.40562200
H	5.62727000	-0.49997500	1.92171600
H	6.58828800	-0.30344000	0.45415100
C	7.99784000	-1.90010200	2.23539200
H	6.11401700	-2.93288100	1.96299600

H	7.07181600	-2.79299400	0.49961500
H	8.56281000	-2.79281200	2.51529800
H	8.66885400	-1.23842600	1.67845000
H	7.71019200	-1.38192500	3.15598700
H	3.22472500	-2.45573400	0.05045900

Coordinates for the chemoselective pathway

TS4RR-HDA

C	-0.70484700	3.63105400	-0.76508200
C	-1.75757000	4.41490300	-1.24246400
C	-1.63829400	5.79635000	-1.28789200
C	-0.44458300	6.38256200	-0.86465000
C	0.61120600	5.59533000	-0.40929600
C	0.48983000	4.20575500	-0.35248400
C	-1.13889200	2.17617600	-0.79615300
C	-2.22606900	2.18612400	-1.89414800
C	-2.90858900	3.53802200	-1.67922100
H	-2.45245600	6.40971500	-1.66207500
H	-0.33252200	7.46135800	-0.90248300
H	1.53829100	6.06418600	-0.09641000
H	1.31166000	3.59456100	0.00913500
H	-2.91475200	1.33527200	-1.81100700
H	-3.39749300	3.87413800	-2.59635200
H	-1.60920100	1.86176800	0.13890500
H	-3.66277300	3.44239000	-0.88982700
C	0.11383100	0.78159800	-2.41554200
C	0.95887700	0.74990700	-0.38406900
N	1.20251300	0.08806600	-2.52546400
N	-0.07367000	1.21832600	-1.12680600
N	1.71771300	0.07314300	-1.26314800
C	-0.89063600	1.07120100	-3.49020400
H	-0.37175600	1.24334500	-4.43420200
H	-1.54429400	0.19425100	-3.60487000
C	2.99896600	-0.52308200	-1.08196900
C	4.11645600	0.27892700	-0.83230500
C	3.17413400	-1.89225100	-1.27785000
C	5.37744800	-0.27744100	-0.69328200
C	4.43482000	-2.46779300	-1.14801600
C	5.51445000	-1.65351300	-0.84280600
H	6.23342400	0.35012200	-0.47923300
H	4.56206500	-3.53375000	-1.28853400
Cl	3.94573900	1.99884600	-0.73078300
Cl	7.08810100	-2.36724500	-0.66781500
Cl	1.84240500	-2.90124200	-1.70948000

O	-1.62723600	2.22817600	-3.18089600
C	1.32263400	0.91203600	1.07888400
O	2.36373300	0.32354400	1.43791700
C	0.50278900	1.71965300	1.86888000
C	1.02745700	2.16638600	3.20324200
H	-0.26913600	2.33121700	1.42601200
C	0.06337100	3.10906900	3.91582900
H	1.25980200	1.29863800	3.83130200
H	1.99425000	2.66799700	3.04548400
H	0.46179700	3.43695800	4.87922900
H	-0.13032800	3.99900700	3.30702800
H	-0.89855000	2.61994200	4.10065800
C	-3.10896600	-0.18457800	0.82411300
O	-3.41570100	1.00800500	0.85528800
C	-1.74720400	-0.64860100	1.19451700
C	-1.24275300	-0.02448700	2.34421400
H	-1.90299700	0.78165100	2.66610200
C	-4.17693900	-1.18796800	0.50311400
C	-4.11203600	-2.50883600	0.95122500
C	-5.27620800	-0.76366000	-0.24742200
C	-5.12320100	-3.40522300	0.62324600
H	-3.26925500	-2.83056200	1.55577500
C	-6.28169600	-1.66162900	-0.58282600
H	-5.31875600	0.27407300	-0.56422800
C	-6.20221700	-2.98536600	-0.15164200
H	-5.06947900	-4.43132900	0.97168600
H	-7.12773100	-1.33432800	-1.17855100
H	-6.98616900	-3.68870400	-0.41449500
C	-0.44932500	-0.52660300	3.48353100
C	0.72493700	-1.29835700	3.44744300
C	-0.95075600	-0.14432500	4.74330600
C	1.34314500	-1.68160300	4.63470200
H	1.16734500	-1.55212200	2.49868400
C	-0.33756800	-0.54263200	5.92284600
H	-1.84842300	0.46674800	4.79167800
C	0.81861700	-1.31822000	5.87129400
H	2.25682600	-2.26544000	4.58619500
H	-0.75646000	-0.24091200	6.87750200
H	1.31217000	-1.62584900	6.78798700
C	-1.00213700	-1.66667400	0.46136200
O	0.16732100	-1.91885200	0.74883900
C	-1.55814700	-2.37828700	-0.74413300
C	-2.26946900	-1.72856600	-1.75063600
C	-1.25816100	-3.73481100	-0.89010900

