

Electronic Supporting Information for
Elucidating the mechanism and regioselectivity of Phosphine-catalyzed
transformation of MBH carbonate

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Part 1: Substituent effect

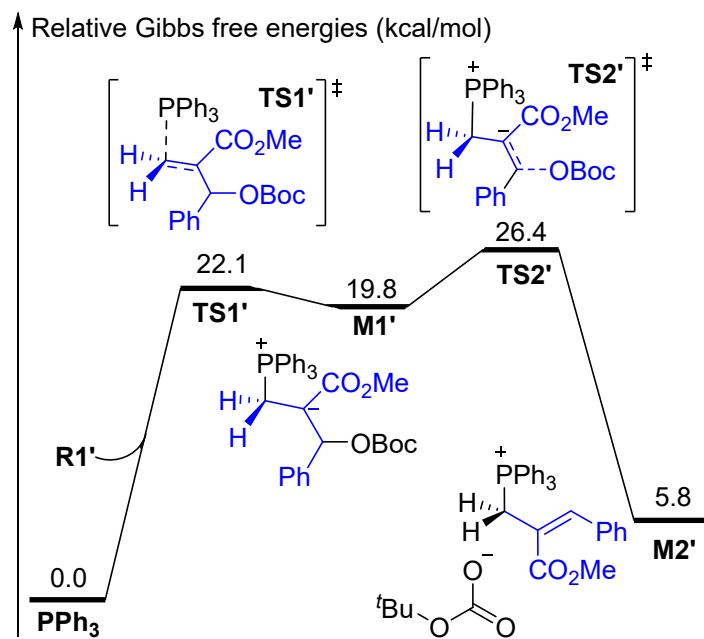


Fig. S1 Gibbs free energy profiles for the formation of complex intermediate **M2'**

Part 2: Different addition modes between ylide and dicyanoheptafulvene

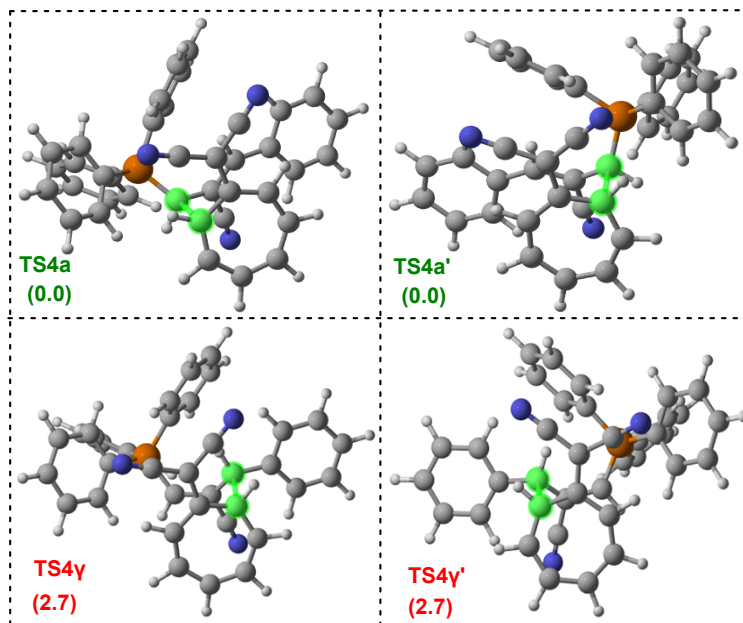


Fig. S2 3D structures and energies barriers involved in C-C bond formation process

Part 3: NBO analysis of allylic phosphorus ylide

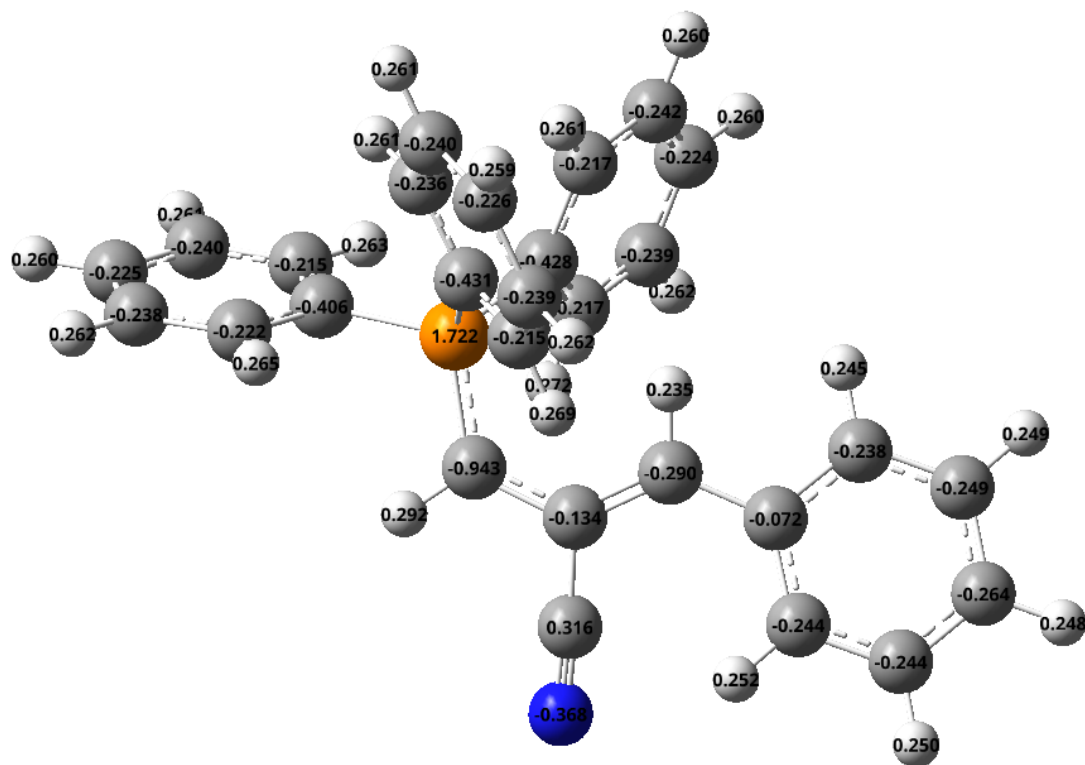


Fig. S3 NPA charge of α - and γ -carbon atoms in the allylic phosphorus ylide

Part 4: Energy profile of the entire reaction

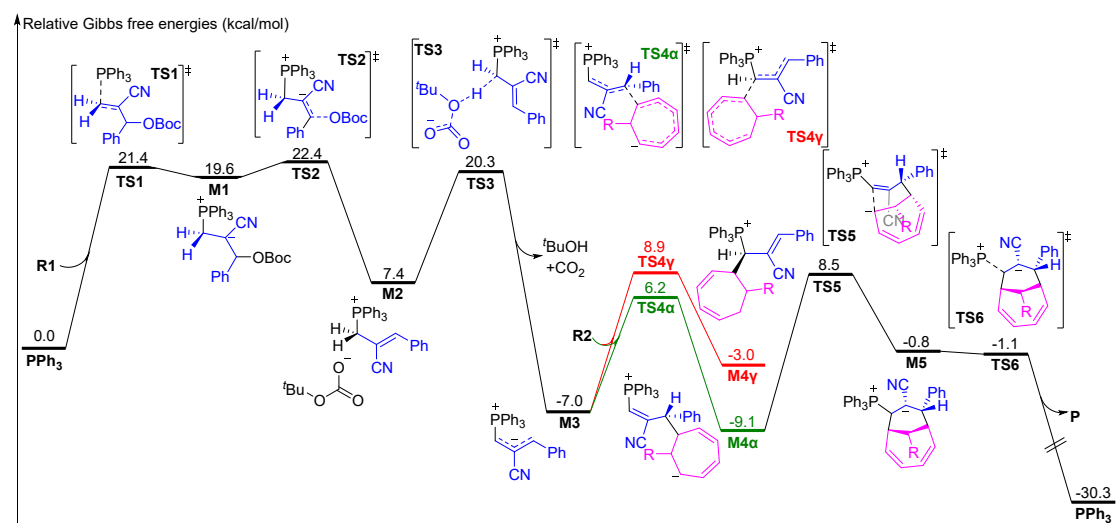


Fig. S4 The energy profile for the entire catalytic cycle

Part 5: Cartesian coordinates of all the stationary points involved in the reaction

R1			
C	0.93849000	1.29456100	-1.00294500
H	1.60484500	1.75162300	-1.74095600
C	0.73371200	2.35451900	0.06834000
C	1.07564100	3.62647200	-0.14567600
H	0.90953800	4.39125800	0.60359100
H	1.51972800	3.92473300	-1.08900800
C	0.16978100	2.01660100	1.35418000
C	1.57070800	-0.00398200	-0.53545100
C	1.38581900	-1.17318100	-1.27632100
C	2.38309300	-0.03360600	0.59643900
C	1.97915300	-2.36296500	-0.87006800
H	0.76562700	-1.15384100	-2.16833200
C	2.98187000	-1.22633300	1.00054400
H	2.55400000	0.87003800	1.17408800
C	2.77616300	-2.39435100	0.27460800
H	1.81922400	-3.26811500	-1.44743600
H	3.60440200	-1.23847900	1.88908700
H	3.23599600	-3.32396800	0.59366600
O	-0.26094100	1.10208900	-1.77158500
C	-1.32819500	0.43992500	-1.27283400
O	-2.32263600	0.30689900	-1.93826000
O	-1.09879200	-0.00349600	-0.04906900
C	-1.99286000	-0.97527300	0.59332400
C	-3.26988500	-0.25692400	1.00271900
C	-2.24522800	-2.15167100	-0.34349000
C	-1.18055000	-1.42908400	1.79985000
H	-3.02388000	0.60659300	1.62703300
H	-3.82424600	0.07722200	0.12382000
H	-3.90044000	-0.93703400	1.58185700
H	-1.28999400	-2.55757600	-0.69177700
H	-2.76733300	-2.93516000	0.21200400
H	-2.85124400	-1.86494200	-1.20207400
H	-1.73815100	-2.19352900	2.34709500
H	-0.22819800	-1.85458600	1.46635700
H	-0.97442900	-0.59002500	2.46653400
N	-0.26039400	1.81480100	2.40949400

R1'

