

Supporting Information

**Understanding the mechanisms, regioselectivities and
enantioselectivities of the DMAP-catalyzed [2+4] cycloaddition of γ -
methyl allenoate and phenyl(phenyldiazenyl)methanone**

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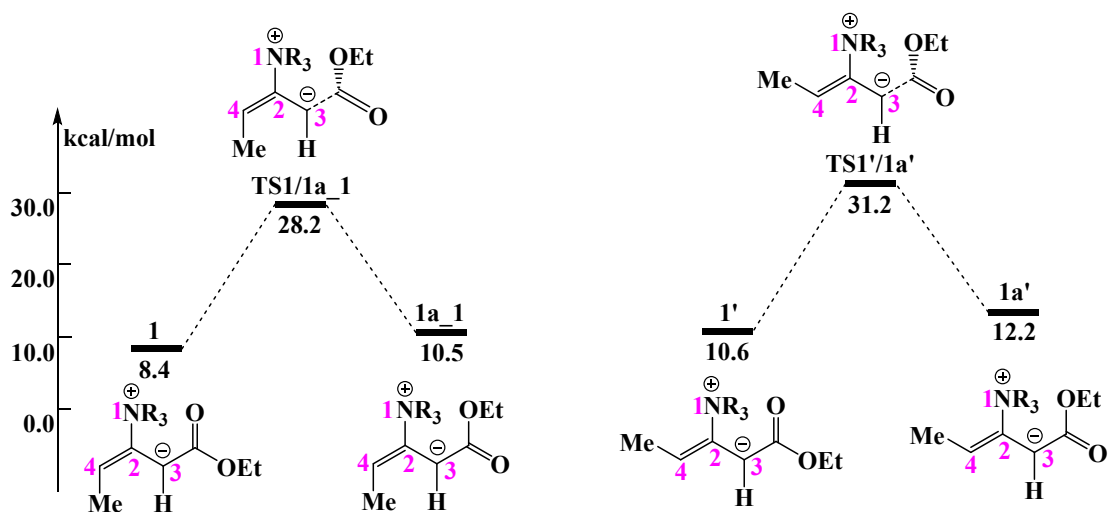
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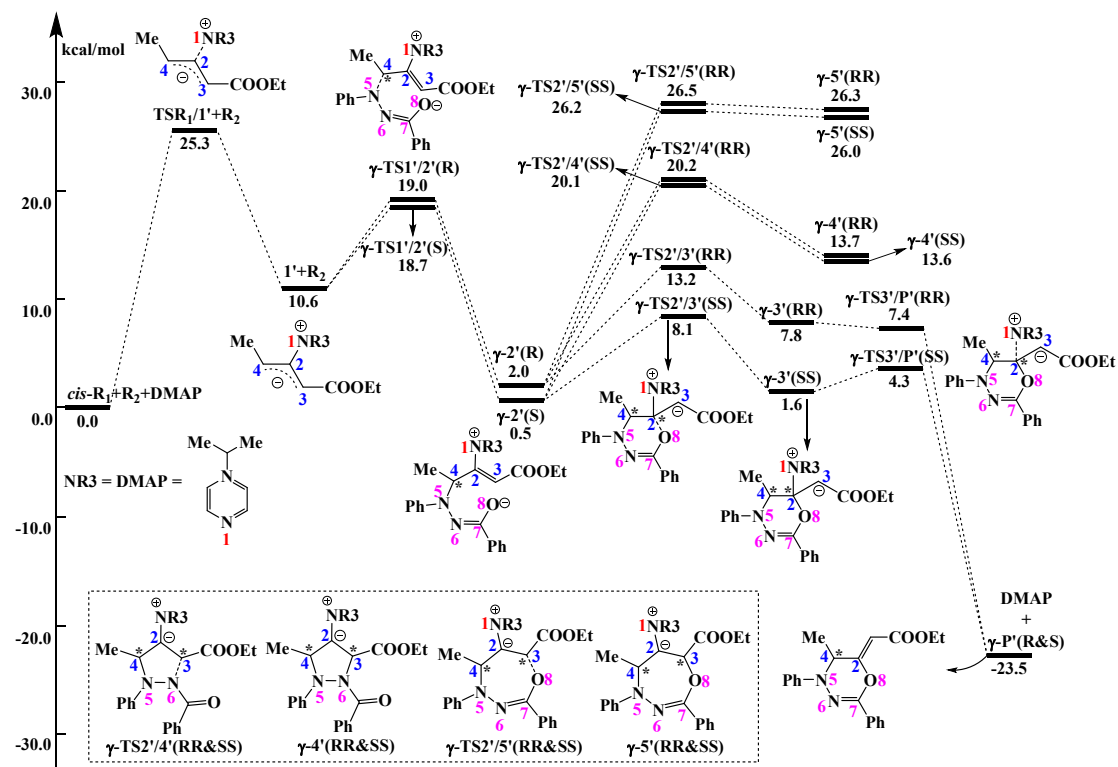
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Fig S1. Free energy profile of the conversion between **1** and **1a** (**1'** and **1a'**). The solvation-corrected relative free energies at SMD(toluene)/M06-2X/6-311++G(d,p) level are given in kcal/mol.



It should be noted that for **1**→**1a** conversion, **1** has to undergo C2-C3 bond rotation to generate **1a_1**, followed by the rotation of C3-ester C bond to afford **1a**. On the basis of our calculations, the C2-C3 bond rotation transition state **TS1/1a_1** is 4.2 kcal/mol higher than **TSR₁/1** (28.2 kcal/mol vs 24.0 kcal/mol), which makes the transformation of **1**→**1a_1** much less favorable, the transition state for the conversion of **1a_1**→**1a** is thus not searched.

Fig S2. Free energy profile of the reaction pathways proceeded via 1'. The solvation-corrected relative free energies at SMD(toluene)/M06-2X/6-311++G(d,p) level are given in kcal/mol.



Cartesian coordinates of all stationary points for the DMAP-catalyzed reaction of γ -methyl allenoate with phenyl(phenyldiazenyl)methanone in toluene:

DMAP

N	-1.90783500	0.00107300	0.00185500
C	1.58988300	-1.13342300	0.00441700
C	0.20447700	-1.19886400	0.00627400
C	-0.54444900	0.00022700	0.00009600
C	-2.63144200	-1.25573800	-0.01156400
H	2.16229200	-2.05880000	0.01032800
H	-0.27681300	-2.16874300	0.01558900
H	-2.37730500	-1.85493300	-0.89462000
H	-2.41990500	-1.85227500	0.88497700
H	-3.70094600	-1.04942700	-0.03959000
C	1.59142200	1.13094300	-0.00988900
C	0.20610900	1.19829300	-0.00801100
C	-2.62994800	1.25869500	0.01538200
H	2.16508400	2.05553200	-0.01733700
H	-0.27384200	2.16884600	-0.01599900
H	-2.41914800	1.85437600	-0.88191200
H	-2.37390500	1.85821300	0.89765100
H	-3.69963300	1.05356400	0.04519400
N	2.30410200	-0.00172800	-0.00373100

cis-R₁

C	-0.76228800	-0.77406300	-0.03357500
H	-0.60132200	-1.84653800	-0.09717300

C	-1.97154600	-0.26003100	-0.00155300
C	-3.16806600	0.25638400	0.03622400
H	-3.63670500	0.51679900	-0.91294200
C	0.43831300	0.09796300	0.02052300
O	1.55710600	-0.64223700	-0.01883900
O	0.43788500	1.30678000	0.09304700
C	2.79797200	0.08396300	0.03562900
C	3.91733200	-0.92932700	-0.02570700
H	2.82226800	0.66561200	0.96226300
H	2.83244100	0.78360700	-0.80501300
H	4.88100000	-0.41516500	0.02742500
H	3.85451600	-1.63096400	0.81042500
H	3.87947400	-1.49551200	-0.96016000
C	-3.93848800	0.52902700	1.30105600
H	-4.17270200	1.59545500	1.37376400
H	-4.88572200	-0.01890100	1.29465800
H	-3.36742500	0.23562300	2.18359900

trans-R₁

C	-0.85426900	0.99964400	0.03004100
H	-1.03709300	2.07029100	0.05931900
C	-1.84303000	0.13432000	-0.00612100
C	-2.82664900	-0.72154700	-0.03830200
H	-3.21447800	-1.07961300	0.91545800
C	0.57583900	0.60663700	0.04269800
O	0.76479000	-0.71625600	-0.02519600

O	1.48129600	1.41113800	0.10960600
C	2.13469200	-1.15691000	-0.01051100
C	2.12507600	-2.66771500	-0.04860100
H	2.61670300	-0.77385500	0.89388400
H	2.64943600	-0.72920200	-0.87654500
H	3.15328900	-3.03991700	-0.04179300
H	1.60449400	-3.07607600	0.82182100
H	1.63189100	-3.03240900	-0.95368000
C	-3.45050700	-1.26044100	-1.29840700
H	-3.32779700	-2.34710500	-1.34290900
H	-4.52392000	-1.04801600	-1.31127800
H	-2.99416800	-0.82016500	-2.18675700

R₂

C	1.71955900	0.67772900	-0.45586800
O	1.96393000	1.84167400	-0.66806200
C	-1.79819100	0.26346900	-0.10345200
C	-2.21115600	-0.56843000	-1.15041700
C	-2.71316000	0.75185700	0.82894100
C	-3.55379200	-0.90910300	-1.24987500
H	-1.48329800	-0.93099800	-1.86866100
C	-4.05715100	0.40025100	0.72495900
H	-2.35409700	1.40053800	1.62227300
C	-4.47597700	-0.42846100	-0.31362600
H	-3.88872100	-1.54959600	-2.05984000
H	-4.77368000	0.77504800	1.44864700

H	-5.52340900	-0.70141700	-0.40001700
C	2.72478500	-0.34466300	-0.06869100
C	2.36639500	-1.68336800	0.12392300
C	4.04769200	0.06622400	0.12868500
C	3.33253800	-2.60645300	0.51574200
H	1.34096500	-2.00113200	-0.03723200
C	5.00772900	-0.85944700	0.51906900
H	4.30361100	1.11000200	-0.02469600
C	4.64990100	-2.19559400	0.71277700
H	3.05771600	-3.64576800	0.66513600
H	6.03456500	-0.54335400	0.67388300
H	5.40152500	-2.91741700	1.01852300
N	-0.44873200	0.68618900	0.09608400
N	0.38532500	0.16489400	-0.65706100