C	-2.70478100	-2.42291700	-2.87529000
H	-2.49536500	-0.67217200	-1.64577400
C	-1.70147300	-4.43601900	-2.00600600
H	-0.67283200	-4.22461100	-0.11798800
C	-2.42711200	-3.78154200	-3.00060300
H	-3.26438200	-1.90545000	-3.64891300
H	-1.47839800	-5.49363100	-2.10384800
H	-2.77114700	-4.32872500	-3.87237000

TS4RS-HDA

C	0.59609000	-2.90207500	-1.83415100
C	1.55817300	-3.32827800	-2.75247100
C	1.59100100	-4.65178100	-3.16818500
C	0.63891600	-5.53940900	-2.66429100
C	-0.33215300	-5.10486700	-1.76424700
C	-0.36189700	-3.77623900	-1.33751500
C	0.82924000	-1.43043900	-1.54254200
C	1.56960000	-0.95758300	-2.81524700
C	2.43130800	-2.16844500	-3.17490800
H	2.33262000	-4.98797300	-3.88658600
H	0.64679600	-6.57560000	-2.98686700
H	-1.07390400	-5.80321500	-1.39131000
H	-1.11618300	-3.44178200	-0.63125600
H	2.15403700	-0.04641300	-2.64336600
H	2.67794300	-2.16521900	-4.23895900
H	1.48579700	-1.27058200	-0.68475500
H	3.36152300	-2.13268900	-2.59660000
C	-0.96394300	0.08432700	-2.34799500
C	-1.24343900	-0.59939100	-0.27861400
N	-2.12130400	0.55388600	-2.00157800
N	-0.39254300	-0.63976100	-1.32982300
N	-2.28399700	0.12614200	-0.71798700
C	-0.24504800	0.28950700	-3.64668100
H	-0.96787600	0.31386300	-4.46316700
H	0.27933600	1.25605200	-3.60951900
C	-3.53425000	0.38920600	-0.08646200
C	-4.45252300	-0.64492100	0.11177000
C	-3.89851100	1.69565200	0.23326800
C	-5.69491000	-0.39647400	0.67125700
C	-5.14368200	1.96567000	0.79201000
C	-6.01980000	0.91298800	1.00976500
H	-6.39510600	-1.20553000	0.83557600
H	-5.41535400	2.98190000	1.04877900
Cl	-4.05117300	-2.26298800	-0.35556400

Cl	-7.57769300	1.23647500	1.70794600
Cl	-2.80912000	2.99970800	-0.06527200
O	0.64675900	-0.77204300	-3.87937200
C	-1.17145100	-1.16980200	1.12150500
O	-2.13381200	-0.87969800	1.85250200
C	-0.05466200	-1.94654600	1.47810900
C	-0.17560900	-2.67984900	2.78966100
H	0.58198900	-2.38063800	0.71905600
C	0.59397100	-3.99811500	2.82417600
H	0.15013200	-2.04048800	3.62413500
H	-1.24292100	-2.85549800	2.97192900
H	0.39811600	-4.53895300	3.75420000
H	0.29226400	-4.64044500	1.98956900
H	1.67273100	-3.83574600	2.75034600
C	2.99562500	0.79618500	0.18428300
O	3.41838400	-0.13238500	-0.50402900
C	1.73433800	0.70446300	0.95542700
C	1.51487000	-0.28088100	1.92633000
H	0.74255100	-0.00104000	2.64108000
C	3.81283000	2.05140500	0.27189400
C	3.65191200	2.97750200	1.30498900
C	4.79090100	2.26695500	-0.70347500
C	4.45356900	4.11403700	1.35256600
H	2.90688400	2.80164400	2.07510700
C	5.58543300	3.40456200	-0.65969000
H	4.91059200	1.52773500	-1.48885100
C	5.41593500	4.33081300	0.36929800
H	4.32830500	4.83000800	2.15807500
H	6.33790100	3.57177900	-1.42356500
H	6.03672600	5.22050700	0.40545000
C	2.53794500	-1.21080700	2.45795200
C	3.33713300	-2.05119400	1.66891700
C	2.68453100	-1.27069500	3.85140300
C	4.26906200	-2.89845900	2.25866800
H	3.21661200	-2.05386900	0.59270500
C	3.61651200	-2.11867200	4.44024400
H	2.06054100	-0.63704000	4.47554400
C	4.41556800	-2.93462200	3.64371800
H	4.87479500	-3.54473600	1.63147900
H	3.71371300	-2.14513400	5.52077200
H	5.13985000	-3.60282800	4.09847800
C	0.67698800	1.71218000	0.85083200
O	-0.34768700	1.62463900	1.52951100
C	0.75744200	2.84928100	-0.13108300