C	0.47725200	-1.23391400	1.35978400
H	0.87396900	-1.88503000	2.14538700
C	-0.68853200	-1.99306400	0.75637700
C	-1.14213900	-3.09521000	1.35241500
H	-2.01149000	-3.62506700	0.97666400
H	-0.65153000	-3.50228500	2.23165600
C	1.63757300	-0.85615500	0.45591200
C	2.43776600	0.24151200	0.78071400
C	1.98084300	-1.64926800	-0.63770400
C	3.54491100	0.56273000	0.00181300
H	2.19452900	0.85261100	1.64544500
C	3.09381800	-1.33076600	-1.41366800
H	1.36387900	-2.50180900	-0.90118200
C	3.87463900	-0.22136000	-1.10192900
H	4.15111700	1.42517100	0.26049300
H	3.34452100	-1.94970200	-2.26912500
H	4.73657900	0.02903700	-1.71172800
O	-0.00992500	-0.12014900	2.14106100
C	-0.46574700	1.01034300	1.57376200
O	-0.79163100	1.94504100	2.26125600
O	-0.49332800	0.93538500	0.24911700
C	-0.67414800	2.15078600	-0.55701900
C	-2.10215800	2.65091800	-0.38826000
C	0.36436600	3.19615600	-0.16413500
C	-0.40977600	1.65873400	-1.97308500
H	-2.80705400	1.83864000	-0.58746800
H	-2.26694400	3.02370500	0.62323300
H	-2.29069600	3.45740200	-1.10204700
H	1.36842600	2.76752700	-0.23696300
H	0.29705000	4.03380100	-0.86361400
H	0.20043700	3.57010400	0.84625600
H	-0.48222600	2.49769300	-2.66976600
H	0.59320200	1.22566100	-2.03509700
H	-1.12675300	0.88768100	-2.26138500
C	-1.38614400	-1.54536000	-0.49648600
O	-0.87828700	-1.46450600	-1.58928100
O	-2.68820400	-1.32680100	-0.26875000
C	-3.47159200	-1.04307600	-1.43218000
H	-4.49431000	-0.92997500	-1.07874000
H	-3.12969500	-0.12179700	-1.90840400
H	-3.39759300	-1.86316800	-2.14870600

R2

C	-3.02370200	0.67947300	-0.00007300
C	-3.02370200	-0.67947300	-0.00007400
C	-1.88804100	-1.54997900	0.00000400
C	-1.88804100	1.54997900	0.00000300
C	-0.55704900	-1.27036800	0.00009200
C	-0.55704800	1.27036700	0.00008900
H	-3.99005800	1.17473200	-0.00013400
H	-3.99005800	-1.17473200	-0.00013500
H	-2.13047500	-2.60928000	0.00002200
H	-2.13047500	2.60928000	-0.00000700
H	0.09754400	-2.13745800	0.00015900
H	0.09754500	2.13745700	0.00012700
C	0.12827400	0.00000000	0.00013100
C	1.52236300	0.00000000	0.00003500
C	2.27911400	-1.20828900	-0.00002400
N	2.88702100	-2.19652600	-0.00007400
C	2.27911300	1.20828900	-0.00003000
N	2.88702000	2.19652600	-0.00006100

PPh₃

P	1.77566000	-0.30846200	0.44358300
C	3.47660900	-0.34985800	1.15498100
C	4.42289600	0.66585200	0.98586900
C	3.82450500	-1.48287300	1.90118700
C	5.69191000	0.54749100	1.54974800
H	4.16819000	1.55191900	0.41158200
C	5.09572000	-1.60621700	2.45416000
H	3.09241300	-2.27304800	2.04968700
C	6.03133600	-0.58813200	2.28139900
H	6.41780400	1.34307900	1.41405400
H	5.35295900	-2.49144300	3.02703200
H	7.02037600	-0.67860300	2.71916800
C	1.64714200	1.44853100	-0.10313000
C	1.98771300	1.89713300	-1.38323100
C	1.17877200	2.37522700	0.83645400
C	1.86326500	3.24492900	-1.71433500
H	2.35182900	1.19151200	-2.12447300
C	1.06490400	3.72313100	0.50909200
H	0.89806700	2.03660100	1.83092000
C	1.40454900	4.15990800	-0.76973500
H	2.12845900	3.58014500	-2.71218700
H	0.70151600	4.43004700	1.24822400
H	1.30812800	5.20920000	-1.02991200

C	2.03196000	-1.16681000	-1.16795600
C	3.28472900	-1.49324100	-1.69590200
C	0.88271600	-1.49571100	-1.89801500
C	3.38383100	-2.13154500	-2.93112500
H	4.18616200	-1.24711800	-1.14217700
C	0.98237100	-2.12174200	-3.13664100
H	-0.09779100	-1.25809800	-1.49180700
C	2.23550600	-2.44329900	-3.65458600
H	4.36206600	-2.38170600	-3.32997800
H	0.08316100	-2.36644200	-3.69300100
H	2.31667400	-2.93829900	-4.61711100

^tBuOH

C	-0.68154900	-1.25388000	-0.52180500
C	0.00585500	-0.00007800	0.01764100
H	-0.21244400	-2.14861300	-0.10371200
H	-1.74212900	-1.25848000	-0.24635900
H	-0.61680900	-1.30055800	-1.61277900
C	-0.66784600	1.26123700	-0.52170500
C	1.49003400	-0.00797700	-0.32653600
H	-0.18905100	2.15045200	-0.10272100
H	-0.60203300	1.30777600	-1.61264400
H	-1.72836100	1.27697900	-0.24654800
H	1.63437800	-0.00797300	-1.41013800
H	1.97744500	0.87644100	0.09284100
H	1.96752100	-0.89833100	0.09163800
O	-0.04849300	0.00017900	1.44544400
H	-0.97953900	0.00506500	1.70129900

CO₂

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16274600
O	0.00000000	0.00000000	-1.16274600

TS1

C	1.46470400	-1.45368000	-0.62974500
H	0.97954200	-2.43358000	-0.54324900
C	0.70647800	-0.67990100	-1.65053600
C	-0.66600600	-0.97736100	-1.81629300
H	-1.18326700	-0.50542500	-2.65185600
H	-0.95272800	-2.02181100	-1.68325200

C	1.22975700	0.48644900	-2.24896200
C	2.94777300	-1.69177300	-0.85949400
C	3.77492600	-2.02135300	0.21888000
C	3.49685000	-1.64415600	-2.13940900
C	5.12966700	-2.26463700	0.02596400
H	3.35437100	-2.07217300	1.21937900
C	4.85585200	-1.89282700	-2.33474600
H	2.86440400	-1.40298300	-2.98712000
C	5.67829800	-2.19617900	-1.25505000
H	5.75842400	-2.50981900	0.87652800
H	5.26973400	-1.84116900	-3.33692700
H	6.73643200	-2.38274900	-1.40806600
O	1.20631800	-0.94122200	0.73325600
C	1.72202400	0.22373400	1.15221100
O	1.40244200	0.68447500	2.22519000
O	2.57996300	0.72796300	0.28174000
C	3.53276200	1.77491000	0.63706500
C	2.79293500	3.09642400	0.77114800
C	4.28653900	1.38945500	1.90513000
C	4.46828500	1.77267300	-0.56588100
H	2.26951300	3.31720600	-0.16298500
H	2.06610400	3.04995000	1.58490800
H	3.50900400	3.89846900	0.97286000
H	4.72592400	0.39420500	1.78451700
H	5.09619800	2.10675100	2.06477900
H	3.63343200	1.39409600	2.77799100
H	5.24361400	2.53248100	-0.43550500
H	4.93896700	0.78865800	-0.66698900
H	3.90147400	1.98275400	-1.47659800
N	1.62722700	1.43974100	-2.79514100
P	-2.04537800	-0.25234600	-0.26037000
C	-3.65674900	0.07796800	-1.04184800
C	-4.43354200	1.18817700	-0.69394400
C	-4.10302900	-0.79390300	-2.04310400
C	-5.64869400	1.41326200	-1.33320700
H	-4.08565200	1.87519800	0.07174000
C	-5.32307200	-0.56778600	-2.67447300
H	-3.50123000	-1.65319400	-2.32960700
C	-6.09476000	0.53648700	-2.32027700
H	-6.24781400	2.27549700	-1.05991900
H	-5.66560800	-1.24884600	-3.44626600
H	-7.04288200	0.71605700	-2.81638700
C	-1.50456400	1.32293500	0.44233400
C	-1.76372600	1.69841900	1.76514000

C	-0.88737000	2.22679300	-0.43107500
C	-1.40969300	2.96938300	2.20592500
H	-2.24625400	1.00434200	2.44592000
C	-0.54869100	3.50074800	0.01388100
H	-0.67797000	1.94856700	-1.45947100
C	-0.80622900	3.87099200	1.33148400
H	-1.61220200	3.25691900	3.23227200
H	-0.07870700	4.19922900	-0.67064300
H	-0.53453100	4.86295200	1.67829100
C	-2.35245600	-1.42068600	1.09659300
C	-3.43383300	-2.30853900	1.02686600
C	-1.44770700	-1.51209400	2.16501200
C	-3.61045200	-3.27317000	2.01362900
H	-4.14683300	-2.24116500	0.21094600
C	-1.63865600	-2.47749700	3.14974000
H	-0.60409300	-0.83220700	2.23190800
C	-2.71380600	-3.35995000	3.07603500
H	-4.45448900	-3.95240300	1.95443300
H	-0.94051400	-2.53728700	3.97822000
H	-2.85495100	-4.11115000	3.84623900

TS1'

C	-1.37373393	1.12792441	-1.01885524
H	-0.89169193	2.03487441	-1.40596324
C	-0.60661793	-0.01558759	-1.60315824
C	0.72351307	0.24786941	-1.95319724
H	1.24415007	-0.51744759	-2.52413724
H	0.99469007	1.27229241	-2.20520424
C	-2.85212293	1.30303041	-1.32142424
C	-3.68716993	1.99257141	-0.44068424
C	-3.36160693	0.90647941	-2.55785124
C	-5.01911993	2.23589241	-0.76723924
H	-3.29459993	2.34668741	0.50811376
C	-4.69062693	1.15466641	-2.89009824
H	-2.71268293	0.38405441	-3.25300924
C	-5.52859793	1.81161541	-1.99202524
H	-5.65666193	2.76314241	-0.06380124
H	-5.07308993	0.82882341	-3.85243824
H	-6.56669093	1.99926041	-2.24744824
O	-1.07001693	1.31677541	0.40972776
C	-1.55426793	0.54257441	1.39034676
O	-1.20506693	0.72749441	2.53335176
O	-2.42781693	-0.35462459	0.95382976

C	-3.38897393	-0.96084959	1.87734176
C	-2.67754093	-1.93899659	2.80125676
C	-4.13052893	0.12525641	2.65202676
C	-4.34525093	-1.68718459	0.94122276
H	-2.18598893	-2.71821159	2.21309076
H	-1.92783493	-1.42745659	3.40615876
H	-3.41281093	-2.41205559	3.45924876
H	-4.60834793	0.82122141	1.95649276
H	-4.91118293	-0.34449659	3.25638276
H	-3.45926493	0.67331441	3.31383276
H	-5.17254293	-2.11112359	1.51672776
H	-4.74124993	-0.99243359	0.19435276
H	-3.82522893	-2.49540059	0.42397476
P	2.19977000	0.18491300	-0.31045800
C	3.68806300	-0.69754600	-0.87558800
C	4.27696200	-1.72060900	-0.12573000
C	4.21759200	-0.36829700	-2.13062600
C	5.38943700	-2.39489500	-0.62027600
H	3.86449500	-1.98814800	0.84229000
C	5.33595800	-1.03903400	-2.61628000
H	3.75834300	0.41736900	-2.72671700
C	5.92113900	-2.05410000	-1.86183400
H	5.84156500	-3.18779200	-0.03339700
H	5.74440000	-0.77555500	-3.58628700
H	6.78831400	-2.58266700	-2.24414900
C	1.61485200	-0.71504800	1.14581700
C	1.86797500	-0.28850100	2.45337600
C	0.93437900	-1.92001600	0.92100400
C	1.45467800	-1.06681600	3.52955100
H	2.39084000	0.64572300	2.63097600
C	0.54756400	-2.70261300	2.00517300
H	0.72486700	-2.25633000	-0.09246800
C	0.80261200	-2.27717500	3.30679000
H	1.65237800	-0.73144200	4.54234600
H	0.03940000	-3.64559200	1.83000700
H	0.48775800	-2.88706800	4.14803600
C	2.75042400	1.82322400	0.26095000
C	4.04281300	2.30600400	0.02955600
C	1.80601200	2.64389500	0.89685300
C	4.38651200	3.59486700	0.42941600
H	4.78361300	1.67777500	-0.45494800
C	2.16128200	3.92769200	1.29792900
H	0.80722400	2.26338600	1.09742000
C	3.44886200	4.40692700	1.06204400