TSR₁/1

C	-2.34235000	0.77113300	-0.67233400
H	-2.88400000	0.70373300	-1.60990100
C	-1.51941800	1.82338300	-0.43027800
C	-1.35897200	3.12322600	-0.25637100
H	-0.37450800	3.56955500	-0.36792700
C	-2.39089100	-0.34379900	0.24640800
O	-3.20561900	-1.33805900	-0.20234500
O	-1.78175300	-0.44356300	1.30168100
C	-3.32036200	-2.48002200	0.65010800
C	-4.26517400	-3.45518300	-0.01708700

H	-3.69391200	-2.16252200	1.62924600
H	-2.32832000	-2.91891900	0.80020400
H	-4.37667200	-4.34831800	0.60500600
H	-5.25246100	-3.00617200	-0.15689700
H	-3.88275100	-3.76203600	-0.99493100
C	-2.50467900	4.03793900	0.08364800
H	-3.42271300	3.47123300	0.25186000
H	-2.28022400	4.61678000	0.98630700
H	-2.68373300	4.75424600	-0.72601200
C	0.63186600	0.00335700	-1.03214900
C	1.82833200	-0.68264700	-0.94752400
C	2.85227300	-0.18777500	-0.10256500
C	2.55767900	0.99585200	0.61846600
C	1.32690500	1.60213100	0.44977500
N	0.38604300	1.13125600	-0.36964400
H	-0.18917700	-0.36496200	-1.64829400
H	1.95482400	-1.59327800	-1.51865500
H	3.26565100	1.42781100	1.31388300
H	1.07096900	2.49999200	1.00882300
N	4.04850500	-0.82073500	0.01927000
C	4.27668800	-2.07666100	-0.67340600
H	3.56664600	-2.84913000	-0.35221300
H	4.19041800	-1.95192000	-1.75892500
H	5.28469000	-2.42530800	-0.45224100
C	5.04915600	-0.30665900	0.93715200

H	5.32367800	0.72347000	0.68371300
H	4.69639400	-0.32981000	1.97608100
H	5.94602100	-0.92075700	0.86574700

TSR₁/1'

C	2.42322600	1.04420100	-0.47969900
H	3.06073900	1.07466700	-1.35651300
C	1.55589300	2.06192100	-0.23384200
C	1.39100100	3.35427400	-0.00093600
H	2.28738500	3.84077000	0.38411600
C	2.40330500	-0.15633000	0.32351600
O	3.24479300	-1.10855200	-0.16659400
O	1.72366200	-0.35715300	1.32042700
C	3.30096200	-2.33216600	0.56997600
C	4.22415800	-3.27033200	-0.17627000
H	2.29178400	-2.74715900	0.65949100
H	3.66704300	-2.12798300	1.58215800
H	4.30014400	-4.22149400	0.35904800
H	3.84343500	-3.46909700	-1.18224500
H	5.22661300	-2.84231600	-0.26433900
C	0.19821000	4.23481100	-0.23132900
H	-0.17138100	4.65857500	0.70939500
H	0.48288500	5.08076200	-0.86676300
H	-0.61399000	3.70043700	-0.72483900
C	-1.15963300	1.40234200	0.70282100
C	-2.27424900	0.59924800	0.85167300

C	-2.53598500	-0.40968700	-0.10820800
C	-1.59771700	-0.53620400	-1.16258100
C	-0.50783800	0.31167000	-1.20184400
N	-0.29824700	1.27879100	-0.30941900
H	-0.92934600	2.17529200	1.43341700
H	-2.91724800	0.74816800	1.70941000
H	-1.70112700	-1.29394400	-1.92850300
H	0.25845100	0.20468100	-1.96866000
N	-3.62062900	-1.22210300	-0.01318400
C	-4.50240500	-1.12221100	1.13634500
H	-3.96626400	-1.32109100	2.07255900
H	-4.96113200	-0.12857700	1.20032400
H	-5.29934300	-1.85805000	1.03567700
C	-3.83207200	-2.26674800	-0.99895500
H	-3.91599800	-1.84647300	-2.00753600
H	-3.01684000	-3.00142500	-0.99119400
H	-4.76246000	-2.78565000	-0.77144100

TSR₁/1a

C	-1.88979100	0.25313200	-1.45431200
H	-1.57496000	0.17696000	-2.48988200
C	-1.35472400	1.17491600	-0.60911400
C	-1.55999400	2.20952200	0.18720200
H	-0.82128200	2.49076100	0.93251200
C	-2.85582700	-0.73078400	-1.01743300
O	-3.19099200	-0.62758400	0.29755000

O	-3.35974200	-1.58648000	-1.73396200
C	-4.16423700	-1.56114000	0.76940700
C	-4.39292500	-1.26839500	2.23667500
H	-3.79563900	-2.58079800	0.61471600
H	-5.08614700	-1.45020400	0.18870300
H	-5.13066400	-1.96488500	2.64597700
H	-3.46364900	-1.37689600	2.80320200
H	-4.76555500	-0.24941500	2.37577800
C	-2.84674300	2.98756200	0.15707000
H	-2.65405500	4.06464400	0.10698100
H	-3.45999800	2.69713100	-0.69855600
H	-3.42373900	2.79910000	1.07000400
C	1.53372100	1.59776100	0.03317400
C	2.85048400	1.22433400	0.22012800
C	3.21719700	-0.13541900	0.05182600
C	2.18161500	-1.02501400	-0.32813000
C	0.89734200	-0.54152700	-0.48658600
N	0.56967700	0.73578400	-0.29979500
H	1.23334300	2.63749800	0.14629100
H	3.57825100	1.98113900	0.48318400
H	2.37063500	-2.07788800	-0.49222800
H	0.07390500	-1.19200900	-0.78231600
N	4.49179800	-0.56009200	0.24017300
C	4.82703800	-1.95813900	0.03178400
H	4.26886300	-2.60887100	0.71586000

H	4.61414600	-2.26807300	-0.99808800
H	5.89091200	-2.10027900	0.21633000
C	5.51456400	0.37997500	0.66409800
H	5.68308900	1.15804900	-0.09030500
H	5.24141700	0.86242400	1.61002600
H	6.45035600	-0.15643300	0.81572700

TSR₁/1a'

C	-1.88979100	0.25313200	-1.45431200
H	-1.57496000	0.17696000	-2.48988200
C	-1.35472400	1.17491600	-0.60911400
C	-1.55999400	2.20952200	0.18720200
H	-0.82128200	2.49076100	0.93251200
C	-2.85582700	-0.73078400	-1.01743300
O	-3.19099200	-0.62758400	0.29755000
O	-3.35974200	-1.58648000	-1.73396200
C	-4.16423700	-1.56114000	0.76940700
C	-4.39292500	-1.26839500	2.23667500
H	-3.79563900	-2.58079800	0.61471600
H	-5.08614700	-1.45020400	0.18870300
H	-5.13066400	-1.96488500	2.64597700
H	-3.46364900	-1.37689600	2.80320200
H	-4.76555500	-0.24941500	2.37577800
C	-2.84674300	2.98756200	0.15707000
H	-2.65405500	4.06464400	0.10698100
H	-3.45999800	2.69713100	-0.69855600

H	-3.42373900	2.79910000	1.07000400
C	1.53372100	1.59776100	0.03317400
C	2.85048400	1.22433400	0.22012800
C	3.21719700	-0.13541900	0.05182600
C	2.18161500	-1.02501400	-0.32813000
C	0.89734200	-0.54152700	-0.48658600
N	0.56967700	0.73578400	-0.29979500
H	1.23334300	2.63749800	0.14629100
H	3.57825100	1.98113900	0.48318400
H	2.37063500	-2.07788800	-0.49222800
H	0.07390500	-1.19200900	-0.78231600
N	4.49179800	-0.56009200	0.24017300
C	4.82703800	-1.95813900	0.03178400
H	4.26886300	-2.60887100	0.71586000
H	4.61414600	-2.26807300	-0.99808800
H	5.89091200	-2.10027900	0.21633000
C	5.51456400	0.37997500	0.66409800
H	5.68308900	1.15804900	-0.09030500
H	5.24141700	0.86242400	1.61002600
H	6.45035600	-0.15643300	0.81572700
1			
C	2.14160200	0.92226800	0.24203800
H	3.07745400	1.37771100	0.53836500
C	0.99288600	1.75835300	0.18043900
C	0.92621500	3.11458300	0.20415600

H	-0.04340200	3.59229100	0.31432700
C	2.16327400	-0.44105600	-0.13216700
O	3.41856800	-0.99280300	0.01541500
O	1.23035900	-1.15158700	-0.53859000
C	3.54540200	-2.36101600	-0.35319300
C	4.99836200	-2.74677000	-0.16864500
H	3.22650200	-2.49605700	-1.39285000
H	2.88917500	-2.97735100	0.27236000
H	5.14643500	-3.79661500	-0.43992200
H	5.64491300	-2.13139700	-0.80089400
H	5.30703000	-2.61232900	0.87229400
C	2.16139200	3.96444300	0.18380800
H	2.88245900	3.59387100	-0.55548000
H	1.92215400	5.00203900	-0.06555700
H	2.68004300	3.97505600	1.15353500
C	-0.61005100	0.15426600	1.07236900
C	-1.81226300	-0.49928500	1.07876600
C	-2.76538200	-0.24865600	0.05472700
C	-2.39676600	0.70362100	-0.93261100
C	-1.17703100	1.32744900	-0.86142100
N	-0.30321900	1.07592400	0.13422700
H	0.15784300	-0.01823400	1.81689800
H	-1.99834500	-1.21731200	1.86528600
H	-3.04185500	0.93837600	-1.76801000
H	-0.84153800	2.04093300	-1.60384500