C	1.28898600	2.71710000	-1.41380100
C	0.19716500	4.07177800	0.24987300
C	1.26962200	3.78873100	-2.30287100
H	1.72160300	1.77033100	-1.72332400
C	0.19009600	5.14818300	-0.62917800
H	-0.23818500	4.15376300	1.24093900
C	0.72428000	5.00769400	-1.90999600
H	1.68563700	3.67179000	-3.29902900
H	-0.23559600	6.09718200	-0.31880900
H	0.71464800	5.84652700	-2.59838000

TS4SR-HDA

C	4.35933600	0.68333400	1.42469500
C	5.41770400	1.56864700	1.23642100
C	6.71496300	1.18065800	1.56146200
C	6.92729400	-0.09784900	2.07217000
C	5.85748600	-0.97389800	2.27257200
C	4.55763800	-0.58791000	1.95512000
C	3.05036800	1.31168300	0.99917300
C	3.46321500	2.64529600	0.28439500
C	4.92989600	2.89331800	0.70601100
H	7.54765300	1.86277300	1.41694900
H	7.93446700	-0.41471100	2.32401800
H	6.04016000	-1.95979200	2.68784800
H	3.70635700	-1.23791500	2.13521700
H	2.78864800	3.44239600	0.59621600
H	5.50584700	3.26540400	-0.14699900
H	2.36212600	1.48943900	1.82319000
H	4.97607500	3.65977100	1.48692400
C	2.73357300	0.35858500	-1.25965100
C	1.38514300	-0.46889100	0.24461800
N	2.08361900	-0.57244500	-1.89485600
N	2.35096500	0.43463400	0.05012600
N	1.24598200	-1.08520900	-0.94021000
C	3.69492900	1.39541900	-1.74450000
H	4.72821300	1.10404300	-1.50629800
H	3.59118100	1.52211900	-2.82267500
C	0.64205400	-2.35482100	-1.17878000
C	-0.55643300	-2.46750100	-1.88280500
C	1.29418800	-3.51071900	-0.74136200
C	-1.11416300	-3.71569200	-2.13188600
C	0.75164100	-4.76582600	-0.97788700
C	-0.45068200	-4.84703200	-1.67259300
H	-2.05231000	-3.79696900	-2.66685500

H	1.25878800	-5.65793900	-0.63223300
Cl	-1.37741500	-1.03572200	-2.36881300
Cl	-1.14144500	-6.40915800	-1.97135400
Cl	2.79863800	-3.37926900	0.10444600
O	3.32154200	2.60696600	-1.12898900
C	0.71744000	-0.76707300	1.56526200
O	1.44145900	-0.60202700	2.56258100
C	-0.62405800	-1.21583100	1.54324100
C	-1.06910200	-1.92284400	2.80470200
H	-1.02990100	-1.56376600	0.59869000
C	-2.01475300	-3.09213400	2.54027300
H	-0.17026100	-2.27540800	3.32423400
H	-1.54367400	-1.21692300	3.50029300
H	-2.24008900	-3.62775600	3.46656200
H	-2.96022200	-2.75362800	2.10829600
H	-1.55949800	-3.80390000	1.84222000
C	-0.37198200	2.12175000	0.26287300
O	0.35966200	2.14067400	1.26978400
C	-1.60860600	1.37539500	0.27061600
C	-1.84267900	0.60955900	1.43795400
H	-1.30412000	0.92114800	2.33133900
C	0.11424900	2.90373000	-0.92611700
C	0.27265700	2.31583900	-2.18213000
C	0.57181400	4.20813700	-0.71740400
C	0.88065300	3.02580700	-3.21553500
H	-0.08035600	1.30431300	-2.34412600
C	1.15400700	4.92513500	-1.75554100
H	0.46460800	4.64931600	0.26965300
C	1.31515100	4.33083900	-3.00693000
H	1.00543600	2.55800500	-4.18772900
H	1.49015100	5.94405700	-1.58971800
H	1.77950200	4.88619200	-3.81616100
C	-3.14780800	-0.04632200	1.66561300
C	-3.74699000	0.01831900	2.92745500
C	-3.81854100	-0.72239200	0.63698200
C	-4.99422000	-0.55768300	3.15337700
H	-3.23712700	0.54415200	3.73038200
C	-5.06468500	-1.29363800	0.85929100
H	-3.35127400	-0.80171000	-0.34175800
C	-5.65762600	-1.21186200	2.11917600
H	-5.44874000	-0.49072400	4.13664700
H	-5.57431300	-1.80806200	0.05079100
H	-6.63089000	-1.65970200	2.29250000
C	-2.65079400	1.65474400	-0.75593500

O	-2.46828700	1.55109500	-1.96290200
C	-3.97917100	2.20586100	-0.29547600
C	-4.14293100	2.83766700	0.93870500
C	-5.06226800	2.12775400	-1.17473300
C	-5.37813000	3.37024500	1.29463400
H	-3.29827700	2.91713800	1.61643000
C	-6.29858600	2.65040100	-0.81648300
H	-4.91135400	1.65096100	-2.13786200
C	-6.45842700	3.27224100	0.42147000
H	-5.49720300	3.86311700	2.25427600
H	-7.13824300	2.57695500	-1.50050200
H	-7.42313500	3.68296000	0.70320200