H	5.39245800	3.96106300	0.25143100
H	1.42918600	4.55430900	1.79688500
H	3.72195300	5.40958600	1.37504600
C	-1.01753893	-1.39367859	-1.75303224
O	-0.24960493	-2.31634459	-2.02825924
O	-2.34701093	-1.62025059	-1.64338924
C	-2.75155093	-2.95063259	-1.93825124
H	-3.83978293	-2.95136259	-1.88052824
H	-2.42405693	-3.24502559	-2.93793324
H	-2.33325393	-3.65644659	-1.21480624
M1			
C	1.48089700	-1.47532900	-0.30482400
H	0.95327700	-2.41417600	-0.08949100
C	0.67355400	-0.71686800	-1.27510100
C	-0.76541000	-1.02746200	-1.42773600
H	-1.16377100	-0.71426800	-2.39979000
H	-0.98098900	-2.09866900	-1.31248100
C	1.19680000	0.31427400	-2.05608200
C	2.91302300	-1.82755800	-0.68380300
C	3.85294100	-2.13244000	0.30629700
C	3.29267900	-1.93299500	-2.02155600
C	5.14593700	-2.51366300	-0.03379600
H	3.56761300	-2.05702300	1.35085900
C	4.58941000	-2.31548500	-2.36401000
H	2.57017600	-1.71099200	-2.79906600
C	5.52187100	-2.60435900	-1.37364900
H	5.86349900	-2.73915800	0.74938200
H	4.86797600	-2.38313000	-3.41121000
H	6.53229400	-2.89802400	-1.64028500
O	1.45412900	-0.89692200	1.08383900
C	1.89621000	0.34272900	1.29563900
O	1.50159200	0.99473000	2.24207000
O	2.79765500	0.71469700	0.40031600
C	3.41812300	2.03428000	0.42806700
C	2.35202000	3.09349700	0.18609700
C	4.16696500	2.23092100	1.74178700
C	4.38828100	1.95573800	-0.74467600
H	1.86238400	2.89566100	-0.77155700
H	1.60569600	3.08574100	0.98370700
H	2.82218500	4.08101100	0.14831300
H	4.84614700	1.38999000	1.91259700
H	4.76335000	3.14551900	1.67821200

H	3.47912000	2.31289600	2.58312700
H	4.91868600	2.90589200	-0.85186900
H	5.11871900	1.15838300	-0.57713900
H	3.83608000	1.74121800	-1.66309900
N	1.57974100	1.17227500	-2.76116500
P	-2.00215300	-0.25154700	-0.20986900
C	-3.63382700	-0.28367500	-1.00183100
C	-4.54466400	0.76091800	-0.81427900
C	-3.97080700	-1.36759400	-1.82277200
C	-5.78778900	0.71339600	-1.43733800
H	-4.28006500	1.61015000	-0.19130200
C	-5.21689300	-1.40870200	-2.44003300
H	-3.26816200	-2.18057500	-1.98324300
C	-6.12376000	-0.36906100	-2.24783700
H	-6.49331200	1.52436800	-1.29230300
H	-5.47557900	-2.24987100	-3.07388100
H	-7.09327600	-0.40111600	-2.73393000
C	-1.59835100	1.47061500	0.12863100
C	-1.88234000	2.06457800	1.36353100
C	-1.11001400	2.24582700	-0.92977400
C	-1.66536900	3.42809100	1.53759900
H	-2.27209200	1.47088300	2.18410300
C	-0.90393900	3.60875000	-0.74782700
H	-0.87928500	1.79732400	-1.89042600
C	-1.17763900	4.19826800	0.48415200
H	-1.87838500	3.88686600	2.49702900
H	-0.51617500	4.20403400	-1.56757400
H	-1.00881200	5.26096400	0.62521600
C	-2.11306000	-1.18953200	1.33065200
C	-3.06362200	-2.21292500	1.44587200
C	-1.20396600	-0.95349300	2.36961600
C	-3.09890500	-2.99804900	2.59264600
H	-3.78126700	-2.39127700	0.65123900
C	-1.25240600	-1.74552700	3.51349700
H	-0.45873400	-0.16866900	2.29490200
C	-2.19288800	-2.76566700	3.62593600
H	-3.83857200	-3.78648500	2.68104000
H	-0.54663900	-1.56023800	4.31609100
H	-2.22336100	-3.37896700	4.52062900
MI'			
C	-1.23693000	-1.40394300	0.36159300
H	-0.67096900	-2.33922300	0.23237100

C	-0.53768700	-0.61325900	1.39414200
C	0.92332100	-0.85128000	1.52044700
H	1.29383500	-0.36605800	2.42910200
H	1.19279800	-1.91799300	1.55031600
C	-2.68280600	-1.83463900	0.54548200
C	-3.54411800	-1.98501600	-0.54166000
C	-3.12852200	-2.22484700	1.80987600
C	-4.83793000	-2.47228000	-0.36462000
H	-3.20480400	-1.72325100	-1.53881200
C	-4.41532400	-2.72262300	1.98838800
H	-2.45774100	-2.11689700	2.65623900
C	-5.28098800	-2.83988200	0.90245000
H	-5.49633400	-2.56915100	-1.22294300
H	-4.74529000	-3.01398300	2.98094500
H	-6.28766800	-3.22104000	1.04226000
O	-1.01092700	-0.86119900	-1.01215200
C	-1.51779100	0.29087700	-1.44680800
O	-1.15946900	0.74626400	-2.51493800
O	-2.42281300	0.80836500	-0.62899100
C	-3.35435500	1.82884100	-1.10262900
C	-2.61889600	3.12981800	-1.39591900
C	-4.11156600	1.30307800	-2.31831700
C	-4.29745300	1.99751000	0.08035800
H	-2.07091100	3.45314000	-0.50747000
H	-1.91585100	3.00948200	-2.22063900
H	-3.34953100	3.90259400	-1.65346200
H	-4.59954900	0.35566300	-2.06964300
H	-4.88319100	2.02465600	-2.60066700
H	-3.44275700	1.15545900	-3.16728800
H	-5.08269400	2.71514500	-0.17257000
H	-4.75406800	1.03716600	0.33630900
H	-3.74590300	2.35991300	0.95006200
P	2.07965200	-0.21586500	0.18412300
C	3.70946300	0.01404200	0.95834200
C	4.59532200	0.97591600	0.46253500
C	4.08455500	-0.78683000	2.04332000
C	5.84880400	1.12954300	1.04587600
H	4.30362700	1.60938900	-0.36981400
C	5.34168100	-0.62945200	2.62002300
H	3.40252900	-1.53103000	2.44352000
C	6.22235600	0.32763300	2.12229000
H	6.53235300	1.87880700	0.66129600
H	5.62790400	-1.25032400	3.46198700
H	7.19977800	0.45221000	2.57653800

C	1.57268200	1.37943300	-0.47213400
C	1.92362600	1.78850400	-1.76348300
C	0.91575300	2.25665600	0.40053400
C	1.60776300	3.07543600	-2.18650000
H	2.44248700	1.11184600	-2.43518500
C	0.61789500	3.54501400	-0.03356900
H	0.65006700	1.94922200	1.41096000
C	0.95556900	3.95176500	-1.32236200
H	1.87428700	3.39179400	-3.18908300
H	0.11579200	4.23128100	0.64083000
H	0.71061900	4.95578400	-1.65435000
C	2.31364800	-1.42717600	-1.14594200
C	3.24714300	-2.45274700	-0.94497200
C	1.54721100	-1.39808500	-2.31839300
C	3.40967900	-3.44462200	-1.90557000
H	3.85684200	-2.47435000	-0.04674500
C	1.72670500	-2.39201400	-3.27711900
H	0.80799300	-0.62112400	-2.48134700
C	2.65083700	-3.41321700	-3.07349700
H	4.13522300	-4.23460800	-1.74450000
H	1.13493300	-2.36571200	-4.18584100
H	2.78227100	-4.18399000	-3.82591600
C	-1.05793400	0.35862600	2.27104400
O	-0.38686900	1.04911600	3.06521800
O	-2.42003800	0.50977600	2.25293400
C	-2.93948300	1.34959300	3.26686100
H	-2.57863600	2.37720100	3.15995500
H	-4.02433500	1.32161500	3.15210800
H	-2.66034600	0.99353500	4.26265000

TS2

C	1.67426500	-1.76021700	-0.10311300
H	1.29952800	-2.62594600	0.44220100
C	0.70428300	-1.20323500	-0.96542700
C	-0.73670100	-1.60500500	-0.88121800
H	-1.16896000	-1.82846100	-1.86573300
H	-0.85457700	-2.50690300	-0.26846400
C	1.06222000	-0.41826500	-2.08114100
C	3.08454100	-1.97003100	-0.55774500
C	3.65563300	-3.23312700	-0.37384800
C	3.85516700	-0.96716300	-1.15937800
C	4.95551300	-3.50045300	-0.79438500
H	3.07326900	-4.01590900	0.10498100

C	5.15691900	-1.23241900	-1.57140800
H	3.43325100	0.02093400	-1.29540800
C	5.71204600	-2.49882500	-1.39569100
H	5.37777200	-4.48946900	-0.64628500
H	5.74107400	-0.44270200	-2.03426300
H	6.72769100	-2.70091100	-1.72094400
O	1.99804500	-0.96926000	1.46485300
C	2.35533500	0.26299200	1.59783800
O	2.80155400	0.74963900	2.62913000
O	2.12634800	1.00332000	0.47623300
C	2.48796000	2.40715600	0.42060000
C	1.70400300	3.21424400	1.45442800
C	3.99557200	2.57094700	0.59205300
C	2.05597800	2.81230500	-0.98421300
H	0.62828000	3.07123200	1.30302200
H	1.97111300	2.92075200	2.46901000
H	1.92117100	4.27822800	1.31930800
H	4.52226800	1.92732800	-0.11971200
H	4.27622500	3.60905400	0.39035000
H	4.30287700	2.30636300	1.60360700
H	2.22651800	3.88246200	-1.13443000
H	2.60881100	2.25130400	-1.74193200
H	0.99210300	2.59567500	-1.12432700
N	1.30451200	0.19494800	-3.04485200
P	-1.94507800	-0.40329100	-0.13486800
C	-3.61079400	-0.97946400	-0.54134400
C	-4.58167100	-0.08346600	-0.99910800
C	-3.91843700	-2.33923700	-0.40080500
C	-5.85652700	-0.54757200	-1.30890200
H	-4.34291700	0.96892600	-1.11810300
C	-5.19594000	-2.79326800	-0.70989100
H	-3.17180100	-3.04379200	-0.04482600
C	-6.16307600	-1.89812200	-1.16411900
H	-6.60841100	0.14745400	-1.66645800
H	-5.43368800	-3.84563300	-0.59976900
H	-7.15758400	-2.25628700	-1.40862700
C	-1.73623000	1.24642000	-0.83169600
C	-1.87133100	2.38659100	-0.03166800
C	-1.53468300	1.37345200	-2.21068300
C	-1.78405800	3.64905100	-0.61135400
H	-2.04157000	2.29235700	1.03622200
C	-1.44740600	2.63856400	-2.78069100
H	-1.42884900	0.49613700	-2.84054800
C	-1.56937500	3.77377300	-1.98205700