N	-3.95098200	-0.88696200	0.01856900
C	-4.25481300	-1.91877000	1.00016400
H	-3.50964900	-2.72142700	0.97104500
H	-4.29132500	-1.50310700	2.01316100
H	-5.22898900	-2.34729100	0.77035100
C	-4.89978400	-0.60574100	-1.04871100
H	-5.14532600	0.46087100	-1.08092700
H	-4.50572900	-0.91137200	-2.02510300
H	-5.81811800	-1.15840000	-0.85753500
1'			
C	-2.16220500	1.20100800	0.22389900
H	-3.05170700	1.74959800	0.50581800
C	-0.94123700	1.93421900	0.13229500
C	-0.75617700	3.27779100	0.08467500
H	-1.66279600	3.86987500	-0.01299000
C	-2.30783900	-0.15209800	-0.14440300
O	-3.60932900	-0.58976700	0.01649800
O	-1.44698900	-0.95029600	-0.55298400
C	-3.85081200	-1.95068100	-0.31611600
C	-5.32391700	-2.21975300	-0.08701900
H	-3.22804500	-2.60194400	0.30817300
H	-3.56990800	-2.13484100	-1.35950500
H	-5.55765800	-3.26261800	-0.32345500
H	-5.59397300	-2.03227300	0.95652000
H	-5.93933900	-1.57551500	-0.72165000

C	0.53375500	4.03285600	0.24349100
H	0.85943900	4.51306100	-0.68950500
H	0.42012200	4.83687000	0.98027500
H	1.35469500	3.39615900	0.58876100
C	1.13838500	1.17930100	-0.90165700
C	2.25032900	0.38126000	-0.97157600
C	2.51239400	-0.56182200	0.05856000
C	1.58385000	-0.60133200	1.13290600
C	0.48631300	0.21695600	1.11950400
N	0.27482700	1.11203400	0.13181200
H	0.88408700	1.89264400	-1.67676500
H	2.89421600	0.47457900	-1.83515300
H	1.69466500	-1.29272700	1.95677600
H	-0.27474800	0.19314100	1.89126000
N	3.58125900	-1.38003000	0.01395000
C	4.47705800	-1.34601700	-1.13284700
H	3.94664600	-1.60132000	-2.05729200
H	4.93385700	-0.35698700	-1.24548800
H	5.27289300	-2.07286000	-0.98074200
C	3.78333200	-2.37357000	1.05896200
H	3.90322000	-1.89596700	2.03713400
H	2.94287500	-3.07552800	1.10442800
H	4.69002300	-2.93557400	0.84090800
1a			
C	-1.53585000	-0.32593500	-1.13409600

H	-0.99009000	-0.79847500	-1.94464800
C	-0.87138400	0.66256100	-0.35661100
C	-1.29060600	1.79700900	0.25846500
H	-0.61486100	2.28584800	0.95792100
C	-2.84798000	-0.82227000	-0.93076500
O	-3.46348300	-0.35375800	0.21051000
O	-3.43463000	-1.64309100	-1.64540100
C	-4.76249400	-0.87587700	0.46653700
C	-5.25548600	-0.26226400	1.76070100
H	-4.71388100	-1.96821300	0.53866000
H	-5.42936600	-0.63487200	-0.36889300
H	-6.24241900	-0.66274000	2.01282600
H	-4.57069800	-0.48912300	2.58343100
H	-5.34027700	0.82500200	1.67263700
C	-2.64386400	2.39980500	0.05554900
H	-2.58596000	3.49396200	0.08610000
H	-3.05479100	2.09295500	-0.91274400
H	-3.36414400	2.07619100	0.81604900
C	1.49296100	1.36126100	-0.46765100
C	2.84083400	1.14963000	-0.32226400
C	3.32027100	-0.11715000	0.10822500
C	2.33444600	-1.11349100	0.35267900
C	1.00620300	-0.82439700	0.18133600
N	0.58252100	0.39822400	-0.21003500
H	1.08469800	2.30374100	-0.81233500

H	3. 51404200	1. 96013100	-0. 56603300
H	2. 60200400	-2. 10884700	0. 68002900
H	0. 21731000	-1. 54837100	0. 35046900
N	4. 63388800	-0. 36453400	0. 26323500
C	5. 08603400	-1. 68978200	0. 66569300
H	4. 71544500	-1. 94795100	1. 66396000
H	4. 75129800	-2. 45167800	-0. 04637200
H	6. 17433800	-1. 69911900	0. 68928800
C	5. 61015600	0. 68555900	0. 00730700
H	5. 60124100	0. 98773600	-1. 04618000
H	5. 41379300	1. 56368700	0. 63147600
H	6. 60292600	0. 31114000	0. 25045400

1a'

C	2. 91368100	0. 08986600	0. 42806200
H	3. 93866900	-0. 03120900	0. 75570000
C	2. 20297300	-1. 09768300	0. 07424500
C	2. 68882900	-2. 32250000	-0. 24821500
H	3. 76507500	-2. 37783300	-0. 39132100
C	2. 49586200	1. 42923400	0. 24918800
O	1. 23941100	1. 57059900	-0. 33307400
O	3. 12725900	2. 44561100	0. 55590300
C	0. 75394100	2. 90248500	-0. 44486200
C	-0. 64334800	2. 82846700	-1. 02822400
H	1. 41981700	3. 48904600	-1. 08732300
H	0. 74912000	3. 38047100	0. 54137700

H	-1.05611300	3.83514600	-1.14753100
H	-0.62875000	2.34333100	-2.00952500
H	-1.31003200	2.25824800	-0.37144200
C	1.92246700	-3.61238800	-0.34088400
H	1.85116800	-3.98397300	-1.37206000
H	2.42035500	-4.40045700	0.23660600
H	0.90276200	-3.52439600	0.04776600
C	0.00742800	-1.13170400	-0.99588700
C	-1.34770000	-0.92350400	-1.01396500
C	-2.01880100	-0.52878200	0.17515700
C	-1.21853100	-0.40377500	1.34417400
C	0.13281600	-0.61750800	1.27489900
N	0.73661600	-0.98624900	0.12707900
H	0.56958200	-1.39828000	-1.88337600
H	-1.86986600	-1.03544600	-1.95417300
H	-1.64355300	-0.11564500	2.29577300
H	0.79454000	-0.48952900	2.12402000
N	-3.33937300	-0.26561100	0.19071200
C	-3.97521400	0.20251200	1.41500200
H	-3.88858300	-0.54329600	2.21242500
H	-3.53085000	1.14430900	1.75724300
H	-5.03276300	0.37281500	1.22043800
C	-4.11331700	-0.34626200	-1.04060700
H	-3.75492900	0.37808200	-1.78144700
H	-4.06026200	-1.35175600	-1.47095100

H	-5.15598100	-0.12703400	-0.81786800
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1a-1

C	-2.77943300	0.03320100	0.45578800
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H	-3.79390500	-0.12368500	0.80039200
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C	-2.02650300	-1.12214000	0.10502600
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C	-2.46761200	-2.37309600	-0.18604600
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H	-1.74684600	-3.18467200	-0.24307200
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C	-2.41000700	1.39152900	0.28962300
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O	-1.16366900	1.58108600	-0.29206800
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O	-3.07933800	2.37864200	0.60522000
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C	-0.75319100	2.93384300	-0.45469400
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C	0.65050400	2.91270000	-1.02459300
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H	-0.78590100	3.45148200	0.51020900
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H	-1.44665500	3.45171300	-1.12674700
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H	1.00677600	3.93440400	-1.18930800
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H	1.34115000	2.41449400	-0.33554300
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H	0.67301000	2.38050900	-1.98077900
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C	-3.92695000	-2.68620800	-0.32690700
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H	-4.42679500	-2.81084000	0.64439800
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H	-4.45053000	-1.87750400	-0.85089400
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H	-4.07882100	-3.61295200	-0.88821500
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C	0.05666100	-0.54303400	1.23522800
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C	1.41409200	-0.37255300	1.28915800
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C	2.21061000	-0.62494600	0.13779400
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C	1.52015900	-1.05921000	-1.02481500
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C	0.15703400	-1.21736900	-0.99369300
N	-0.56387600	-0.97939800	0.11893200
H	-0.59634100	-0.33554400	2.07539200
H	1.84997000	-0.03170000	2.21832600
H	2.03582000	-1.25506800	-1.95476800
H	-0.41544900	-1.52151000	-1.86143800
N	3.54529900	-0.44569400	0.14783100
C	4.32452900	-0.70085300	-1.05526000
H	4.23553500	-1.74685300	-1.36964200
H	4.00154200	-0.05322600	-1.87778000
H	5.37275200	-0.49326800	-0.84776200
C	4.21407500	-0.00684200	1.36499000
H	3.84447400	0.97233100	1.68887300
H	4.06882400	-0.72865200	2.17651200
H	5.28168300	0.07821800	1.16968800

TS1/1a-1

C	2.38992000	-0.70668800	0.83302200
H	3.41978100	-1.00269700	0.99672300
C	1.54712500	-1.55716400	0.11290100
C	1.77032200	-2.75562100	-0.51692100
H	0.92152200	-3.38274100	-0.77445900
C	2.09202000	0.73928900	0.94651800
O	2.43094900	1.44895600	-0.16259400
O	1.58888300	1.31257800	1.89748900
C	2.17654700	2.85950400	-0.11989200

C	2.62926800	3.44638600	-1.43874400
H	2.71784700	3.29588700	0.72593700
H	1.10703100	3.02426000	0.05134100
H	2.44957000	4.52565400	-1.44706100
H	3.69736100	3.27213600	-1.59511300
H	2.08161200	2.99782000	-2.27259600
C	3.15953400	-3.30836500	-0.62200000
H	3.54513400	-3.70319100	0.33217400
H	3.20953600	-4.12530800	-1.34901400
H	3.86761000	-2.53105200	-0.94350300
C	-0.45884800	-0.90181400	-1.13743300
C	-1.75810000	-0.46860300	-1.22940000
C	-2.50283700	-0.20003900	-0.04897400
C	-1.82996300	-0.40610400	1.18634200
C	-0.52900500	-0.83733400	1.19714000
N	0.14740000	-1.08928200	0.05383200
H	0.15719400	-1.11170200	-2.00380800
H	-2.18105600	-0.32451000	-2.21418500
H	-2.31744600	-0.23287400	2.13588400
H	0.03589100	-0.99893400	2.10815400
N	-3.77886700	0.22871600	-0.09818800
C	-4.44010200	0.40741000	-1.38290500
H	-3.95470400	1.19208000	-1.97439700
H	-4.43779700	-0.52469900	-1.95802000
H	-5.47504700	0.69716600	-1.20924400