TS4SS-HDA

C	0.42098600	-1.55255700	1.03039300
O	1.50372600	-1.96060100	1.50485900
C	-0.85181300	-1.58695100	1.59074200
C	-1.10579000	-2.53083000	2.73386300
H	-1.69809800	-1.24805100	0.99907500
C	-2.55686600	-2.50780800	3.20563500
H	-0.42071700	-2.31361100	3.56221200
H	-0.84512400	-3.54894600	2.40627700
H	-2.72205000	-3.22487800	4.01366700
H	-3.23415900	-2.75978000	2.38279200
H	-2.84626900	-1.51881600	3.57332300
C	-2.08893000	1.76398400	0.89469400
O	-2.92498300	0.86442200	0.79983000
C	-0.76182500	1.51293700	1.49753700
C	-0.81510500	0.53796300	2.51569800
H	-1.84901100	0.28524300	2.74059400
C	-2.49986400	3.15529800	0.49718200
C	-1.92586300	4.29295300	1.06863100
C	-3.54299100	3.29913300	-0.42080600
C	-2.36959000	5.55963200	0.70229700
H	-1.13954500	4.18418900	1.80970200
C	-3.97801900	4.56437000	-0.79680800
H	-4.00101200	2.40183100	-0.82444600
C	-3.38827100	5.69719300	-0.23780800
H	-1.92208300	6.43979100	1.15261800
H	-4.77891800	4.67073400	-1.52169000
H	-3.72860700	6.68619600	-0.52847100
C	0.05293300	0.23904100	3.67229300
C	1.44769600	0.09427300	3.66125100
C	-0.62304300	0.00337500	4.88378700

C	2.12953300	-0.26476700	4.81910900
H	1.99452000	0.27376100	2.75148700
C	0.06097100	-0.32965900	6.04557500
H	-1.70562100	0.09617400	4.91046300
C	1.44642900	-0.47113100	6.01383400
H	3.20785800	-0.38180000	4.78389500
H	-0.48645800	-0.48944300	6.96889300
H	1.98918600	-0.74346400	6.91362100
C	0.45347900	2.16951600	1.04703000
O	1.53111800	2.10027700	1.65284600
C	0.47886100	2.89990200	-0.27171400
C	-0.19612400	2.41909500	-1.39164600
C	1.30442700	4.01891600	-0.40066500
C	-0.06290200	3.05003500	-2.62521100
H	-0.82339900	1.53762400	-1.30256100
C	1.42794700	4.66124800	-1.62628500
H	1.84376200	4.37112000	0.47393100
C	0.74576800	4.17659400	-2.74242300
H	-0.58862300	2.65566000	-3.49068000
H	2.05974700	5.53946300	-1.71577700
H	0.84825400	4.67629900	-3.70073600
C	3.96137300	-1.02226000	-0.56654400
C	5.11545100	-0.40094700	-1.03966400
C	6.21529400	-1.16803500	-1.41321500
C	6.13493800	-2.55478000	-1.30744300
C	4.97727200	-3.16845500	-0.82358200
C	3.87615800	-2.40542600	-0.44177200
C	2.90246800	0.00919800	-0.23601800
C	3.44938000	1.34396300	-0.85143900
C	4.96125500	1.09906200	-1.04122900
H	7.11881600	-0.69436600	-1.78570500
H	6.98309500	-3.16512900	-1.60119100
H	4.93777500	-4.24949900	-0.73824600
H	2.97805500	-2.85671900	-0.03095400
H	3.22721300	2.16715700	-0.17200300
H	5.30374200	1.57738600	-1.96345200
H	2.72782700	0.11496800	0.83408400
H	5.52297900	1.54443400	-0.21292200
C	1.41486600	-0.14516100	-2.19480600
C	0.54174000	-0.97079200	-0.36511300
N	0.27437000	-0.63502900	-2.58089200
N	1.61726200	-0.34155400	-0.85592200
N	-0.26292700	-1.14594400	-1.43029300
C	2.44314600	0.65650900	-2.92719500

H	3.29298100	0.02027800	-3.21214300
H	2.00094300	1.09528700	-3.82245400
C	-1.44068200	-1.94700100	-1.49216200
C	-1.36668600	-3.31707400	-1.20780900
C	-2.67421400	-1.39767100	-1.85084400
C	-2.50813300	-4.10486800	-1.18864600
C	-3.82630600	-2.17599400	-1.84299000
C	-3.73000700	-3.51490000	-1.49149600
H	-2.44000400	-5.15933100	-0.95201200
H	-4.77945600	-1.73483600	-2.10645100
Cl	0.15958500	-4.07119600	-0.90062700
Cl	-5.16518000	-4.48504400	-1.45893100
Cl	-2.80502800	0.24785300	-2.35219000
O	2.82214300	1.71197900	-2.07385800