H	-1.87922800	4.53256800	0.01066500
H	-1.27317200	2.73424700	-3.84657600
H	-1.49347700	4.75931300	-2.42961000
C	-1.75964100	-0.32580400	1.65120200
C	-2.67676100	-0.93520300	2.51457800
C	-0.62081500	0.30797500	2.15645900
C	-2.44016200	-0.90801500	3.88490000
H	-3.56809100	-1.41689200	2.12547000
C	-0.38640600	0.32103800	3.52709900
H	0.06962100	0.79079800	1.47301700
C	-1.29691000	-0.28770400	4.38785300
H	-3.15000400	-1.37212000	4.56109000
H	0.51894000	0.78713600	3.90179200
H	-1.11622600	-0.27959600	5.45778600

TS2'

C	1.62128300	-1.57924300	0.47099300
H	1.16305000	-2.21599000	1.22735100
C	0.72212700	-1.25074400	-0.55700600
C	-0.71159600	-1.68247300	-0.45119700
H	-1.05999900	-2.08800300	-1.40830700
H	-0.84258700	-2.45509300	0.31525900
C	3.04135700	-2.00619200	0.22249500
C	3.28613600	-3.37987100	0.18436400
C	4.11206700	-1.12778400	0.04006000
C	4.56912400	-3.87293300	-0.04939200
H	2.46194500	-4.07278500	0.33587900
C	5.39273800	-1.61653000	-0.18766800
H	3.92100800	-0.06091700	0.05595200
C	5.62815500	-2.99119900	-0.23456500
H	4.73802500	-4.94496300	-0.07680900
H	6.21419100	-0.92017900	-0.32714000
H	6.63066700	-3.36918100	-0.40924300
O	1.96426000	-0.38708400	1.85196100
C	2.16856900	0.87389200	1.75005500
O	2.48422200	1.61583600	2.67685500
O	1.95383900	1.34386300	0.48427100
C	2.15610400	2.73968700	0.16016500
C	1.23142500	3.64241800	0.97640800
C	3.62265400	3.11722800	0.34927800
C	1.77156200	2.80144600	-1.31473000
H	0.18948400	3.33791500	0.83364900
H	1.47938100	3.60317200	2.03630500
H	1.32892600	4.67273900	0.62010100

H	4.25848200	2.43657100	-0.22622300
H	3.79200800	4.13419700	-0.01754200
H	3.90036300	3.06420100	1.40212600
H	1.80313800	3.83428100	-1.67364100
H	2.45838600	2.19292700	-1.90713000
H	0.75819300	2.40846200	-1.45174900
P	-2.00444100	-0.43392400	0.00315400
C	-3.61751700	-1.17881100	-0.34512500
C	-4.65819000	-0.40636000	-0.86970200
C	-3.81917900	-2.53818000	-0.07417100
C	-5.89463300	-0.99397300	-1.12066600
H	-4.50179400	0.64584100	-1.08673100
C	-5.05825400	-3.11695600	-0.32741700
H	-3.01933600	-3.14741500	0.33620200
C	-6.09369100	-2.34574200	-0.85138900
H	-6.70072800	-0.39485900	-1.53012200
H	-5.21289100	-4.16989400	-0.11866100
H	-7.05828900	-2.80089300	-1.05041700
C	-1.89388700	1.09989100	-0.94213000
C	-2.09235400	2.34221400	-0.32930400
C	-1.71609000	1.01651600	-2.32837600
C	-2.08355400	3.50049700	-1.10247700
H	-2.25117400	2.41055100	0.74222100
C	-1.71029600	2.17997000	-3.09042700
H	-1.54565700	0.05603800	-2.80145700
C	-1.88920500	3.41958000	-2.47902600
H	-2.22638300	4.46404500	-0.62510500
H	-1.55959700	2.11569400	-4.16259900
H	-1.87896100	4.32474400	-3.07739100
C	-1.90860400	-0.05309000	1.75852100
C	-2.83669400	-0.55900100	2.67473200
C	-0.82502100	0.71486700	2.19388800
C	-2.66813000	-0.28957800	4.02930200
H	-3.68180800	-1.15089200	2.33747700
C	-0.65888500	0.97284100	3.55022600
H	-0.12419400	1.10908000	1.46547700
C	-1.58214100	0.46943100	4.46461100
H	-3.38551500	-0.67491600	4.74584800
H	0.20494500	1.54524800	3.87236000
H	-1.45482400	0.66734800	5.52398100
C	1.10752100	-0.83876300	-1.88593000
O	0.39455300	-0.93329200	-2.88599900
O	2.36356000	-0.35769500	-1.98757500
C	2.81411100	-0.09891900	-3.30932900

H	3.84268000	0.24859100	-3.20742700
H	2.78042300	-1.00416300	-3.92033900
H	2.19950900	0.66953600	-3.78601100
M2			
C	-0.80290000	-3.05651800	0.13802400
H	-0.30733400	-3.55824800	-0.69304000
C	0.00017500	-2.38595700	0.98822300
C	1.47930900	-2.25021600	0.72754800
H	2.07515900	-2.40120100	1.63400600
H	1.79180600	-2.98467800	-0.01945700
C	-0.48153800	-1.78654900	2.20462400
C	-2.25998000	-3.20410400	0.19286900
C	-2.82321100	-4.40107400	-0.27492000
C	-3.09634800	-2.17089900	0.63934400
C	-4.19890900	-4.58685300	-0.25116700
H	-2.17295500	-5.18840000	-0.64669500
C	-4.47571100	-2.35988200	0.63907900
H	-2.69590200	-1.19870000	0.93073900
C	-5.02823500	-3.56398700	0.20948800
H	-4.62522400	-5.52097400	-0.60213600
H	-5.11841500	-1.54819000	0.96365500
H	-6.10493500	-3.70147400	0.21484200
O	-2.21734300	0.84414900	1.10497600
C	-2.59593700	1.61376200	0.19681800
O	-3.38496900	1.41506100	-0.74179600
O	-1.96954300	2.87345700	0.29920400
C	-2.16292500	3.89850600	-0.68488500
C	-1.70108400	3.43167200	-2.06565600
C	-3.61596500	4.37093300	-0.71005400
C	-1.25653700	5.02686400	-0.19390800
H	-0.68184200	3.03283700	-2.00085200
H	-2.35885500	2.64826400	-2.44089500
H	-1.69760900	4.27437000	-2.76496200
H	-3.92059500	4.68024100	0.29458000
H	-3.71990800	5.22955000	-1.38156800
H	-4.26573400	3.56395100	-1.04642900
H	-1.30581000	5.88628600	-0.86908700
H	-1.56362100	5.34923800	0.80566400
H	-0.21929200	4.67996600	-0.14185500
N	-0.78429500	-1.33999800	3.22938000
P	1.92851700	-0.58468200	0.07309300
C	3.69315700	-0.61312200	-0.30405800
C	4.47203200	0.51482000	-0.02409700

C	4.26934800	-1.73655200	-0.91000900
C	5.82607200	0.51228600	-0.34433100
H	4.02499400	1.38482500	0.44659100
C	5.62342600	-1.72913800	-1.22562900
H	3.67352400	-2.61251900	-1.14787400
C	6.40012600	-0.60726900	-0.94106000
H	6.43057600	1.38502900	-0.12359000
H	6.07131600	-2.59941800	-1.69236000
H	7.45688900	-0.60685000	-1.18641900
C	1.62115000	0.61307900	1.37414500
C	0.66094100	1.61276600	1.23387500
C	2.32750000	0.45945900	2.58007800
C	0.38984300	2.45542200	2.31111500
H	0.09218500	1.74520900	0.32193900
C	2.06354000	1.31622100	3.63626800
H	3.08230000	-0.31547500	2.68960300
C	1.08747200	2.30942100	3.50212100
H	-0.39267100	3.19552600	2.18934100
H	2.60565400	1.20514700	4.56898800
H	0.87064200	2.96312700	4.34076900
C	0.97297000	-0.27921100	-1.41796600
C	1.61505900	-0.21514300	-2.66114700
C	-0.42263600	-0.16354900	-1.32779100
C	0.85352200	-0.04666100	-3.81280100
H	2.69538500	-0.29160400	-2.73175600
C	-1.17160100	0.00333300	-2.48897600
H	-0.93360800	-0.16292200	-0.36673100
C	-0.53400200	0.05642400	-3.72668900
H	1.34686800	0.00872800	-4.77723900
H	-2.24502200	0.12580400	-2.38915400
H	-1.11955500	0.19172500	-4.63058800
M2'			
C	-0.61149200	-2.84423000	0.47251600
H	0.02549400	-3.43545000	-0.18904100
C	0.04854000	-2.01511600	1.30524300
C	1.54180400	-1.86659800	1.16085000
H	2.03194100	-1.69836300	2.12431500
H	1.96317000	-2.75890700	0.69217600
C	-2.04760000	-3.05933800	0.22729100
C	-2.46890000	-4.34529300	-0.13802700
C	-2.96984400	-2.00355300	0.20560900
C	-3.79727700	-4.58792800	-0.46945500
H	-1.74839200	-5.15925400	-0.15619800