C	-4.49682000	0.52815400	1.13293600
H	-4.60745200	-0.36760500	1.75431200
H	-3.97976800	1.30096300	1.71164400
H	-5.48957400	0.89696700	0.88102200

TS1'/1a'

C	-2.74418300	0.62215400	-0.33806000
H	-3.78193700	0.91668300	-0.46194900
C	-1.78905000	1.64717300	-0.24805100
C	-1.88308900	3.01317000	-0.24392600
H	-2.88400000	3.41506700	-0.11178100
C	-2.53144300	-0.61039200	0.46245300
O	-2.15123400	-1.68106000	-0.28661100
O	-2.65097600	-0.73477700	1.66903700
C	-1.90429100	-2.89744500	0.42759300
C	-1.48551400	-3.94311700	-0.58230800
H	-2.81317400	-3.19154400	0.96265900
H	-1.12361700	-2.72118900	1.17615600
H	-1.28672000	-4.89262200	-0.07646000
H	-2.27282600	-4.10517500	-1.32365000
H	-0.57638900	-3.63433200	-1.10728600
C	-0.79594300	3.98780000	-0.61370300
H	-1.08870900	4.61559000	-1.46664900
H	-0.54495900	4.67854900	0.20357200
H	0.13294200	3.48447700	-0.90539300
C	0.05686300	0.28031900	-1.13252700

C	1. 32768200	-0. 23606800	-1. 09051300
C	2. 19275100	0. 08758500	-0. 00965300
C	1. 66621100	0. 95420300	0. 98760800
C	0. 38831400	1. 43781100	0. 86854900
N	-0. 40357000	1. 11254600	-0. 17472400
H	-0. 65545300	0. 05396400	-1. 91779400
H	1. 64213300	-0. 88650200	-1. 89520600
H	2. 24305700	1. 23799300	1. 85710400
H	-0. 06394600	2. 09876800	1. 59945300
N	3. 44394900	-0. 40440800	0. 06864600
C	3. 94116800	-1. 30352400	-0. 96296900
H	3. 34358700	-2. 22084900	-1. 01085600
H	3. 93115500	-0. 81984700	-1. 94583700
H	4. 96858100	-1. 57536600	-0. 72732800
C	4. 29316000	-0. 06386300	1. 20139200
H	4. 44870400	1. 01865400	1. 26446500
H	3. 85753400	-0. 41669800	2. 14285100
H	5. 26325100	-0. 54073000	1. 07175300

TSR₂/1b

C	0. 97490500	-0. 79162700	-0. 71033000
O	0. 49290000	0. 30319300	-1. 00983000
C	-1. 68196100	-3. 10070600	-0. 99417200
C	-1. 03090500	-4. 33294800	-1. 03942300
C	-3. 07631600	-3. 04171500	-0. 94849300
C	-1. 78582500	-5. 50663700	-1. 05064400

H	0.05276300	-4.35728300	-1.04462200
C	-3.82246200	-4.21473900	-0.96503800
H	-3.56013800	-2.07028700	-0.89356900
C	-3.17759000	-5.45264500	-1.01743800
H	-1.28032600	-6.46757200	-1.07963400
H	-4.90644900	-4.16578800	-0.92647200
H	-3.75904600	-6.36960200	-1.02155700
C	2.40824200	-0.90351600	-0.26491500
C	2.94651600	-2.10852100	0.19914800
C	3.20666100	0.24352900	-0.28330800
C	4.26723600	-2.16226500	0.63866100
H	2.32084200	-2.99456200	0.21452100
C	4.52889300	0.18810600	0.15024800
H	2.77049600	1.17208400	-0.63862800
C	5.06165100	-1.01535700	0.61367100
H	4.67716200	-3.09957900	1.00341100
H	5.14324100	1.08352000	0.13213300
H	6.09173600	-1.05926600	0.95547000
N	-0.98014900	-1.83457100	-0.94410900
N	0.32313000	-1.99598400	-0.80428300
C	-0.67679500	-1.82861900	-3.64714800
C	-0.75714100	-1.30180300	-4.91840000
C	-1.49908100	-0.10802200	-5.12982200
C	-2.09903500	0.48693000	-3.98888600
C	-1.95758200	-0.11462800	-2.75548200

N	-1.28958300	-1.25529700	-2.61595500
H	-0.10028700	-2.72496500	-3.41851200
H	-0.24646400	-1.80608900	-5.72798900
H	-2.64494200	1.41849100	-4.05523300
H	-2.35878500	0.31201700	-1.84090800
N	-1.61659900	0.44492500	-6.36063400
C	-0.95348200	-0.16660400	-7.50052100
H	0.13364300	-0.19559700	-7.36146000
H	-1.31508800	-1.18760200	-7.66811100
H	-1.16912100	0.42064200	-8.39203900
C	-2.35803300	1.68327900	-6.53188600
H	-3.39510700	1.57189900	-6.19550500
H	-1.89424700	2.50775900	-5.97693500
H	-2.37022700	1.94508000	-7.58878400

TSR₂/1b'

C	1.85748000	-2.07009100	-1.36758100
O	2.13311100	-0.90326300	-1.65694300
C	-1.56430500	-2.03296100	-0.50034700
C	-1.73533800	-3.22770000	0.19781900
C	-2.66544200	-1.22999600	-0.80439900
C	-3.01553700	-3.60801500	0.60166400
H	-0.87008500	-3.84939500	0.39786500
C	-3.93831900	-1.61351500	-0.39685400
H	-2.50771800	-0.31193800	-1.36382000
C	-4.11652000	-2.80531700	0.30917200

H	-3.15223600	-4.54151700	1.13968200
H	-4.79372900	-0.99020300	-0.63888600
H	-5.11109200	-3.10999300	0.62048200
C	2.88890500	-3.15719500	-1.51012700
C	2.59692300	-4.50015700	-1.24922500
C	4.16898100	-2.80585000	-1.94719900
C	3.57593400	-5.47648000	-1.42326200
H	1.60094000	-4.77019400	-0.91496800
C	5.14818600	-3.78136100	-2.11816900
H	4.37605900	-1.76016200	-2.15236200
C	4.85310800	-5.11968800	-1.85648400
H	3.34167400	-6.51766700	-1.22138400
H	6.14055300	-3.49885900	-2.45729700
H	5.61510300	-5.88199600	-1.99069200
N	-0.27914600	-1.57490900	-0.98628900
N	0.66033100	-2.49408800	-0.84804300
C	0.31057800	-0.56155700	1.47236000
C	0.74475800	0.40001000	2.35932800
C	0.93355000	1.73229200	1.90131900
C	0.66836900	1.98467200	0.52968800
C	0.24086600	0.95372600	-0.28114700
N	0.04445200	-0.26933600	0.20197300
H	0.17738400	-1.60406400	1.76090800
H	0.94492800	0.11617700	3.38410700
H	0.81880100	2.96222700	0.09197100

H	0.06456200	1.07404300	-1.34596300
N	1.36051000	2.71370500	2.73122400
C	1.64388700	2.41718700	4.12563400
H	0.75648500	2.02165500	4.63247200
H	2.45957000	1.69075200	4.22362700
H	1.94076600	3.33585600	4.62993400
C	1.58929300	4.05301200	2.21435400
H	2.34927300	4.05073400	1.42405000
H	0.66551800	4.48702300	1.81445900
H	1.94166000	4.68880600	3.02504100

1b

C	1.82278700	-1.91857400	-1.19916500
O	2.01608800	-0.68138500	-1.20417400
C	-1.67521500	-2.16586100	-0.88644300
C	-2.87697000	-1.60152000	-1.33794300
C	-1.71363000	-3.24585400	0.00520900
C	-4.09507600	-2.11113700	-0.89380300
H	-2.87016000	-0.76134700	-2.02531800
C	-2.93968200	-3.74036500	0.44002800
H	-0.77940600	-3.67592200	0.34393500
C	-4.13840400	-3.18254800	-0.00431000
H	-5.01688800	-1.66278700	-1.25308500
H	-2.95395000	-4.57692600	1.13268900
H	-5.09019600	-3.57490500	0.33896700
C	3.01650400	-2.84905200	-1.17825400

C	2.88827300	-4.24246900	-1.18348300
C	4.29260400	-2.28293800	-1.14414800
C	4.02127800	-5.05298600	-1.15413100
H	1.89534700	-4.67908400	-1.21203400
C	5.42688000	-3.09290500	-1.11575400
H	4.37075600	-1.20032600	-1.13748100
C	5.29411500	-4.48077100	-1.12144100
H	3.91169900	-6.13382300	-1.15706900
H	6.41458700	-2.64125600	-1.08715400
H	6.17652000	-5.11391000	-1.09925800
N	-0.41594200	-1.62154400	-1.24482300
N	0.64810300	-2.55433000	-1.24523500
C	-0.62787800	-1.56386600	-3.63694900
C	-0.59770200	-0.89792200	-4.82999200
C	-0.36227300	0.50991000	-4.85163000
C	-0.18112200	1.15135000	-3.59558100
C	-0.21722800	0.41852200	-2.43699800
N	-0.46262700	-0.90450600	-2.46819900
H	-0.77494000	-2.63480300	-3.54826700
H	-0.74257100	-1.46488500	-5.73927400
H	0.02198700	2.21042300	-3.52275900
H	-0.04633200	0.82577200	-1.44924100
N	-0.30311500	1.19326400	-6.00707000
C	-0.46554400	0.50180700	-7.27957700
H	0.30828900	-0.26157300	-7.41492300

H	-1.45098400	0.02910400	-7.34838400
H	-0.37756600	1.22721500	-8.08625100
C	-0.02966900	2.62478600	-5.99498400
H	-0.80665900	3.16790800	-5.44636000
H	0.94357900	2.83489800	-5.53840400
H	-0.01511900	2.98914600	-7.02046900