TS5R-Stetter

C	-0.47752500	4.05829600	-0.16571200
C	-0.39314800	5.31976100	0.41783700
C	-0.77414500	6.44773000	-0.30461800
C	-1.23323200	6.28887400	-1.61038400
C	-1.29480500	5.02203500	-2.19589900
C	-0.90950300	3.89247200	-1.47799400
C	-0.01493700	2.98522600	0.79236800
C	0.20452500	3.72889100	2.15670900
C	0.17102800	5.23796200	1.81461000
H	-0.71278700	7.43620700	0.14142900
H	-1.53697700	7.15973500	-2.18269200
H	-1.63763100	4.91918700	-3.22048800
H	-0.91977700	2.90387300	-1.92833700
H	1.16298400	3.41750300	2.57345700
H	-0.42331900	5.77761100	2.55925500
H	0.92006300	2.51864800	0.47739500
H	1.18257200	5.65513600	1.84658500
C	-2.10851700	2.11037200	1.76368900
C	-1.18537800	0.75286900	0.29455500
N	-2.96160400	1.14567500	1.67235200
N	-1.01724600	1.93008900	0.95089400
N	-2.39348100	0.29261400	0.73847800
C	-2.07530400	3.29422400	2.67323100
H	-2.38371300	4.20265700	2.13614800
H	-2.74074400	3.13615500	3.52196700
C	-3.27651100	-0.57291700	0.04111800
C	-3.67417300	-1.79294300	0.59106100
C	-3.79493300	-0.19628100	-1.20246800

C	-4.54458100	-2.63605900	-0.08972400
C	-4.65408200	-1.02761300	-1.90703200
C	-5.01561000	-2.24160200	-1.33572400
H	-4.83849000	-3.58401900	0.34371000
H	-5.03787100	-0.72775100	-2.87406400
Cl	-3.02683000	-2.28799100	2.10976200
Cl	-6.08947000	-3.29360500	-2.20505900
Cl	-3.36559400	1.33718400	-1.88236600
O	-0.75058600	3.38859300	3.15537200
C	-0.24355600	0.09141000	-0.54555900
O	0.48197800	0.97835400	-1.31349600
C	-0.64274400	-1.16588500	-1.19915300
C	-0.25174000	-1.52339900	-2.42575000
H	-1.21416000	-1.86820100	-0.59773100
C	-0.55377500	-2.85655400	-3.03680500
H	1.38577900	0.61121500	-1.41228600
H	0.34209800	-0.82618900	-3.01237400
H	-1.06790900	-2.74673700	-3.99734800
H	0.37183400	-3.40918300	-3.23542800
H	-1.18050900	-3.46419200	-2.37764100
C	2.84997100	-1.37013800	-0.83159400
O	2.88342000	-1.05174500	-2.01472900
C	2.40941200	-0.37873100	0.19171400
C	1.19170900	-0.47728800	0.91564900
H	1.07131600	0.40497200	1.54663500
C	3.29154800	-2.74286300	-0.42451700
C	3.62881100	-3.03587900	0.89913200
C	3.37839600	-3.73772900	-1.40210500
C	4.04233500	-4.31860700	1.24413800
H	3.55142500	-2.25501500	1.65090600
C	3.77753800	-5.02230900	-1.05386300
H	3.12617500	-3.47938200	-2.42578200
C	4.10903100	-5.31251400	0.27016200
H	4.30393300	-4.54500100	2.27257800
H	3.83678800	-5.79814200	-1.81056500
H	4.42256300	-6.31578900	0.54165800
C	0.64412800	-1.68702900	1.58734700
C	0.29787100	-1.54809300	2.93852700
C	0.52576500	-2.95907600	1.00569600
C	-0.10089500	-2.64294900	3.70037200
H	0.37156600	-0.56764200	3.40293600
C	0.11330300	-4.05056200	1.76122800
H	0.76908900	-3.10067200	-0.04112700
C	-0.18796500	-3.90214700	3.11392000

H	-0.34158000	-2.50873600	4.75036000
H	0.04016100	-5.02645000	1.29137000
H	-0.49396700	-4.76093700	3.70303800
C	3.10631000	0.88959000	0.28081200
O	2.68931400	1.84367600	0.96188700
C	4.42511400	1.09119800	-0.42111600
C	5.41054000	0.10533900	-0.50285500
C	4.68762900	2.36184000	-0.93892600
C	6.63122300	0.38178300	-1.11122000
H	5.23633700	-0.87769700	-0.07440700
C	5.89858000	2.63305600	-1.56502400
H	3.92594800	3.12831200	-0.83897400
C	6.87431700	1.64189700	-1.65193400
H	7.39383800	-0.38886500	-1.16266400
H	6.08462200	3.61858800	-1.98043800
H	7.82369100	1.85218100	-2.13452000