C	-4.28857400	-2.24600800	-0.16263000
H	-2.66522100	-0.99070600	0.45943000
C	-4.71020300	-3.53468500	-0.48648800
H	-4.11464600	-5.59194000	-0.73240100
H	-4.97810100	-1.40906900	-0.20630400
H	-5.74320300	-3.71741100	-0.76661300
O	-2.01656300	0.97692600	1.04518500
C	-2.52435900	1.55536400	0.05800100
O	-3.35378800	1.12800400	-0.76274600
O	-2.00825200	2.85072800	-0.10435400
C	-2.39825100	3.68620600	-1.20545200
C	-2.02275500	3.04963600	-2.54359100
C	-3.88883500	4.01681100	-1.14125500
C	-1.57081200	4.95220200	-0.99000100
H	-0.97123200	2.74141100	-2.52483100
H	-2.64088400	2.17396900	-2.73838400
H	-2.15473400	3.77615700	-3.35212400
H	-4.12838700	4.46296100	-0.17095200
H	-4.14662000	4.73704800	-1.92453000
H	-4.47835200	3.10977900	-1.27269500
H	-1.77855000	5.68836600	-1.77198700
H	-1.80660300	5.39703200	-0.01850900
H	-0.50300100	4.71092700	-1.00999300
P	2.04178300	-0.44128100	0.09750500
C	3.78775400	-0.65422800	-0.33048900
C	4.57178300	0.48410500	-0.55477100
C	4.33651700	-1.92781900	-0.51674600
C	5.89824100	0.34429600	-0.94841300
H	4.14888300	1.47411700	-0.41564400
C	5.66576000	-2.05874700	-0.90662600
H	3.74194300	-2.82302000	-0.36931700
C	6.44591200	-0.92516300	-1.11948500
H	6.50290400	1.22816200	-1.11983200
H	6.08988800	-3.04740400	-1.04311500
H	7.48240200	-1.03102600	-1.42202100
C	1.89269100	1.09192900	1.02486100
C	0.85923700	1.99811900	0.79696200
C	2.79609500	1.28775800	2.08053200
C	0.72341000	3.10139700	1.63764900
H	0.13357600	1.86378200	0.00470000
C	2.66406800	2.39993400	2.89690600
H	3.59967600	0.57830500	2.26123400
C	1.62086400	3.30329300	2.67882000
H	-0.11111100	3.77324000	1.46638900

H	3.36521200	2.55815800	3.70919500
H	1.51059900	4.16345100	3.33161400
C	1.07024200	-0.45451500	-1.41964300
C	1.69448100	-0.69003300	-2.65129000
C	-0.32005900	-0.28607800	-1.34855500
C	0.92102500	-0.75896800	-3.80570300
H	2.77055700	-0.81822500	-2.71147000
C	-1.08325300	-0.36286100	-2.50985300
H	-0.81410200	-0.08732000	-0.40058300
C	-0.46232300	-0.60040700	-3.73421700
H	1.40144500	-0.93755200	-4.76171400
H	-2.15581500	-0.21911100	-2.42464200
H	-1.05745000	-0.65851200	-4.64006100
C	-0.53168700	-1.18690400	2.40499300
O	0.12216900	-0.34755400	2.98791800
O	-1.77197100	-1.52680700	2.73259700
C	-2.41441800	-0.65146000	3.66522900
H	-1.87762800	-0.65124900	4.61618700
H	-2.44088200	0.35076900	3.23698900
H	-3.41896500	-1.05099000	3.79272700

TS3

C	2.45011900	-0.33222100	-1.03348000
H	2.38639000	0.46065500	-1.77805100
C	1.31335000	-0.60706500	-0.35868400
C	0.05061800	0.14475700	-0.61494000
H	0.33798300	1.43905900	-0.05125800
H	-0.05156100	0.40001500	-1.67514300
C	1.33279100	-1.55750400	0.72820700
C	3.78361300	-0.91689700	-0.83530800
C	4.90028500	-0.07722400	-0.95134100
C	3.98474500	-2.27750200	-0.56978900
C	6.18440700	-0.58100500	-0.78098600
H	4.74325900	0.98017900	-1.14432400
C	5.27130600	-2.77960800	-0.40328300
H	3.13331500	-2.94791400	-0.51295600
C	6.37372800	-1.93447700	-0.50589800
H	7.03889000	0.08339100	-0.86063600
H	5.41306700	-3.83664900	-0.20217400
H	7.37613900	-2.33005700	-0.37751600
O	1.97043600	1.27776900	1.98329200
C	2.27656700	2.00487700	1.07467800
O	3.21543600	2.50346800	0.50593500

O	0.81646900	2.45124500	0.35249700
C	0.71731100	3.56296700	-0.56618700
C	1.27366700	4.80209800	0.13069000
C	1.46869900	3.27103400	-1.86506400
C	-0.77336800	3.75044800	-0.84484300
H	0.75774500	4.95306300	1.08351200
H	2.34239300	4.69425400	0.31817700
H	1.10874100	5.68367700	-0.49582500
H	1.02619700	2.41148600	-2.37983200
H	1.39798800	4.13238500	-2.53627800
H	2.51932300	3.06513200	-1.65722700
H	-0.92683700	4.62042600	-1.49066200
H	-1.19516600	2.87419300	-1.34800300
H	-1.31801500	3.90704800	0.09055300
N	1.28008200	-2.34110000	1.58026000
P	-1.50673000	-0.48396500	-0.08117000
C	-2.74454700	0.73489300	-0.59478600
C	-3.32139000	1.60933200	0.32711500
C	-3.05198800	0.83991500	-1.95682300
C	-4.19523700	2.59928300	-0.11701800
H	-3.08524800	1.52502100	1.38330900
C	-3.91927100	1.83456300	-2.39293800
H	-2.61893400	0.14574100	-2.67254700
C	-4.48714300	2.71619900	-1.47281600
H	-4.64239100	3.28114000	0.59835500
H	-4.15479300	1.92056500	-3.44825100
H	-5.16413600	3.49168300	-1.81581300
C	-1.56143700	-0.66595200	1.71383400
C	-2.20825000	-1.75236300	2.31005000
C	-0.92564100	0.30249300	2.49939200
C	-2.22253500	-1.86531300	3.69612600
H	-2.68077800	-2.51619800	1.70125900
C	-0.94358300	0.17573800	3.88452800
H	-0.38831500	1.12832300	2.04280900
C	-1.59023700	-0.90403100	4.48147700
H	-2.71630500	-2.71152100	4.16145400
H	-0.43537700	0.91565900	4.49328000
H	-1.59305300	-1.00300700	5.56213000
C	-2.02339200	-2.04898200	-0.84364400
C	-3.37750500	-2.40735500	-0.87345900
C	-1.06256600	-2.89395200	-1.40489200
C	-3.76009600	-3.61474100	-1.44650200
H	-4.12870200	-1.74158500	-0.45608200
C	-1.45344000	-4.10094800	-1.97924100

H	-0.01478100	-2.60873200	-1.40775700
C	-2.79784200	-4.46133900	-1.99633700
H	-4.80833400	-3.89287900	-1.46893600
H	-0.70723400	-4.75616100	-2.41527400
H	-3.10026100	-5.40178900	-2.44536700

M3

C	-2.08831400	0.16908400	-0.50587500
C	-1.30336200	-0.22822700	-1.55351400
C	0.12930600	-0.30532200	-1.60965300
C	-1.92687600	-0.72195500	-2.76520700
C	-3.54493600	0.16018900	-0.37295700
C	-4.08231700	0.04471600	0.92260800
C	-4.44679800	0.29440300	-1.44304400
C	-5.45418200	0.03305400	1.13939600
H	-3.39971400	-0.05170700	1.76371300
C	-5.82014300	0.27693400	-1.22361000
H	-4.07542600	0.43211700	-2.45178000
C	-6.33460500	0.14306600	0.06430100
H	-5.83824100	-0.06440400	2.15033200
H	-6.49444000	0.38214800	-2.06817200
H	-7.40708400	0.13410100	0.22910100
N	-2.36547200	-1.13267800	-3.75553400
P	1.15846700	-0.06143500	-0.26835800
C	0.56570800	-0.93857100	1.21927500
C	0.73430700	-0.43379100	2.51129300
C	-0.10392500	-2.15213700	1.02533300
C	0.25165200	-1.15054700	3.60357700
H	1.22527900	0.52083900	2.66905200
C	-0.58479400	-2.86277000	2.11990600
H	-0.25653600	-2.52054800	0.01436400
C	-0.40602300	-2.36251200	3.40870800
H	0.38301100	-0.75589200	4.60556800
H	-1.10708200	-3.80103500	1.96612100
H	-0.78677500	-2.91481000	4.26187100
C	1.41951900	1.67203200	0.24530000
C	2.52777600	2.05053600	1.01232800
C	0.49636800	2.63412400	-0.17175400
C	2.69656200	3.38278900	1.37562900
H	3.26342200	1.30862400	1.31406500
C	0.66759700	3.96564500	0.19916500
H	-0.34567600	2.33682600	-0.79135800
C	1.76443800	4.33823400	0.97271500

H	3.55836500	3.67650000	1.96568300
H	-0.05031800	4.71201300	-0.12426600
H	1.90009100	5.37735900	1.25476000
C	2.80933500	-0.67576900	-0.69529800
C	3.26882800	-1.90555600	-0.21926300
C	3.60174200	0.08501100	-1.56209300
C	4.51879300	-2.37426600	-0.61567000
H	2.65498900	-2.49346500	0.45657300
C	4.84613200	-0.39263300	-1.95883100
H	3.24855200	1.04798900	-1.92065700
C	5.30397000	-1.62118600	-1.48512800
H	4.87833200	-3.32793800	-0.24425700
H	5.45948800	0.19546600	-2.63311000
H	6.27662900	-1.99047300	-1.79339100
H	0.62209100	-0.57813000	-2.53236000
H	-1.56220500	0.47723300	0.39642400

TS4a

C	1.80388000	0.45699200	-0.00453800
C	0.98826800	0.59532800	-1.08923400
C	-0.33721600	-0.01636800	-1.21189800
C	1.42705000	1.28859200	-2.27591400
C	3.16458000	0.93479900	0.24148800
C	3.61953800	0.87402000	1.57071000
C	4.05659900	1.38202400	-0.74778500
C	4.90351900	1.27909300	1.90976600
H	2.94777700	0.49150500	2.33594500
C	5.34368300	1.78287000	-0.40365400
H	3.75916500	1.40694200	-1.78914700
C	5.77126500	1.74159500	0.92172700
H	5.23045600	1.22629500	2.94325500
H	6.01992600	2.12523900	-1.18062100
H	6.77694500	2.05619400	1.18108100
N	1.68792300	1.87825600	-3.24033500
P	-1.58459600	0.47092700	-0.04683500
C	-0.89932500	0.76451400	1.59750600
C	-0.36475700	2.02848600	1.87113100
C	-0.73966100	-0.28293700	2.51219800
C	0.33957300	2.23879000	3.05156100
H	-0.48342800	2.83905200	1.15807400
C	-0.02922100	-0.06398600	3.68914600
H	-1.16422100	-1.26135000	2.31029700
C	0.51205600	1.19216300	3.95586400