1b'

C	1.80138900	-2.10345400	-1.25162700
O	1.99060400	-0.98074700	-1.77191200
C	-1.58593200	-1.94713800	-0.31599900
C	-1.93604300	-3.27253600	-0.60273100
C	-2.56519500	-1.06254400	0.16031600
C	-3.25003600	-3.69496300	-0.41772700
H	-1.17135500	-3.94625600	-0.96825900
C	-3.87299900	-1.50279800	0.34107400
H	-2.31508800	-0.02964700	0.38291100
C	-4.22777600	-2.82028000	0.05431100
H	-3.50760100	-4.72527500	-0.64594400
H	-4.61870400	-0.80450800	0.70988400
H	-5.24921500	-3.15851400	0.19580400
C	2.89794600	-3.14351000	-1.32539700
C	2.79295800	-4.39423400	-0.70634200
C	4.05221800	-2.83730600	-2.04983000
C	3.82716300	-5.32129500	-0.81501600
H	1.89565200	-4.62817600	-0.14312400

C	5.08643600	-3.76520100	-2.16130100
H	4.11604300	-1.86246600	-2.52314200
C	4.97727500	-5.01014400	-1.54252900
H	3.73637200	-6.29002700	-0.33158400
H	5.97715600	-3.51711400	-2.73157000
H	5.78128700	-5.73563800	-1.62791700
N	-0.26919100	-1.49991000	-0.59410100
N	0.71597200	-2.51349500	-0.58664400
C	0.32527200	-0.60365600	1.55406400
C	0.74004000	0.42294400	2.35510700
C	0.97336100	1.71369700	1.79189100
C	0.75994800	1.85383300	0.39304600
C	0.35114100	0.77712000	-0.35167300
N	0.11215100	-0.41140700	0.23293200
H	0.14865600	-1.61229700	1.91173300
H	0.89365300	0.22448900	3.40678600
H	0.93880900	2.78896700	-0.11869200
H	0.20129400	0.79297100	-1.42300900
N	1.38145700	2.74455200	2.55149500
C	1.60259200	2.56033100	3.98015800
H	0.68263400	2.24180800	4.48206900
H	2.38630600	1.81781800	4.16492200
H	1.91919200	3.50727000	4.41327800
C	1.61908200	4.04844500	1.94586800
H	2.40140500	3.99057600	1.18149100

H	0.70353700	4.44205300	1.49088600
H	1.94481500	4.74310800	2.71794000

γ -TS1/2(R)

C	0.42817300	-0.67511100	1.54666600
H	1.36502100	-0.46025500	2.04381700
C	-0.44819100	0.36398000	1.34942400
C	-0.08996000	1.71404300	1.51332300
H	-0.89510600	2.44114900	1.45349900
C	0.22390400	-2.06218400	1.13857100
O	1.29381700	-2.81531600	1.46790700
O	-0.75630800	-2.53102200	0.58300400
C	1.23012600	-4.19677100	1.09255500
C	2.50788200	-4.85333000	1.56377900
H	1.11765100	-4.26202600	0.00585700
H	0.34592200	-4.65038400	1.55353400
H	2.50406700	-5.91081800	1.28303800
H	3.37727000	-4.37528100	1.10431400
H	2.60440900	-4.78499300	2.65129100
C	1.10484900	2.05801200	2.35111400
H	2.02690400	1.69578100	1.87300000
H	1.19135500	3.13857300	2.48432500
H	1.04162600	1.59536400	3.34416100
C	-2.63561300	-0.69213500	1.44433800
C	-3.90408300	-0.91003600	0.98387100
C	-4.34083700	-0.28535800	-0.21820600

C	-3.40696100	0.56739700	-0.86424500
C	-2.15144100	0.74448600	-0.34476500
N	-1.76969400	0.12109800	0.79673000
H	-2.26276100	-1.15069300	2.35178400
H	-4.54478200	-1.57076200	1.55111100
H	-3.64636600	1.07728600	-1.78706100
H	-1.38171000	1.34548400	-0.81984100
N	-5.57514900	-0.48901700	-0.71293600
C	-6.49640300	-1.38933300	-0.03353100
H	-6.08399300	-2.40231100	0.02870100
H	-6.72106200	-1.03277200	0.97781600
H	-7.42815100	-1.43205500	-0.59480500
C	-5.97297700	0.14847400	-1.96121800
H	-5.91734700	1.23917600	-1.87976800
H	-5.33756500	-0.17893300	-2.79139600
H	-7.00253800	-0.12443300	-2.18622000
C	1.23502100	-0.05661100	-1.16477500
N	0.72727100	1.99901200	-0.44718700
N	1.67920600	1.10339200	-0.54730100
O	0.12405900	-0.22971800	-1.67013600
C	2.28520200	-1.13201700	-1.26390800
C	1.96803400	-2.29756200	-1.96583600
C	3.54646500	-1.01014400	-0.66912000
C	2.90170200	-3.32595000	-2.08485800
H	0.98018100	-2.37899700	-2.40918600

C	4.47858500	-2.03762700	-0.78745000
H	3.78215200	-0.10892900	-0.11334900
C	4.15991500	-3.19754300	-1.49684000
H	2.64761900	-4.22709200	-2.63607800
H	5.45536100	-1.93602100	-0.32311600
H	4.88961100	-3.99734600	-1.58841200
C	1.22229800	3.31801500	-0.23998600
C	0.27261700	4.34645900	-0.15581700
C	2.58431600	3.63701600	-0.17932800
C	0.67292900	5.66524700	0.01649400
H	-0.78173800	4.09274000	-0.23204400
C	2.97926400	4.96363100	-0.01157800
H	3.31414900	2.84189200	-0.28027300
C	2.03247700	5.98111000	0.09570400
H	-0.07385800	6.45139700	0.08146300
H	4.03811400	5.20336000	0.03113100
H	2.34782400	7.01199500	0.22507600

γ -2(R)

C	0.49834400	1.94206900	-1.42914600
H	1.41417500	1.95256000	-2.00945200
C	-0.25684400	0.84250900	-1.43468500
C	0.06032400	-0.46533100	-2.13673200
H	-0.86969600	-0.80618300	-2.60292400
C	0.20361400	3.16377500	-0.63531600
O	1.26228300	3.97797400	-0.63440000

O	-0.83993100	3.41707600	-0.07059400
C	1.12882700	5.19860500	0.11926800
C	2.43795800	5.94380200	0.00276000
H	0.89271400	4.94262200	1.15614700
H	0.29125700	5.77065500	-0.29171300
H	2.37481600	6.88314200	0.55898600
H	3.25941800	5.35236400	0.41518300
H	2.66313400	6.17582600	-1.04160500
C	1.10832700	-0.34473300	-3.23888300
H	2.06950500	-0.00933800	-2.84890200
H	1.25939600	-1.33074800	-3.68547800
H	0.75875300	0.34395500	-4.01446000
C	-2.62980000	1.25135200	-1.17974400
C	-3.81466800	1.16184300	-0.50651600
C	-3.85274100	0.56547900	0.78900600
C	-2.61793200	0.09580200	1.30858600
C	-1.46026500	0.21422100	0.58371800
N	-1.47488000	0.78073600	-0.65030500
H	-2.55302200	1.70313300	-2.16238400
H	-4.70428400	1.55273200	-0.98066900
H	-2.54892100	-0.36606800	2.28405800
H	-0.48356300	-0.14585900	0.93276700
N	-5.00094600	0.45580900	1.47650300
C	-6.23785600	1.00251400	0.93517600
H	-6.12384500	2.06574700	0.69987300

H	-6.54776200	0.46555400	0.03142300
H	-7.02259800	0.90255400	1.68298600
C	-5.01298500	-0.20248200	2.77741500
H	-4.60618300	-1.21574100	2.70343600
H	-4.43125100	0.36357000	3.51324400
H	-6.04195700	-0.27143800	3.12608000
C	2.05380500	-1.01450000	0.45724200
N	0.42403900	-1.41383600	-1.09341600
N	1.80588200	-1.40356900	-0.78881100
O	1.23599300	-0.69451300	1.35902800
C	3.53148600	-0.98005100	0.79671100
C	3.91120300	-0.52851700	2.06296000
C	4.52203900	-1.37988500	-0.10766500
C	5.25693600	-0.47152000	2.42270400
H	3.12937400	-0.22746500	2.75317600
C	5.86717600	-1.32487200	0.25114500
H	4.22244200	-1.73384900	-1.08852800
C	6.23943600	-0.86996800	1.51723500
H	5.53956800	-0.11956800	3.41100200
H	6.62787300	-1.64101400	-0.45744900
H	7.28876700	-0.82983600	1.79596300
C	-0.31931200	-2.55575100	-0.84348900
C	-1.68904100	-2.66063000	-1.17719000
C	0.27640400	-3.65101900	-0.18144700
C	-2.40360500	-3.82296800	-0.89952100

H	-2.21865900	-1.82989100	-1.63309800
C	-0.45515800	-4.80005700	0.08993000
H	1.31878700	-3.58186800	0.10407600
C	-1.80003700	-4.90937700	-0.26951300
H	-3.45416300	-3.86828800	-1.17575200
H	0.04008000	-5.62622100	0.59315600
H	-2.36339700	-5.81118800	-0.05326800

γ -TS2/3(RS)

C	-2.39207100	0.27453900	-1.47495000
H	-2.62089400	0.68324200	-2.44966800
C	-1.07100900	0.13968000	-1.12257800
C	0.02110900	0.04474700	-2.19231100
H	-0.10654600	-0.93057000	-2.66559700
C	-3.52189800	0.02460800	-0.60856500
O	-4.68799500	0.28545600	-1.25381000
O	-3.51981900	-0.38468700	0.54653600
C	-5.88525200	0.06863000	-0.50040700
C	-7.05270000	0.44370000	-1.38605600
H	-5.85423700	0.67953300	0.40749200
H	-5.93245400	-0.98151800	-0.19391000
H	-7.99158400	0.29122900	-0.84562400
H	-6.99338900	1.49424600	-1.68389700
H	-7.07033400	-0.17211000	-2.28951700
C	-0.10387400	1.11292600	-3.27824700
H	-0.10697600	2.11188600	-2.83735500