TS5S-Stetter

C	0.50576500	3.75486600	-1.12155300
C	0.90031100	5.05505700	-0.81703700
C	0.73940400	6.07003100	-1.75740600
C	0.18068000	5.75953700	-2.99459400
C	-0.20150900	4.45001400	-3.29701000
C	-0.03765000	3.43186700	-2.36129000
C	0.75912400	2.82088100	0.03898400
C	1.23645100	3.75508100	1.21130000
C	1.49564900	5.13805000	0.56602100
H	1.04203300	7.08790200	-1.52909100
H	0.04508900	6.54171400	-3.73478100
H	-0.62328400	4.22512000	-4.27136700
H	-0.30404900	2.40365200	-2.58877700
H	2.14155700	3.33043800	1.64821600
H	1.05268700	5.92719000	1.18289300
H	1.52715000	2.07781700	-0.16550900
H	2.57066400	5.33777900	0.51649200
C	-1.40666700	2.69992700	1.21175500
C	-0.95198600	0.89492800	0.03235500
N	-2.47110000	1.98196100	1.34255600
N	-0.46211100	2.10297400	0.41660700
N	-2.19738900	0.85614000	0.58809100
C	-1.02701100	3.97920700	1.88045900
H	-1.15470700	4.83084900	1.19683200
H	-1.64323800	4.13421300	2.76605400
C	-3.29741800	0.05859700	0.18750800

C	-3.91994200	-0.80059300	1.09560200
C	-3.80713800	0.14824900	-1.11326700
C	-4.99369500	-1.59460600	0.71024300
C	-4.86748200	-0.64798800	-1.52369700
C	-5.44381100	-1.51410500	-0.60126900
H	-5.46137900	-2.26409700	1.42136100
H	-5.24349500	-0.58062900	-2.53692900
Cl	-3.32613000	-0.89971300	2.71111600
Cl	-6.77443600	-2.51117900	-1.09867800
Cl	-3.12162600	1.27294800	-2.23433900
O	0.31686000	3.83264700	2.29259500
C	-0.25742800	-0.12618700	-0.68569400
O	0.65348700	0.42010800	-1.56882800
C	-0.99757300	-1.30573400	-1.16925700
C	-0.75541000	-1.90713500	-2.33763000
H	-1.69845900	-1.76118000	-0.46959400
C	-1.43612800	-3.16492900	-2.78162400
H	1.50575300	-0.05337400	-1.47137500
H	-0.02354600	-1.46027500	-3.00838200
H	-1.91355100	-3.02945600	-3.75772400
H	-0.71655100	-3.98476800	-2.88662900
H	-2.20126500	-3.47606500	-2.06463700
C	2.45539500	-2.12482900	-0.96429100
O	2.94184200	-1.78566400	-2.03943400
C	2.23296200	-1.14345100	0.12703800
C	0.95517900	-1.15945600	0.74423200
H	0.43229900	-2.08259300	0.50604900
C	2.07962000	-3.56790900	-0.75800500
C	2.00590600	-4.14334800	0.51425700
C	1.87434100	-4.36559400	-1.88658900
C	1.71155000	-5.49700800	0.65425200
H	2.19423800	-3.52857400	1.39086200
C	1.57049600	-5.71476800	-1.74652600
H	1.96164700	-3.90335900	-2.86525900
C	1.48660300	-6.28116300	-0.47466100
H	1.66247900	-5.94021700	1.64374500
H	1.40215800	-6.32768400	-2.62663400
H	1.25313500	-7.33556000	-0.36460500
C	0.57803000	-0.74776800	2.12762900
C	-0.03251400	-1.74303900	2.90685100
C	0.76172700	0.51617900	2.70781700
C	-0.42919200	-1.49874100	4.21734100
H	-0.19162500	-2.72894900	2.47514100
C	0.31837900	0.77560900	4.00035500

H	1.27384200	1.28548800	2.15150600
C	-0.27198700	-0.22865200	4.76469500
H	-0.88409200	-2.29482900	4.79915400
H	0.44986100	1.77330600	4.40796600
H	-0.60251300	-0.02393500	5.77818600
C	3.23259200	-0.11632600	0.35186900
O	2.96428500	0.98600000	0.85155200
C	4.67624200	-0.38785800	0.02128500
C	5.24198100	-1.66375200	0.07727400
C	5.49113100	0.70812200	-0.26947500
C	6.59931300	-1.84025600	-0.17010200
H	4.62488600	-2.52102700	0.33268700
C	6.84467800	0.53184200	-0.53112300
H	5.04146600	1.69544500	-0.28498500
C	7.40139000	-0.74455700	-0.48182700
H	7.03212900	-2.83400700	-0.11597400
H	7.46693300	1.38826400	-0.77100700
H	8.45925100	-0.88556000	-0.68060700