H	0.76015000	3.21660100	3.25978600
H	0.10712200	-0.87892300	4.39121200
H	1.07004700	1.35607100	4.87207700
C	-2.38243500	2.03374100	-0.55307200
C	-3.60876200	2.40208800	0.01252400
C	-1.75544900	2.87674000	-1.47395100
C	-4.19720700	3.61131600	-0.33780700
H	-4.10767700	1.74380300	0.71800100
C	-2.35165700	4.08744000	-1.82087800
H	-0.80754100	2.59662900	-1.92404000
C	-3.56833900	4.45400800	-1.25386800
H	-5.14826000	3.89455000	0.10055900
H	-1.86332900	4.73996300	-2.53660500
H	-4.03157600	5.39630600	-1.52773300
C	-2.91110700	-0.75183800	0.04657100
C	-3.66416900	-0.90932200	1.21322600
C	-3.22754500	-1.49294000	-1.09709600
C	-4.71531700	-1.82048500	1.23973200
H	-3.42598500	-0.33470100	2.10354600
C	-4.27645200	-2.40440900	-1.06192700
H	-2.65944500	-1.36151900	-2.01438400
C	-5.01598800	-2.57117200	0.10701000
H	-5.29135900	-1.94911000	2.14965200
H	-4.51617700	-2.98436300	-1.94653100
H	-5.83033000	-3.28764700	0.13370000
H	-0.76154900	0.08406500	-2.21188800
H	1.36651200	-0.06680400	0.84239600
C	2.78053600	-1.77230900	-3.25271100
C	1.47733500	-2.02409200	-3.70404000
C	0.34212100	-2.27191900	-2.95596900
C	3.23755900	-1.83084500	-1.94526200
C	0.15699500	-2.23331500	-1.55628300
C	2.54825700	-2.12079500	-0.76602500
H	3.52151400	-1.54994900	-4.01487300
H	1.34045700	-2.02502700	-4.78254400
H	-0.57076500	-2.43699300	-3.52469000
H	4.30007300	-1.64418400	-1.80789000
H	-0.83000500	-2.54299000	-1.22690300
H	3.17427800	-2.18228300	0.12156800
C	1.18370900	-2.39968500	-0.54887700
C	0.74539100	-2.75682900	0.75505900
C	-0.56930800	-3.21905200	1.00722700
N	-1.64933600	-3.59689100	1.22587000
C	1.61047300	-2.68570300	1.87607200

N	2.31788800	-2.58291600	2.79487200
TS4a'			
C	-1.80388000	0.45699200	-0.00453800
C	-0.98826800	0.59532800	-1.08923400
C	0.33721600	-0.01636800	-1.21189800
C	-1.42705000	1.28859200	-2.27591400
C	-3.16458000	0.93479900	0.24148800
C	-3.61953800	0.87402000	1.57071000
C	-4.05659900	1.38202400	-0.74778500
C	-4.90351900	1.27909300	1.90976600
H	-2.94777700	0.49150500	2.33594500
C	-5.34368300	1.78287000	-0.40365400
H	-3.75916500	1.40694200	-1.78914700
C	-5.77126500	1.74159500	0.92172700
H	-5.23045600	1.22629500	2.94325500
H	-6.01992600	2.12523900	-1.18062100
H	-6.77694500	2.05619400	1.18108100
N	-1.68792300	1.87825600	-3.24033500
P	1.58459600	0.47092700	-0.04683500
C	0.89932500	0.76451400	1.59750600
C	0.36475700	2.02848600	1.87113100
C	0.73966100	-0.28293700	2.51219800
C	-0.33957300	2.23879000	3.05156100
H	0.48342800	2.83905200	1.15807400
C	0.02922100	-0.06398600	3.68914600
H	1.16422100	-1.26135000	2.31029700
C	-0.51205600	1.19216300	3.95586400
H	-0.76015000	3.21660100	3.25978600
H	-0.10712200	-0.87892300	4.39121200
H	-1.07004700	1.35607100	4.87207700
C	2.38243500	2.03374100	-0.55307200
C	3.60876200	2.40208800	0.01252400
C	1.75544900	2.87674000	-1.47395100
C	4.19720700	3.61131600	-0.33780700
H	4.10767700	1.74380300	0.71800100
C	2.35165700	4.08744000	-1.82087800
H	0.80754100	2.59662900	-1.92404000
C	3.56833900	4.45400800	-1.25386800
H	5.14826000	3.89455000	0.10055900
H	1.86332900	4.73996300	-2.53660500
H	4.03157600	5.39630600	-1.52773300
C	2.91110700	-0.75183800	0.04657100

C	3.66416900	-0.90932200	1.21322600
C	3.22754500	-1.49294000	-1.09709600
C	4.71531700	-1.82048500	1.23973200
H	3.42598500	-0.33470100	2.10354600
C	4.27645200	-2.40440900	-1.06192700
H	2.65944500	-1.36151900	-2.01438400
C	5.01598800	-2.57117200	0.10701000
H	5.29135900	-1.94911000	2.14965200
H	4.51617700	-2.98436300	-1.94653100
H	5.83033000	-3.28764700	0.13370000
H	0.76154900	0.08406500	-2.21188800
H	-1.36651200	-0.06680400	0.84239600
C	-2.78053600	-1.77230900	-3.25271100
C	-1.47733500	-2.02409200	-3.70404000
C	-0.34212100	-2.27191900	-2.95596900
C	-3.23755900	-1.83084500	-1.94526200
C	-0.15699500	-2.23331500	-1.55628300
C	-2.54825700	-2.12079500	-0.76602500
H	-3.52151400	-1.54994900	-4.01487300
H	-1.34045700	-2.02502700	-4.78254400
H	0.57076500	-2.43699300	-3.52469000
H	-4.30007300	-1.64418400	-1.80789000
H	0.83000500	-2.54299000	-1.22690300
H	-3.17427800	-2.18228300	0.12156800
C	-1.18370900	-2.39968500	-0.54887700
C	-0.74539100	-2.75682900	0.75505900
C	0.56930800	-3.21905200	1.00722700
N	1.64933600	-3.59689100	1.22587000
C	-1.61047300	-2.68570300	1.87607200
N	-2.31788800	-2.58291600	2.79487200

TS4 γ

C	-1.84603300	-0.28332500	-0.18864200
C	-1.01724500	-0.39129700	-1.32894400
C	0.35574600	-0.16916800	-1.40654300
C	-1.62115300	-0.65713200	-2.61938900
C	-3.14463400	-0.94981900	0.03736200
C	-3.44517300	-1.30578500	1.36312900
C	-4.12110600	-1.17368400	-0.94609000
C	-4.65992700	-1.89451300	1.69195200
H	-2.70914900	-1.10662700	2.13937700
C	-5.33648700	-1.76573700	-0.61188700
H	-3.94613600	-0.87937700	-1.97366500
C	-5.61150200	-2.13449500	0.70225500

H	-4.86470200	-2.16304700	2.72364100
H	-6.07667100	-1.93253100	-1.38831300
H	-6.56101400	-2.59566100	0.95412100
N	-2.05214000	-0.90865000	-3.66490300
P	1.57555100	-0.54291900	-0.19604800
C	2.68143500	0.83752300	0.17209100
C	3.45936500	0.85391200	1.33574900
C	2.84352000	1.83437900	-0.79451200
C	4.37600400	1.87984500	1.53683300
H	3.34996900	0.07452400	2.08437800
C	3.76557100	2.85459200	-0.58679400
H	2.24538300	1.81583300	-1.70063700
C	4.52594500	2.87985100	0.57918000
H	4.96892500	1.89952000	2.44460200
H	3.88645000	3.63088300	-1.33467800
H	5.23874400	3.68114400	0.74273700
C	0.87505100	-1.20412300	1.33379500
C	0.40119200	-2.52157900	1.32202500
C	0.71451200	-0.40558200	2.46990200
C	-0.23383100	-3.03469400	2.44646600
H	0.52365300	-3.14211100	0.43917100
C	0.08023600	-0.93032000	3.59305400
H	1.06631100	0.62168400	2.47799300
C	-0.39169600	-2.24017900	3.58136000
H	-0.60575900	-4.05333900	2.43572000
H	-0.05887800	-0.30449000	4.46719800
H	-0.88971500	-2.64232300	4.45752900
C	2.62099600	-1.85105400	-0.92032300
C	3.96461100	-1.97251200	-0.55178200
C	2.05589100	-2.76556200	-1.81645300
C	4.73286200	-3.00998300	-1.06934200
H	4.41543000	-1.25633200	0.12759300
C	2.83089400	-3.80185300	-2.32863500
H	1.01711800	-2.66376700	-2.11811700
C	4.16676200	-3.92478400	-1.95481200
H	5.77563000	-3.09936800	-0.78451100
H	2.39135800	-4.50846500	-3.02427300
H	4.76999600	-4.73111400	-2.35889700
H	0.79189400	-0.09023100	-2.39926200
H	-1.29236200	-0.13821600	0.73487100
C	-2.99040500	2.39682900	-2.67345000
C	-1.75204200	2.83042900	-3.18038500
C	-0.59675600	3.06937600	-2.45774000
C	-3.29183300	1.98409800	-1.39541700

C	-0.33476100	2.93042300	-1.09014400
C	-2.42654700	1.76807000	-0.28521000
H	-3.81851100	2.39646200	-3.37840400
H	-1.71523400	3.05438400	-4.24215000
H	0.23958000	3.46351200	-3.03255100
H	-4.32779700	1.71419400	-1.20994100
H	0.62607800	3.31808300	-0.76131300
H	-2.97545100	1.57632900	0.63372900
C	-1.14814900	2.42728400	-0.05980900
C	-0.69074000	2.48839300	1.28676500
C	0.52207700	3.13043600	1.64427100
N	1.51695400	3.65031500	1.95258200
C	-1.45061800	1.96240100	2.35985900
N	-2.07489600	1.50980300	3.23322200

TS4γ'

C	1.84621300	-0.28309700	-0.18903200
C	1.01741400	-0.39025000	-1.32941700
C	-0.35575500	-0.16951300	-1.40707400
C	1.62169600	-0.65456300	-2.62001600
C	3.14472700	-0.95005800	0.03611000
C	3.44450300	-1.30936800	1.36112700
C	4.12179400	-1.17132000	-0.94735800
C	4.65905300	-1.89896900	1.68914400
H	2.70802100	-1.11213800	2.13741900
C	5.33695200	-1.76429400	-0.61398100
H	3.94740100	-0.87419400	-1.97422600
C	5.61117300	-2.13647600	0.69935400
H	4.86328200	-2.17004200	2.72027900
H	6.07759400	-1.92912500	-1.39038400
H	6.56050700	-2.59836900	0.95055400
N	2.05315800	-0.90450400	-3.66570600
P	-1.57535900	-0.54311100	-0.19637100
C	-2.67962500	0.83801100	0.17415000
C	-3.45730100	0.85375800	1.33801100
C	-2.84162900	1.83565000	-0.79165000
C	-4.37339600	1.87997500	1.54016900
H	-3.34833400	0.07352200	2.08582300
C	-3.76322400	2.85606000	-0.58290600
H	-2.24380000	1.81745400	-1.69798800
C	-4.52320800	2.88077600	0.58331800
H	-4.96610600	1.89917800	2.44808600
H	-3.88405600	3.63290900	-1.33021700