H	0.74807900	1.02391100	-3.95827600
H	-1.01912100	0.98060400	-3.85981500
C	-0.34495800	-1.93690600	-0.08244400
C	-0.04315900	-2.74362700	0.97823800
C	-0.15962000	-2.24428200	2.30594400
C	-0.61853000	-0.90752000	2.43701100
C	-0.90957300	-0.16181800	1.32631600
N	-0.75577600	-0.65620100	0.07611700
H	-0.26363500	-2.29945700	-1.09961400
H	0.29056200	-3.75112800	0.77113000
H	-0.75833300	-0.44468900	3.40397400
H	-1.26092800	0.85751900	1.38401400
N	0.14661500	-2.99999400	3.37408400
C	0.60987300	-4.36954300	3.19369700
H	-0.15164300	-4.98251500	2.69905800
H	1.53081400	-4.39656200	2.60203100
H	0.81745700	-4.80468400	4.16977800
C	-0.01308800	-2.45970200	4.71781500
H	0.59773100	-1.56080300	4.85243000
H	-1.06098500	-2.21328900	4.92165100
H	0.31345400	-3.20576100	5.43992900
C	0.87475400	1.90758700	-0.31046700
N	1.33353300	0.03348600	-1.56333700
N	1.77016600	1.10710200	-0.80385000
O	-0.41975900	1.80569700	-0.42421300

C	1. 38829900	3. 06698700	0. 48623000
C	2. 76005500	3. 32000100	0. 61728900
C	0. 47540400	3. 90828000	1. 12879200
C	3. 20570000	4. 38735200	1. 38977300
H	3. 46540000	2. 67381200	0. 10509200
C	0. 92462200	4. 97923900	1. 90113300
H	-0. 58578500	3. 71401000	1. 01006700
C	2. 28994800	5. 22074000	2. 03660500
H	4. 27141500	4. 57492700	1. 48486600
H	0. 20548500	5. 62685600	2. 39454200
H	2. 64003300	6. 05519100	2. 63725700
C	2. 28927800	-0. 93835200	-1. 83206000
C	2. 14735800	-1. 88418000	-2. 86916400
C	3. 44624000	-1. 01365900	-1. 02585100
C	3. 10757300	-2. 87710100	-3. 05877500
H	1. 31322900	-1. 84014100	-3. 56057500
C	4. 39536700	-2. 00455600	-1. 23846200
H	3. 57504000	-0. 28696700	-0. 23445400
C	4. 23726700	-2. 95593800	-2. 24861200
H	2. 96942100	-3. 58777500	-3. 86898400
H	5. 27210400	-2. 03448300	-0. 59716300
H	4. 98276200	-3. 72799200	-2. 40743200
γ-3(RS)			
C	-1. 94261400	-0. 13126100	-1. 90571000
H	-1. 94133200	-0. 23210900	-2. 98097400

C	-0.70717800	0.19747300	-1.21672600
C	0.55141400	0.17506900	-2.11577800
H	0.64894200	-0.81596400	-2.55843600
C	-3.13357300	-0.22826400	-1.17428800
O	-4.23047000	-0.52412100	-1.95683900
O	-3.27516500	-0.09299500	0.05479400
C	-5.47231600	-0.62176200	-1.26979500
C	-6.53799700	-0.94150700	-2.29740000
H	-5.68722500	0.32232400	-0.75619500
H	-5.41245200	-1.40302100	-0.50354100
H	-7.51507000	-1.02707100	-1.81175800
H	-6.59616800	-0.15369800	-3.05412000
H	-6.32029800	-1.88742700	-2.80233300
C	0.47347400	1.22221200	-3.22731500
H	0.33581300	2.22198700	-2.80743000
H	1.40703800	1.21251000	-3.79731200
H	-0.35605800	1.01765000	-3.90618200
C	-0.04768500	-2.03030500	-0.27872400
C	0.13377900	-2.96031300	0.70780200
C	-0.13674200	-2.61883600	2.06277400
C	-0.61957300	-1.30739100	2.29115200
C	-0.77143100	-0.43185400	1.24294600
N	-0.45755700	-0.76996600	-0.02342500
H	0.11449700	-2.28472800	-1.31841800
H	0.47119400	-3.94741600	0.42303900

H	-0.89693900	-0.96523500	3.27840800
H	-1.17038300	0.56136200	1.38968400
N	0.04669800	-3.49928500	3.06504000
C	0.53732000	-4.84010800	2.78105100
H	-0.17271400	-5.40393600	2.16492200
H	1.50313100	-4.80127100	2.26657200
H	0.67421300	-5.37117300	3.72165300
C	-0.29801400	-3.12908000	4.43048900
H	0.28486100	-2.26259500	4.76098000
H	-1.36473900	-2.89464400	4.51983700
H	-0.07237500	-3.96557300	5.08971100
C	0.46545700	1.92396200	-0.07813000
N	1.69314100	0.40392400	-1.24494100
N	1.61433100	1.41569400	-0.33556200
O	-0.72129100	1.49563400	-0.59062500
C	0.33392600	3.05573700	0.86275100
C	1.47332400	3.68006400	1.38764500
C	-0.93705800	3.49747300	1.24782900
C	1.33879400	4.72595100	2.29256400
H	2.45514400	3.34104700	1.07356500
C	-1.06371100	4.55074700	2.15262200
H	-1.81942400	3.01783300	0.83570400
C	0.06993500	5.16470000	2.67948000
H	2.22610700	5.20489100	2.69555900
H	-2.05313700	4.88829900	2.44557400

H	-0.03106500	5.98351600	3.38537000
C	2.94317200	-0.18730500	-1.43001500
C	3.22102200	-0.96496400	-2.56702200
C	3.94823400	-0.02554300	-0.45872800
C	4.46441200	-1.57816100	-2.71001000
H	2.48681900	-1.07779400	-3.35668800
C	5.18496600	-0.63595800	-0.62528100
H	3.74053500	0.57442500	0.41867900
C	5.45734900	-1.42198500	-1.74635800
H	4.65747300	-2.17094900	-3.59956400
H	5.94518300	-0.49813400	0.13832700
H	6.42542500	-1.89655600	-1.86799300

γ -TS3/P(RS)

C	1.72691100	-0.22256300	-2.01583000
H	1.59372600	0.14441000	-3.02504600
C	0.57668000	-0.48299700	-1.24238200
C	-0.74413800	-0.64801900	-1.99782200
H	-0.89910400	0.24301300	-2.61152500
C	3.03504200	-0.29891100	-1.47166900
O	3.99921500	-0.04623700	-2.41447000
O	3.36091900	-0.54807400	-0.30680300
C	5.34762600	-0.10174900	-1.95384600
C	6.24769600	0.15241200	-3.14429900
H	5.54180000	-1.08320200	-1.50851800
H	5.49858800	0.65057300	-1.17149700

H	6.04676500	1.13410000	-3.58309900
H	7.29629500	0.12260900	-2.83267800
H	6.09538000	-0.60812800	-3.91548300
C	-0.70344300	-1.89333700	-2.88874000
H	-0.45764900	-2.77700200	-2.29264900
H	-1.68379200	-2.04815700	-3.34865100
H	0.04869000	-1.78802600	-3.67241300
C	-0.52396400	1.93316000	-0.43830200
C	-0.55346600	3.09263400	0.30382900
C	0.25647400	3.20438400	1.46355500
C	1.05801300	2.07949600	1.78029400
C	1.02569400	0.96314900	0.97367100
N	0.24321300	0.88160300	-0.11636500
H	-1.14651200	1.83863500	-1.32236100
H	-1.20691400	3.89354200	-0.01529300
H	1.71034700	2.07010100	2.64314300
H	1.65481400	0.10084300	1.16945800
N	0.26119100	4.32318900	2.22469000
C	-0.56792600	5.45873700	1.85552100
H	-0.28867600	5.85202800	0.87098200
H	-1.62961600	5.18694700	1.83896100
H	-0.43157000	6.25042800	2.59091800
C	1.11311700	4.39646700	3.40058700
H	0.84955100	3.62217800	4.13029200
H	2.17028400	4.28289200	3.13352100

H	0.98201300	5.36913300	3.87221100
C	-0.40403100	-1.77457600	0.44162200
N	-1.81397700	-0.73260800	-1.01467300
N	-1.59587600	-1.42294300	0.13757400
O	0.71245700	-1.48845800	-0.28890800
C	-0.10999200	-2.54038100	1.66794400
C	1.22078300	-2.76967000	2.03729000
C	-1.14965800	-3.02588700	2.47110600
C	1.50344600	-3.47768600	3.20467000
H	2.02372900	-2.39226200	1.40983300
C	-0.85835400	-3.72621600	3.63556400
H	-2.17807000	-2.85165100	2.17091700
C	0.46911100	-3.95452500	4.00658800
H	2.53734100	-3.65463300	3.48529600
H	-1.66810300	-4.10007100	4.25495000
H	0.69308800	-4.50585900	4.91487200
C	-3.13048400	-0.36057500	-1.29110700
C	-3.49530700	0.12275800	-2.55989600
C	-4.11684100	-0.44472800	-0.29109900
C	-4.80820600	0.51949500	-2.80813800
H	-2.77540200	0.17096400	-3.36895300
C	-5.42118800	-0.05173600	-0.56191700
H	-3.84340400	-0.81271200	0.68959800
C	-5.78350300	0.43616500	-1.81875200
H	-5.06609000	0.88360900	-3.79851600