TS5R'-Stetter

C	-0.39793100	4.01727300	-0.08476200
C	-0.28975400	5.25216900	0.54968300
C	-0.63585200	6.41640400	-0.13171800
C	-1.08381100	6.31938700	-1.44738300
C	-1.16784300	5.07858600	-2.08388200
C	-0.81730100	3.91312800	-1.40705400
C	0.03162500	2.89639000	0.83219700
C	0.25486600	3.57909200	2.22752100
C	0.25794100	5.10097500	1.94717800
H	-0.55638700	7.38517200	0.35299200
H	-1.36119500	7.21871600	-1.98810600
H	-1.50051000	5.02496100	-3.11552800
H	-0.84507900	2.94309200	-1.89550200
H	1.20189900	3.22996200	2.64078400
H	-0.33167300	5.62314000	2.70786100
H	0.96079400	2.42562200	0.50273000
H	1.27819000	5.49315600	2.00542000
C	-2.09137700	2.02861500	1.75038400
C	-1.16013200	0.69137100	0.27062300
N	-2.95010000	1.07137200	1.63174900
N	-0.99434900	1.85881400	0.94306600
N	-2.37712000	0.23196800	0.68745400
C	-2.04159900	3.17912000	2.70111400
H	-2.31793600	4.11504600	2.19509900

H	-2.72070800	3.00765000	3.53619300
C	-3.25936000	-0.59656200	-0.05651500
C	-3.71615700	-1.81101400	0.45919900
C	-3.72542400	-0.18552200	-1.31007900
C	-4.59655400	-2.61108100	-0.25946200
C	-4.59286200	-0.97387400	-2.05254000
C	-5.01652100	-2.18157200	-1.51175600
H	-4.93674100	-3.55407900	0.15005800
H	-4.93533500	-0.64627000	-3.02597800
Cl	-3.13410500	-2.35032200	1.98835600
Cl	-6.10048500	-3.18054500	-2.42897100
Cl	-3.22056400	1.33810600	-1.95990400
O	-0.71930300	3.21804700	3.20092900
C	-0.20913000	0.02205900	-0.55206800
O	0.52244900	0.90220300	-1.32203200
C	-0.59935900	-1.27769000	-1.12867200
C	-0.42607600	-1.72443500	-2.38076500
H	-1.02103000	-1.97000700	-0.40364400
C	0.10069700	-0.99429300	-3.58087800
H	1.38946500	0.48561200	-1.50648800
H	-0.70561100	-2.76337900	-2.55280900
H	-0.45633900	-1.29779200	-4.47193400
H	0.02743300	0.08657900	-3.46940000
H	1.15460900	-1.24693800	-3.74443200
C	2.77319100	-1.45821100	-0.80015700
O	2.79361700	-1.12607100	-1.98270100
C	2.41360000	-0.45285000	0.23451500
C	1.18772200	-0.46882500	0.95722100
H	1.10428500	0.46916200	1.50779300
C	3.14414900	-2.85706400	-0.42236900
C	3.55241700	-3.16811800	0.87700400
C	3.09180500	-3.85832000	-1.39566100
C	3.90114800	-4.47487300	1.20264700
H	3.58140700	-2.37945700	1.62452500
C	3.42535800	-5.16640300	-1.06527200
H	2.78079000	-3.58941200	-2.40026900
C	3.83068500	-5.47411800	0.23390800
H	4.21924700	-4.71553600	2.21169100
H	3.37243900	-5.94752200	-1.81696300
H	4.09326000	-6.49586100	0.49027200
C	0.57378500	-1.56660000	1.75167400
C	0.08156000	-1.20824100	3.01640500
C	0.50105900	-2.91844000	1.37954700
C	-0.39821400	-2.16469500	3.90571700

H	0.10417400	-0.16170900	3.31427400
C	0.01673600	-3.87447700	2.26569300
H	0.83164400	-3.23004100	0.39618100
C	-0.41813400	-3.50715500	3.53791200
H	-0.75137700	-1.85868000	4.88536100
H	-0.01308300	-4.91549000	1.95927800
H	-0.78135600	-4.25976800	4.23069900
C	3.14610800	0.79744100	0.26209200
O	2.77338100	1.79231600	0.91045200
C	4.46907300	0.92163100	-0.45177800
C	5.40729700	-0.11093200	-0.50863300
C	4.79110700	2.16416900	-1.00316200
C	6.63839700	0.09015300	-1.12559700
H	5.18865600	-1.07283000	-0.05375500
C	6.01263300	2.36058000	-1.63715200
H	4.06742000	2.96873300	-0.92234500
C	6.94031900	1.32250600	-1.69913100
H	7.36335900	-0.71711700	-1.15579400
H	6.24501700	3.32541700	-2.07720500
H	7.89839500	1.47567100	-2.18604800