H	-5.23561500	3.68224800	0.74769200
C	-0.87465800	-1.20725400	1.33213200
C	-0.40188200	-2.52507000	1.31798200
C	-0.71310600	-0.41080700	2.46955300
C	0.23284900	-3.04072700	2.44141200
H	-0.52506100	-3.14392700	0.43406100
C	-0.07908600	-0.93805800	3.59168500
H	-1.06369300	0.61686300	2.47933500
C	0.39156600	-2.24836300	3.57768000
H	0.60388600	-4.05967600	2.42878000
H	0.06092000	-0.31381800	4.46682900
H	0.88930800	-2.65251900	4.45308100
C	-2.62277900	-1.84886400	-0.92200600
C	-3.96681400	-1.96812000	-0.55431600
C	-2.05885400	-2.76377700	-1.81850700
C	-4.73665500	-3.00388000	-1.07295500
H	-4.41669700	-1.25160300	0.12529800
C	-2.83544800	-3.79833000	-2.33177200
H	-1.01977800	-2.66357100	-2.11969100
C	-4.17172800	-3.91913600	-1.95870700
H	-5.77974200	-3.09154000	-0.78875100
H	-2.39683700	-4.50524300	-3.02768500
H	-4.77620600	-4.72410300	-2.36364500
H	-0.79186800	-0.09059700	-2.39978700
H	1.29264000	-0.13913100	0.73471700
C	2.98989500	2.39992600	-2.67149600
C	1.75145500	2.83418600	-3.17759600
C	0.59660400	3.07299500	-2.45416700
C	3.29165500	1.98586400	-1.39394200
C	0.33524700	2.93302000	-1.08657900
C	2.42664700	1.76840400	-0.28380900
H	3.81781100	2.40024800	-3.37667700
H	1.71426600	3.05911300	-4.23914200
H	-0.23978500	3.46818100	-3.02818700
H	4.32769700	1.71592500	-1.20897500
H	-0.62520200	3.32087900	-0.75687800
H	2.97584600	1.57555800	0.63471400
C	1.14844600	2.42768100	-0.05721300
C	0.69134700	2.48702300	1.28956200
C	-0.52055100	3.13015100	1.64832800
N	-1.51449300	3.65126500	1.95755300
C	1.45104600	1.95859200	2.36157700
N	2.07511900	1.50374300	3.23391700

M4 α

C	1.90046200	0.26537600	0.03074400
C	1.09700700	0.69292500	-0.97048400
C	-0.27303000	0.09207400	-1.20038800
C	1.49957800	1.69528900	-1.91613400
C	3.28856200	0.62940000	0.31847100
C	3.74049100	0.46199000	1.63614400
C	4.18705200	1.08869200	-0.65636900
C	5.04518400	0.78603900	1.98483400
H	3.05298000	0.07639600	2.38482500
C	5.49587200	1.40117900	-0.30508400
H	3.87362100	1.17155700	-1.69110900
C	5.92503200	1.26059500	1.01324800
H	5.38002900	0.65886400	3.00889200
H	6.18628600	1.74859700	-1.06655900
H	6.94771900	1.50718000	1.27975200
N	1.75062500	2.54581200	-2.66388900
P	-1.41544100	0.59104400	0.19119500
C	-0.70678500	0.33446900	1.83153900
C	-0.03937500	1.37799200	2.48369800
C	-0.73408000	-0.94877900	2.39348800
C	0.61241800	1.13035100	3.68760500
H	-0.02933300	2.37859000	2.06639400
C	-0.07283500	-1.18537700	3.59444000
H	-1.28163000	-1.75219300	1.91207900
C	0.60411700	-0.15042600	4.23696400
H	1.12826200	1.93939200	4.19305300
H	-0.08994100	-2.18076900	4.02459200
H	1.11959600	-0.34064900	5.17258200
C	-1.78381700	2.35295600	-0.04934200
C	-3.12199800	2.76055800	-0.10284000
C	-0.76040200	3.30206800	-0.18879300
C	-3.43063200	4.10408400	-0.29453500
H	-3.92287000	2.03663400	0.00126000
C	-1.08016500	4.64068400	-0.38351500
H	0.28277900	3.01093900	-0.14060200
C	-2.41328000	5.04248000	-0.43778100
H	-4.46946600	4.41277700	-0.33486500
H	-0.28380200	5.36786000	-0.49627800
H	-2.65696400	6.08816500	-0.59292400
C	-2.97359800	-0.30151100	0.05472000
C	-3.71795500	-0.59724700	1.20052500
C	-3.47897500	-0.60928000	-1.21494500

C	-4.94950300	-1.23082600	1.07458500
H	-3.34010100	-0.34161200	2.18510900
C	-4.70669100	-1.24884600	-1.32956300
H	-2.92272900	-0.35541700	-2.11384700
C	-5.43641300	-1.56568200	-0.18501900
H	-5.52233500	-1.47064300	1.96336900
H	-5.09220100	-1.50017200	-2.31135500
H	-6.39203300	-2.07066200	-0.27836500
H	-0.73781400	0.62730900	-2.03745500
H	1.46855200	-0.44980200	0.72728000
C	2.17599000	-1.04482700	-3.50905200
C	0.80819700	-1.21361900	-3.92725800
C	-0.25335300	-1.50578300	-3.14901300
C	2.71790900	-1.58158000	-2.37749100
C	-0.29572300	-1.43832400	-1.64429500
C	2.07366600	-2.29682200	-1.32574800
H	2.85329100	-0.58510500	-4.22336700
H	0.63033400	-1.15875100	-5.00022400
H	-1.19888800	-1.74151400	-3.63301500
H	3.80042400	-1.50974700	-2.28003100
H	-1.27685900	-1.81357300	-1.34866500
H	2.73402000	-2.89552400	-0.70196700
C	0.73260700	-2.34592100	-1.00375300
C	0.24308900	-3.24543000	0.00943500
C	-1.12896100	-3.41069200	0.28279700
N	-2.26801400	-3.51928100	0.52047000
C	1.12712000	-4.09197700	0.71992800
N	1.87310200	-4.76386100	1.31098200

M4γ

C	-1.84160600	-0.08909200	-0.29544900
C	-0.98336400	-0.34598900	-1.50909000
C	0.35417200	-0.51459900	-1.54208200
C	-1.63172400	-0.54974500	-2.79114400
C	-2.88522600	-1.18034700	-0.11203200
C	-2.77821300	-2.02253200	0.99801500
C	-3.96045300	-1.35098500	-0.99098900
C	-3.72159300	-3.02113200	1.22565800
H	-1.95736900	-1.88248500	1.69771500
C	-4.90263400	-2.35016400	-0.76189200
H	-4.06797400	-0.70218900	-1.85337600
C	-4.78556100	-3.18916000	0.34331300
H	-3.62557400	-3.66322400	2.09563400

H	-5.73181500	-2.47046100	-1.45162000
H	-5.52262500	-3.96636400	0.51774100
N	-2.10481800	-0.78886000	-3.81974500
P	1.56133500	-0.55266500	-0.20070500
C	2.27689800	1.08059000	0.04139600
C	2.86164800	1.45472500	1.25637500
C	2.34946900	1.92306300	-1.07379700
C	3.48802500	2.69272800	1.35683900
H	2.82697900	0.79522400	2.11752400
C	2.99674600	3.14824800	-0.96618100
H	1.89216400	1.63261100	-2.01526800
C	3.55380900	3.53584600	0.25020600
H	3.91746400	3.00063200	2.30324000
H	3.04718000	3.80602700	-1.82728300
H	4.03748500	4.50269800	0.33919200
C	0.95808300	-1.26195100	1.34940800
C	0.95640200	-2.65481400	1.49374300
C	0.47722200	-0.44194700	2.37674600
C	0.46874700	-3.22081400	2.66674600
H	1.33721600	-3.29587000	0.70566900
C	-0.00675200	-1.01898100	3.54670600
H	0.45990700	0.63749000	2.25709000
C	-0.00868900	-2.40505200	3.69119900
H	0.46561500	-4.29925600	2.77968900
H	-0.40403100	-0.37725300	4.32416800
H	-0.38907600	-2.85074200	4.60429800
C	2.85592900	-1.64560200	-0.83936300
C	4.19062000	-1.38639600	-0.51429400
C	2.51838500	-2.76675300	-1.60774000
C	5.18532400	-2.25299800	-0.95577700
H	4.45487400	-0.51005500	0.06953400
C	3.52050000	-3.62785500	-2.04202300
H	1.48275300	-2.97093700	-1.86688500
C	4.85097400	-3.37095500	-1.71638800
H	6.22166600	-2.04992800	-0.70933500
H	3.26072400	-4.49594300	-2.63756500
H	5.62975100	-4.04278700	-2.06138800
H	0.82772000	-0.70026000	-2.50398300
H	-1.17246400	-0.14741100	0.56543200
C	-3.12975000	2.20818100	-2.49815300
C	-1.82792000	2.53600200	-3.02263700
C	-0.75179600	2.89647400	-2.27079900
C	-3.42534500	1.77636500	-1.25645200
C	-0.62011900	2.97357900	-0.84822000

C	-2.46323900	1.35651600	-0.17825800
H	-3.96692500	2.36070200	-3.17789600
H	-1.73863700	2.60496300	-4.10322300
H	0.12222700	3.24516600	-2.82235700
H	-4.47652900	1.67899600	-0.99690800
H	0.21304300	3.57732300	-0.49669800
H	-3.06271100	1.25064600	0.73090100
C	-1.38078400	2.37686300	0.12564000
C	-1.11638600	2.61408100	1.52482800
C	-0.12667800	3.53647800	1.93558100
N	0.70361100	4.29060900	2.25539800
C	-1.77456600	1.90337400	2.54972400
N	-2.30513600	1.29127400	3.39154300

TS5

C	2.14759400	0.63097100	-0.96201200
C	1.03146400	0.70871000	-0.03840700
C	-0.10721000	-0.10160300	-0.56291100
C	1.24747100	0.81310000	1.35289900
C	3.48502200	1.19685600	-0.60981700
C	4.18330800	0.81408900	0.54211700
C	4.08239500	2.10831100	-1.48590000
C	5.44044700	1.34442200	0.81178000
H	3.74326900	0.09863500	1.22925000
C	5.33691200	2.64599000	-1.21231600
H	3.55357500	2.40078700	-2.38947700
C	6.01972700	2.26486400	-0.06065200
H	5.97089200	1.03507400	1.70660500
H	5.78094100	3.35758000	-1.90128600
H	7.00030500	2.67757100	0.15420500
N	1.41359600	0.96755500	2.49972000
P	-1.74820200	0.37051800	0.09880700
C	-2.96304000	-0.83135500	-0.49933800
C	-3.54523400	-1.77519300	0.34870400
C	-3.23935000	-0.85245900	-1.87343500
C	-4.38717500	-2.75117000	-0.18179600
H	-3.35435000	-1.75239400	1.41616200
C	-4.08671000	-1.82227400	-2.39224900
H	-2.79080900	-0.11714500	-2.53641900
C	-4.65347400	-2.77696600	-1.54729600
H	-4.83608400	-3.48608200	0.47727800
H	-4.30042900	-1.83761900	-3.45540400