H	-6.16525600	-0.12752800	0.22602400
H	-6.80537200	0.73888900	-2.02207000
γ-P(R)			
C	1.92151700	-1.56554200	0.17955100
H	1.85882900	-2.63413800	0.34503900
C	0.79443300	-0.84417000	0.27488000
C	-0.54486600	-1.41919400	0.65045600
H	-0.52796000	-2.48706900	0.43316200
C	3.25079100	-1.00107300	-0.10444500
O	4.17954700	-1.97674300	-0.09668300
O	3.51823600	0.16363800	-0.31223200
C	5.53336500	-1.56074300	-0.33999900
C	6.40975000	-2.78602500	-0.21450600
H	5.80109800	-0.78983300	0.38888700
H	5.59134200	-1.11650400	-1.33862900
H	7.45275600	-2.51431300	-0.39949200
H	6.33678700	-3.21452700	0.78881300
H	6.11811900	-3.54884100	-0.94150100
C	-0.85375600	-1.18784600	2.13537000
H	-0.84821500	-0.12205700	2.38257400
H	-1.84167200	-1.59327600	2.37197500
H	-0.10845400	-1.69028300	2.75703900
C	-0.38232200	1.16324500	-0.04312500
N	-1.53272600	-0.77902800	-0.23047700
N	-1.50883400	0.59329200	-0.21641700

O	0.80876200	0.49902900	0.11709300
C	-0.22071200	2.62826400	-0.05842300
C	1.05788000	3.19552800	-0.05057700
C	-1.35229600	3.45296000	-0.08616600
C	1.19764900	4.58214000	-0.07153100
H	1.93177700	2.55168600	-0.03856300
C	-1.20290600	4.83402400	-0.10695300
H	-2.33924200	3.00167100	-0.09001300
C	0.07255800	5.40328300	-0.09874600
H	2.19143200	5.01912500	-0.06882700
H	-2.08290300	5.46942600	-0.12678300
H	0.18658700	6.48289100	-0.11394300
C	-2.83549600	-1.34439700	-0.26851900
C	-2.97089100	-2.70918400	-0.55276200
C	-3.97909600	-0.57167500	-0.04436400
C	-4.23316100	-3.29208000	-0.59354800
H	-2.09303600	-3.31028300	-0.76839900
C	-5.23850000	-1.16597300	-0.09806600
H	-3.87411900	0.48551900	0.16667000
C	-5.37628000	-2.52613000	-0.36547400
H	-4.32169100	-4.35036700	-0.82044500
H	-6.11893000	-0.55556800	0.08066800
H	-6.35991900	-2.98295500	-0.40371500
γ-TS2/4(RS)			
C	-0.32551500	0.42687400	1.63429700

H	-1.14835200	0.50651100	2.33473300
C	0.58588900	-0.61558200	1.85130900
C	-0.17250100	-1.90004600	1.72365600
H	0.52516900	-2.73007700	1.57133500
C	0.10872700	1.76460500	1.09992000
O	-0.57790300	2.75601900	1.67115600
O	0.94994400	1.93457400	0.24533100
C	-0.37721800	4.06312300	1.09984400
C	-1.24677500	5.03153100	1.86601600
H	-0.65142400	4.01247900	0.03993700
H	0.68403400	4.31981000	1.16961600
H	-1.14113000	6.03321000	1.43959500
H	-2.29830200	4.73895700	1.80365300
H	-0.95537700	5.07029500	2.91939500
C	-1.08946000	-2.20718700	2.90918600
H	-1.81148800	-1.40099500	3.06902100
H	-1.65648600	-3.12593500	2.73923200
H	-0.49558800	-2.32754700	3.81909900
C	2.97135800	-0.22467200	1.66744900
C	4.16691500	-0.14322300	1.00069600
C	4.22819400	-0.45185600	-0.38500800
C	3.00549700	-0.83348900	-0.99719500
C	1.84553000	-0.87589800	-0.26713000
N	1.82067400	-0.58361300	1.05882600
H	2.88034000	-0.00438300	2.72417400

H	5.04327700	0.15489300	1.56006000
H	2.94556000	-1.07523300	-2.04974300
H	0.89321300	-1.13916600	-0.72104800
N	5.38137600	-0.38413400	-1.07794000
C	6.61152200	0.01660600	-0.41183300
H	6.52759500	1.02925200	-0.00164600
H	6.86635300	-0.67544700	0.39868800
H	7.42317500	0.00766500	-1.13720900
C	5.39813600	-0.69658700	-2.50053300
H	5.08320600	-1.73015600	-2.68178800
H	4.74131600	-0.02209300	-3.06055700
H	6.41361000	-0.57747200	-2.87479500
C	-1.32272800	0.08399700	-0.98960100
N	-0.95781400	-1.72646600	0.43111000
N	-1.41266900	-0.39480100	0.28801000
O	-0.87848100	-0.52680400	-1.96690900
C	-1.92444900	1.45500200	-1.16413900
C	-1.55488200	2.20932400	-2.28259400
C	-2.87086000	1.96908000	-0.27137200
C	-2.11645700	3.46425700	-2.50213300
H	-0.82811400	1.79183700	-2.97243600
C	-3.44224300	3.22087200	-0.49821200
H	-3.16662800	1.37483200	0.58769400
C	-3.06510400	3.97172400	-1.61102100
H	-1.82255200	4.04508900	-3.37147200

H	-4.18904000	3.60506900	0.19065400
H	-3.51421700	4.94496800	-1.78801900
C	-1.85096600	-2.73075400	0.04960700
C	-1.51828300	-4.08303100	0.27535900
C	-3.05972600	-2.45444800	-0.61379800
C	-2.36482300	-5.10494100	-0.13590700
H	-0.58752000	-4.33709700	0.77163000
C	-3.89766300	-3.49021900	-1.02079800
H	-3.34316800	-1.42846100	-0.81300300
C	-3.56584500	-4.82274200	-0.78861500
H	-2.07775500	-6.13541000	0.05558000
H	-4.82376500	-3.24271400	-1.53248200
H	-4.22301000	-5.62381700	-1.11126500

γ -4(RS)

C	-0.23409700	0.31373100	0.25423900
H	-0.12265600	0.80874600	1.23135200
C	0.62974200	-0.87954400	0.05639000
C	-0.16740000	-2.12100200	-0.13420800
H	0.16819400	-2.70780800	-1.00229600
C	-0.00755700	1.39121600	-0.83712700
O	0.43988600	2.53601600	-0.31093100
O	-0.20243100	1.21515500	-2.01436400
C	0.67365300	3.60801700	-1.24542500
C	1.13507600	4.80883100	-0.45407700
H	-0.26116600	3.80322700	-1.78028300

H	1.42343900	3.27791100	-1.97134900
H	1.31928700	5.64534100	-1.13403300
H	0.37317400	5.11155400	0.26974200
H	2.06298500	4.59188100	0.08295200
C	-0.16873500	-3.00956300	1.12351400
H	-0.66495100	-2.48517000	1.94663700
H	-0.68066400	-3.96222200	0.95736400
H	0.86066900	-3.22277800	1.43019800
C	2.68477900	0.30880900	0.39037300
C	4.06157000	0.36061500	0.38181700
C	4.85501000	-0.75409300	0.06179300
C	4.12556600	-1.92693400	-0.20201400
C	2.74962800	-1.95933300	-0.18993400
N	1.97511700	-0.84189900	0.08323700
H	2.09719300	1.17575900	0.65587300
H	4.50240000	1.31624300	0.63854700
H	4.62068900	-2.86285600	-0.42927900
H	2.20951200	-2.86852800	-0.40722400
N	6.24961300	-0.69822900	-0.01238200
C	6.90014800	0.39562100	0.68529100
H	6.58016200	1.35800300	0.27754000
H	6.69943800	0.38862800	1.76969900
H	7.97743800	0.32043900	0.52893100
C	6.95718200	-1.96471900	0.02593000
H	6.75470300	-2.53779700	0.94630000

H	6.69006900	-2.58256600	-0.83574900
H	8.02897200	-1.76977500	-0.03410200
C	-2.62423200	0.52745600	-0.33683400
N	-1.50022700	-1.56482700	-0.48492300
N	-1.58686400	-0.27147500	0.13383300
O	-3.48980500	0.11270300	-1.08360100
C	-2.64421000	1.92821400	0.20116400
C	-2.95469600	2.96042800	-0.68796200
C	-2.39214800	2.21408400	1.54567300
C	-2.98069900	4.27810600	-0.23960500
H	-3.16346600	2.71791900	-1.72603900
C	-2.43884800	3.53181000	1.99551500
H	-2.17416300	1.40564800	2.23882500
C	-2.72249900	4.56440500	1.10199700
H	-3.20797400	5.08147500	-0.93403300
H	-2.25450400	3.75255900	3.04240200
H	-2.75001200	5.59207400	1.45225300
C	-2.59091600	-2.43728100	-0.20316400
C	-2.68710300	-3.57797100	-1.00743500
C	-3.52206800	-2.23510800	0.81736700
C	-3.68562300	-4.51748100	-0.77864900
H	-1.97707200	-3.70985700	-1.81879500
C	-4.53184300	-3.17398800	1.02914400
H	-3.46428400	-1.34800600	1.43975900
C	-4.61692300	-4.32049200	0.24231400

H	-3.74583100	-5.39825300	-1.41109100
H	-5.25757700	-3.00403100	1.81916800
H	-5.40522600	-5.04676200	0.41301200

γ -TS2/5(RS)

C	0.88387300	-1.30043300	0.88428200
H	1.75371500	-1.17976400	1.52738500
C	-0.27827500	-0.70706800	1.42037700
C	-0.13275100	0.74698600	1.80678900
H	-1.09255700	1.09632800	2.19526700
C	0.78942700	-2.71099900	0.35986600
O	1.76568800	-3.47619200	0.86304700
O	-0.05094900	-3.12412400	-0.40785400
C	1.76035700	-4.85566900	0.45452200
C	2.93420600	-5.53186200	1.12433600
H	1.83037400	-4.89828100	-0.63649600
H	0.80665500	-5.30312500	0.75139500
H	2.95802000	-6.58809200	0.84147700
H	3.87666200	-5.07057600	0.81740900
H	2.85194900	-5.46706000	2.21259000
C	0.90909500	1.02076400	2.89333200
H	1.91714000	0.71757000	2.60182200
H	0.94174800	2.09314000	3.11197600
H	0.63508100	0.48177400	3.80396600
C	-2.64878500	-1.21528000	1.30948800
C	-3.86705300	-1.30953500	0.68553900