TS5S'-Stetter

C	0.37160700	3.75795400	-1.01980400
C	0.71584700	5.06549800	-0.68657700
C	0.53415500	6.09115300	-1.61131000
C	0.00552500	5.78437200	-2.86258000
C	-0.32727400	4.46831500	-3.19363400
C	-0.14222200	3.43999200	-2.27327700
C	0.64270100	2.81202500	0.12744800
C	1.06118700	3.74251000	1.32466400
C	1.28743000	5.14342400	0.70661700
H	0.79820500	7.11445700	-1.36050300
H	-0.14509400	6.57462600	-3.59116000
H	-0.72695700	4.24668600	-4.17799500
H	-0.37169900	2.40796200	-2.52209900
H	1.97156800	3.34406600	1.77520200
H	0.81175600	5.90816200	1.32975400
H	1.44480800	2.10532800	-0.07827400
H	2.35657500	5.37586400	0.67643900
C	-1.53763700	2.58277400	1.25533300
C	-0.99265400	0.82091300	0.05105300
N	-2.57669900	1.82300800	1.34933900
N	-0.55536500	2.03740400	0.46911600
N	-2.24544100	0.72354900	0.57944400

C	-1.22392000	3.86613600	1.95013700
H	-1.37630400	4.72152800	1.27622900
H	-1.86283500	3.98075200	2.82575400
C	-3.30836400	-0.10825000	0.14719700
C	-3.93204100	-0.98365700	1.03920400
C	-3.79426200	-0.02374500	-1.16298100
C	-4.98472000	-1.79385400	0.63087900
C	-4.83414000	-0.83489200	-1.59558000
C	-5.41352000	-1.71369400	-0.68763400
H	-5.45355300	-2.47432200	1.33066200
H	-5.19199200	-0.76959000	-2.61547200
Cl	-3.37275100	-1.07710600	2.66774700
Cl	-6.71970100	-2.72908200	-1.21291700
Cl	-3.11064200	1.11801700	-2.26854400
O	0.11667800	3.77228800	2.38654300
C	-0.24638700	-0.15787400	-0.67787300
O	0.66470400	0.44941600	-1.51994500
C	-0.93152300	-1.36372500	-1.18177400
C	-0.77240800	-1.94659000	-2.37817500
H	-1.53303900	-1.88843900	-0.43975800
C	-0.00075500	-1.44085500	-3.56704600
H	1.52452200	-0.01275200	-1.42847300
H	-1.26231200	-2.91039100	-2.50265500
H	1.07863700	-1.58070800	-3.42935700
H	-0.29987500	-1.98431200	-4.46601000
H	-0.16481700	-0.37437100	-3.72925400
C	2.49216700	-2.09183400	-0.93978100
O	2.98321500	-1.75291500	-2.01522100
C	2.25313200	-1.11210200	0.14574000
C	0.97003400	-1.15666700	0.75760800
H	0.47737300	-2.09609900	0.52198900
C	2.12070700	-3.53644200	-0.73624100
C	2.07359300	-4.11727000	0.53463700
C	1.88186300	-4.32644500	-1.86355200
C	1.77669700	-5.47032300	0.67550400
H	2.28185100	-3.50596800	1.40930400
C	1.57282200	-5.67379100	-1.72215700
H	1.94558700	-3.86155500	-2.84270000
C	1.51932000	-6.24695200	-0.45162600
H	1.74989400	-5.91822800	1.66376200
H	1.37629700	-6.28095800	-2.60012800
H	1.28285300	-7.30068800	-0.34126800
C	0.57732200	-0.76062000	2.14104700
C	-0.03469300	-1.76627900	2.90603900

C	0.74809000	0.49914300	2.73373200
C	-0.44728200	-1.53459500	4.21375900
H	-0.18152600	-2.75027900	2.46563200
C	0.29058500	0.74553700	4.02388900
H	1.26411000	1.27274300	2.18707400
C	-0.30312900	-0.26810500	4.77295200
H	-0.90355100	-2.33796600	4.78443800
H	0.41116300	1.74053000	4.44107100
H	-0.64618400	-0.07360400	5.78428700
C	3.22888900	-0.06288300	0.37018400
O	2.93728400	1.03518300	0.86733200
C	4.67878600	-0.30582900	0.04453800
C	5.26939000	-1.57018700	0.10669800
C	5.47337900	0.80512700	-0.24606200
C	6.63081900	-1.72114200	-0.13458400
H	4.66844600	-2.43856300	0.36270700
C	6.83118200	0.65423400	-0.50170300
H	5.00481700	1.78356700	-0.26603900
C	7.41255500	-0.61087600	-0.44625800
H	7.08257200	-2.70614000	-0.07535000
H	7.43776800	1.52184800	-0.74149600
H	8.47386800	-0.73154900	-0.64003100