H	-5.31048400	-3.53755800	-1.95589600
C	-1.78856800	0.45239500	1.89964500
C	-2.15350900	1.65113400	2.51980300
C	-1.41005200	-0.65289000	2.67374800
C	-2.14156100	1.73862600	3.90849800
H	-2.43305800	2.51608700	1.92766500
C	-1.39953000	-0.55478900	4.05805400
H	-1.10052800	-1.58717600	2.21799400
C	-1.76368400	0.64054800	4.67526300
H	-2.41933900	2.67063000	4.38845700
H	-1.09000500	-1.41016200	4.64839000
H	-1.74626900	0.71698000	5.75735200
C	-2.21638900	1.97496200	-0.58870900
C	-3.57775100	2.26745500	-0.74298400
C	-1.24452400	2.92680800	-0.91466200
C	-3.96188900	3.51220600	-1.22840200
H	-4.33158400	1.52674600	-0.49165600
C	-1.64268300	4.16620800	-1.40822100
H	-0.19288400	2.69351600	-0.76812500
C	-2.99511300	4.45878300	-1.56346800
H	-5.01533900	3.74025900	-1.34856900
H	-0.89157100	4.90529900	-1.66533600
H	-3.29941000	5.42817400	-1.94445600
C	1.01797500	-1.72070200	-3.49528500
C	-0.11283500	-2.41268000	-2.90742600
C	-0.47001900	-2.45938900	-1.61060500
C	2.11289900	-1.23475900	-2.86908500
C	0.16708600	-1.69534400	-0.48738600
C	2.44757700	-1.17960300	-1.44526200
H	1.00129500	-1.63651300	-4.57876100
H	-0.74081200	-2.96134200	-3.60625900
H	-1.33055300	-3.06457700	-1.33681500
H	2.86780000	-0.76633700	-3.49967500
H	3.52011100	-1.27294300	-1.27808400
C	1.65694000	-1.88449800	-0.45408700
C	2.24026400	-2.47564700	0.64225500
C	3.65520500	-2.67924900	0.73360700
N	4.80056500	-2.84137100	0.80885400
C	1.46997500	-2.92507300	1.76201100
N	0.82745700	-3.27983800	2.66033400
H	1.84806000	0.95556800	-1.96117200
H	-0.21447000	0.11280100	-1.63927400
H	-0.24831100	-2.07282500	0.44881000

M5

C	1.98817600	-0.06536300	-0.07584200
C	1.09189300	0.71981600	-0.97859800
C	-0.24361100	0.15737500	-1.27683100
C	1.54577400	1.74338500	-1.80961800
C	3.36303300	0.50694300	0.19765400
C	3.80636000	0.58238800	1.52146000
C	4.23172900	0.92175200	-0.81953900
C	5.07335200	1.07000200	1.83095900
H	3.14462400	0.25267300	2.31892700
C	5.49865300	1.41023000	-0.51211900
H	3.91648000	0.86540200	-1.85546000
C	5.92426700	1.48854200	0.81220900
H	5.39366200	1.12178700	2.86695400
H	6.15631500	1.73135700	-1.31382300
H	6.91254500	1.87142400	1.04672600
N	1.85297100	2.65011700	-2.48880600
P	-1.50078600	0.58846900	0.07117900
C	-2.04320700	2.30219800	-0.18622100
C	-3.34443100	2.64841600	0.20214700
C	-1.19395600	3.27361700	-0.73052000
C	-3.78959300	3.95635200	0.04711000
H	-4.01310400	1.90089100	0.61706300
C	-1.65424300	4.57839900	-0.88580300
H	-0.18251500	3.03225500	-1.03616700
C	-2.94630100	4.92189200	-0.49792600
H	-4.79859900	4.21766200	0.34729800
H	-0.99293600	5.32418500	-1.31334700
H	-3.29842700	5.94071600	-0.62183100
C	-3.00127600	-0.42454100	0.00462700
C	-3.68649700	-0.83107000	1.15406300
C	-3.50881200	-0.74787300	-1.26118300
C	-4.85142100	-1.58370900	1.03393100
H	-3.32177100	-0.55739500	2.13874200
C	-4.66949600	-1.50293100	-1.37254100
H	-3.00303300	-0.40864100	-2.16264600
C	-5.33572400	-1.92783900	-0.22444100
H	-5.37822400	-1.90152800	1.92709800
H	-5.05342000	-1.75857500	-2.35404000
H	-6.23884100	-2.52252800	-0.31196200
C	-0.74712600	0.45872800	1.70576300
C	-0.05002800	1.56602400	2.19971200
C	-0.70299300	-0.76477300	2.38801800

C	0.69605900	1.44390700	3.36829300
H	-0.07765400	2.51272700	1.66980700
C	0.04349100	-0.87694900	3.55528600
H	-1.24389300	-1.62795300	2.01144900
C	0.74645300	0.22533900	4.04127200
H	1.24411000	2.30019900	3.74625600
H	0.08257300	-1.82610200	4.07869200
H	1.33450000	0.13315700	4.94868600
C	2.59468600	-1.69127100	-3.09540000
C	1.25511500	-1.62653400	-3.67581400
C	0.06295900	-1.55217200	-3.06864500
C	2.96419700	-1.72346500	-1.80668900
C	-0.23137600	-1.39965300	-1.60348600
C	2.12041400	-1.59954100	-0.57979000
H	3.39581200	-1.75770200	-3.82747800
H	1.23389000	-1.67843700	-4.76178300
H	-0.82612600	-1.55307900	-3.69531100
H	4.02702400	-1.80682700	-1.59563600
H	-1.22988600	-1.81075300	-1.43723100
H	2.62987000	-2.12882300	0.23187200
C	0.72495200	-2.10592400	-0.69227100
C	0.26838300	-3.09578100	0.13046800
C	1.10813900	-3.74529100	1.09737000
N	1.76605400	-4.26441100	1.89692400
C	-1.10311400	-3.52477800	0.13124300
N	-2.21487300	-3.85217400	0.14923300
H	1.52083300	-0.20352500	0.90653800
H	-0.68035000	0.66059000	-2.14840600

TS6

C	2.06281500	-0.01646400	-0.02009100
C	1.17064500	0.75171600	-0.96186500
C	-0.12188900	0.21663600	-1.33333400
C	1.53193500	2.00523200	-1.46143200
C	3.46016100	0.53988100	0.16726500
C	4.00411800	0.58065100	1.45305800
C	4.24954500	0.96746000	-0.90693300
C	5.30083400	1.04109800	1.66982900
H	3.39840200	0.24892000	2.29335300
C	5.54397800	1.43091400	-0.69286200
H	3.84580100	0.93517400	-1.91354900
C	6.07430400	1.47033400	0.59541100
H	5.70323700	1.06773700	2.67771100

H	6.14073100	1.76251100	-1.53678900
H	7.08346800	1.83499700	0.75917700
N	1.78801600	3.06444200	-1.89433600
P	-1.57317200	0.57662700	0.05372200
C	-2.25110500	2.24275300	-0.21486500
C	-3.59177500	2.49197300	0.11150100
C	-1.46058900	3.27449900	-0.73500400
C	-4.12981100	3.75963600	-0.07927100
H	-4.21751100	1.70016400	0.51018500
C	-2.01085400	4.54033600	-0.92319100
H	-0.42001400	3.11487000	-0.99465500
C	-3.34150800	4.78476700	-0.59813200
H	-5.16806200	3.94442100	0.17527300
H	-1.38957400	5.33186300	-1.32840900
H	-3.76626600	5.77180800	-0.74906900
C	-3.02022500	-0.51863900	0.05850100
C	-3.64402800	-0.95885300	1.23087200
C	-3.56154100	-0.86301200	-1.18773100
C	-4.77929700	-1.76072300	1.15115200
H	-3.25790100	-0.66736700	2.20222700
C	-4.69660100	-1.66125500	-1.25944900
H	-3.10429200	-0.49989500	-2.10596600
C	-5.30051100	-2.11709300	-0.08932300
H	-5.25777000	-2.10302500	2.06253100
H	-5.10777700	-1.92776600	-2.22705000
H	-6.18266800	-2.74607800	-0.14449800
C	-0.75992800	0.52929100	1.66328700
C	-0.06349100	1.66619100	2.08729500
C	-0.61855100	-0.67910800	2.36083200
C	0.77673500	1.58839400	3.19522100
H	-0.16448400	2.60507000	1.55152200
C	0.21425500	-0.74641400	3.47120400
H	-1.14763400	-1.56973700	2.03475900
C	0.91904800	0.38557400	3.88265000
H	1.32578500	2.46785400	3.51401100
H	0.32308800	-1.68505500	4.00400200
H	1.57933200	0.32860900	4.74202700
C	2.72110700	-1.81611300	-2.95213700
C	1.41320400	-1.73294700	-3.60442900
C	0.20276000	-1.55288400	-3.06345200
C	3.03496900	-1.75919000	-1.65096900
C	-0.14662300	-1.32497100	-1.61479500
C	2.14504400	-1.54308600	-0.46062700
H	3.55157700	-1.95990500	-3.63890200

H	1.44286100	-1.84755700	-4.68529300
H	-0.65735500	-1.53181700	-3.72853200
H	4.08596900	-1.85215700	-1.39013100
H	-1.16320900	-1.70370700	-1.47992400
H	2.60133800	-2.07231900	0.38286900
C	0.74819500	-2.03937900	-0.64467900
C	0.25758600	-3.05571800	0.11589900
C	1.04127000	-3.70583900	1.13095400
N	1.64856200	-4.22172400	1.97106500
C	-1.09459200	-3.53223400	0.00223600
N	-2.18246900	-3.92356300	-0.06931400
H	1.62704000	-0.07479300	0.98576100
H	-0.56284000	0.74320800	-2.18594200

P

C	-0.33334500	1.24765200	0.65638600
C	0.39536400	1.95148800	-0.47103600
C	1.34926400	1.37096900	-1.20960400
C	0.00605400	3.30738500	-0.75254100
C	-1.69848300	0.70944000	0.26143200
C	-2.68127600	0.57641200	1.24628700
C	-1.97339400	0.26995700	-1.03456400
C	-3.91555500	0.01256100	0.94259700
H	-2.47393300	0.91583000	2.25836300
C	-3.21051700	-0.29251900	-1.34084200
H	-1.22279600	0.37437100	-1.81344200
C	-4.18283100	-0.42363300	-0.35365300
H	-4.66955600	-0.08515300	1.71668400
H	-3.41229700	-0.62760800	-2.35300800
H	-5.14598200	-0.86268800	-0.59223300
N	-0.32537300	4.39742300	-0.95883400
C	3.06286400	0.71347300	1.65065500
C	3.76466100	0.15833200	0.48964800
C	3.24202900	-0.18884900	-0.69270000
C	1.75552400	0.70694400	1.94422200
C	1.76690700	-0.06968900	-1.03636300
C	0.58878800	0.10592100	1.20249600
H	3.71211800	1.19354900	2.37855600
H	4.83914800	0.04775400	0.61035600
H	3.88652800	-0.59386200	-1.46599700
H	1.45030700	1.20593600	2.86202900
H	1.60126700	-0.57450300	-1.99478000
C	0.95706300	-0.74995000	0.03478300

C	0.54640700	-2.03281800	-0.08649400
C	0.86751400	-2.81621500	-1.24911200
N	1.14071300	-3.43239100	-2.18959100
C	-0.23500400	-2.68346800	0.93040500
N	-0.86866200	-3.20033500	1.74896500
H	-0.46919900	1.96052500	1.47733100
H	1.85286300	1.92472400	-1.99619100
H	-0.00741200	-0.47211700	1.91655300