C	-3.96652300	-1.07791300	-0.71318600
C	-2.76225800	-0.73685600	-1.38027900
C	-1.58404000	-0.64626400	-0.68106500
N	-1.51502800	-0.88828800	0.65174100
H	-2.52227000	-1.40239300	2.36962100
H	-4.72760400	-1.57952900	1.28232600
H	-2.73727200	-0.53720200	-2.44289800
H	-0.64424400	-0.38464700	-1.15058800
N	-5.14104000	-1.18212100	-1.36787500
C	-6.35197800	-1.53623900	-0.64323000
H	-6.25944600	-2.52394500	-0.17766700
H	-6.58049200	-0.79785400	0.13360000
H	-7.18566200	-1.56502000	-1.34265700
C	-5.19959200	-0.93891500	-2.80215600
H	-4.90727100	0.08980800	-3.04129800
H	-4.54557800	-1.62940900	-3.34601900
H	-6.22163100	-1.09354900	-3.14461200
C	2.02291300	0.63646800	-0.32937400
N	0.11754300	1.58377500	0.58860700
N	1.46224700	1.67787000	0.18214800
O	1.50013500	-0.57118600	-0.51329300
C	3.43895300	0.79155200	-0.79066600
C	4.17071500	-0.34042900	-1.16094500
C	4.05191000	2.05000600	-0.84649500
C	5.49715900	-0.21819800	-1.57508300

H	3.68986700	-1.31222100	-1.12036600
C	5.37203500	2.17029700	-1.26598800
H	3.48122800	2.92481500	-0.55398800
C	6.10144900	1.03531500	-1.62848500
H	6.05778000	-1.10512000	-1.85537500
H	5.83674100	3.15108900	-1.30814300
H	7.13396600	1.13082700	-1.95156900
C	-0.55159500	2.82561500	0.52711600
C	-1.94578800	2.85994600	0.71935200
C	0.10664800	4.02686800	0.22088900
C	-2.64440900	4.05995300	0.64960300
H	-2.48752200	1.93434300	0.89748700
C	-0.60656100	5.22193000	0.14909400
H	1.17342300	4.01095900	0.04084000
C	-1.98187800	5.25570300	0.36836600
H	-3.72026100	4.05575300	0.80181300
H	-0.07147000	6.13942900	-0.08049900
H	-2.52962900	6.19085200	0.30966200

γ -5(RS)

C	0.79336600	1.44839200	-0.77824900
H	1.59218200	1.51453000	-1.52180100
C	-0.34525500	0.74123500	-1.36941900
C	-0.01716500	-0.66340900	-1.79245600
H	-0.92903800	-1.13009900	-2.17636500
C	0.42386800	2.84967800	-0.33403600

O	0.86509400	3.77272200	-1.19680100
O	-0.21645900	3.11600600	0.65883400
C	0.47281900	5.12940400	-0.92546100
C	1.04625300	5.99486800	-2.02387500
H	0.85211600	5.41550000	0.06043800
H	-0.62019800	5.17834000	-0.89557300
H	0.76728900	7.03845200	-1.85242800
H	2.13750300	5.92848200	-2.04165900
H	0.66247400	5.68838100	-3.00062400
C	1.04239100	-0.76702400	-2.89132700
H	2.00464300	-0.34385400	-2.59019400
H	1.21281300	-1.81804100	-3.14830000
H	0.69847400	-0.23511900	-3.78173300
C	-2.75488400	0.87153300	-1.09462200
C	-3.94142800	0.75660600	-0.41313600
C	-3.93556800	0.47258000	0.97851900
C	-2.66092000	0.31650100	1.57700000
C	-1.52004700	0.42146100	0.81830300
N	-1.54784000	0.70144500	-0.50921700
H	-2.71204600	1.11261400	-2.15015500
H	-4.86228100	0.90870400	-0.95996100
H	-2.54950500	0.10626000	2.63203900
H	-0.53843500	0.29758600	1.25182000
N	-5.07792400	0.36314600	1.68996700
C	-6.36399800	0.56210100	1.04090700

H	-6.44284900	1.56935200	0.61583400
H	-6.52370300	-0.17250800	0.24341500
H	-7.15428500	0.44026100	1.78001300
C	-5.02107500	0.07832300	3.11582600
H	-4.51954600	-0.87660600	3.30766100
H	-4.49307600	0.87082700	3.65855000
H	-6.03654500	0.01410400	3.50354800
C	2.09711900	-0.31652800	0.33843200
N	0.36422800	-1.54415600	-0.61740600
N	1.66348400	-1.42120500	-0.13814100
O	1.45085300	0.86802300	0.44688300
C	3.45942800	-0.30288100	0.94502700
C	4.06882800	0.91272100	1.27028200
C	4.14395600	-1.49980400	1.19769100
C	5.34559100	0.93302300	1.83082300
H	3.53518500	1.83887600	1.08640700
C	5.41373000	-1.47618500	1.76199200
H	3.66500200	-2.44135500	0.95040900
C	6.02187300	-0.25890600	2.07805100
H	5.80999700	1.88377400	2.07547900
H	5.93278300	-2.40986600	1.95763500
H	7.01493600	-0.24269300	2.51730800
C	-0.01856100	-2.90565800	-0.74718900
C	-1.38684100	-3.20019300	-0.85929900
C	0.89998500	-3.96317100	-0.74277900

C	-1.81952700	-4.51520900	-0.99230300
H	-2.11089400	-2.38954300	-0.81632800
C	0.45509100	-5.27833600	-0.86852700
H	1.95557200	-3.74341900	-0.63996700
C	-0.90189000	-5.56674100	-0.99926300
H	-2.88332100	-4.72008900	-1.07434800
H	1.18371000	-6.08452800	-0.86867000
H	-1.24133100	-6.59322300	-1.09566900

γ -TS1/2(S)

C	0.21556400	0.79758200	1.52362500
H	1.16301800	0.91184400	2.03357000
C	-0.25803400	-0.47681000	1.32891500
C	0.53478100	-1.62529600	1.51072000
H	0.02481100	-2.58252100	1.44487700
C	-0.42592800	2.03286300	1.08208200
O	0.34184400	3.09793800	1.39727100
O	-1.49606100	2.14072700	0.50540100
C	-0.14474100	4.38538700	0.99523900
C	-1.11784500	4.94413000	2.01658100
H	-0.60727000	4.30173200	0.00907900
H	0.75074500	5.00554700	0.91722100
H	-0.64814500	5.00953600	3.00224000
H	-1.43195600	5.94915900	1.71803300
H	-2.00784300	4.31348000	2.08799200
C	1.75253200	-1.54063100	2.38180000

H	2.20272100	-2.52567100	2.52172600
H	2.50543400	-0.88027900	1.92789800
H	1.50609300	-1.13361600	3.37056300
C	-1.70884600	-1.43200000	-0.37455200
C	-2.94364400	-1.69424600	-0.90727800
C	-4.11738300	-1.18315600	-0.29147800
C	-3.93202800	-0.42228600	0.89699700
C	-2.67123900	-0.20285600	1.37651900
N	-1.57447300	-0.69793700	0.75735800
H	-0.77575400	-1.74717300	-0.83220200
H	-2.98667400	-2.26891300	-1.82200600
H	-4.76549300	0.00222600	1.43900600
H	-2.48586800	0.36901700	2.27718100
N	-5.34176000	-1.41077300	-0.79996200
C	-5.49279100	-2.20346400	-2.01289700
H	-5.00852800	-1.71744000	-2.86703400
H	-5.06480100	-3.20273300	-1.88257700
H	-6.55340000	-2.31194700	-2.23214300
C	-6.51683600	-0.82314900	-0.17161600
H	-6.65521700	-1.20681100	0.84522500
H	-6.43667100	0.26843400	-0.13314800
H	-7.39659800	-1.08186400	-0.75827500
C	1.22314000	0.47703800	-1.16464200
N	1.43971600	-1.62104700	-0.42218400
N	2.02560100	-0.45096800	-0.51965900

O	0.12753900	0.25353500	-1.68405500
C	1.84186300	1.84690400	-1.26978100
C	1.14990300	2.82699900	-1.98664100
C	3.06165700	2.17156200	-0.66539800
C	1.67318600	4.11295900	-2.10965600
H	0.20016300	2.55914000	-2.43933900
C	3.58206600	3.45781700	-0.78467000
H	3.58869900	1.41043700	-0.10017900
C	2.89087400	4.43143700	-1.50854300
H	1.12954400	4.86759200	-2.67126800
H	4.52874100	3.70276100	-0.31194100
H	3.30036700	5.43330600	-1.60179700
C	2.35849600	-2.68445700	-0.18979700
C	1.82848700	-3.98146300	-0.13296300
C	3.74270600	-2.50485200	-0.07801500
C	2.66155200	-5.07647600	0.06028000
H	0.75570500	-4.11419500	-0.24816100
C	4.57318600	-3.60818600	0.11313100
H	4.14709100	-1.50247800	-0.15711000
C	4.04150300	-4.89463200	0.19041700
H	2.23767600	-6.07554100	0.10056400
H	5.64607200	-3.46014400	0.19684700
H	4.69408400	-5.74971700	0.33710200
γ-2(S)			
C	-2.35468300	-1.11295200	-1.28504300

H	-2.32333200	-1.83966500	-2.08711300
C	-1.26178700	-0.37554500	-1.04478500
C	-0.03566500	-0.38077600	-1.96971100
H	-0.31965200	0.24702500	-2.81713200
C	-3.65422000	-1.00438300	-0.58690500
O	-4.52030000	-1.89290400	-1.09652100
O	-3.95129800	-0.22482900	0.29591200
C	-5.84597200	-1.88315600	-0.53725300
C	-6.65014900	-2.93329100	-1.26837900
H	-6.27069000	-0.88240500	-0.66028400
H	-5.77575400	-2.09350600	0.53427800
H	-7.66967600	-2.95538400	-0.87368600
H	-6.69860100	-2.71083700	-2.33770000
H	-6.20703100	-3.92401300	-1.13734400
C	0.23264000	-1.77079400	-2.56012700
H	-0.55527100	-2.04381700	-3.26624700
H	1.17919900	-1.73976800	-3.10404600
H	0.29280700	-2.52717600	-1.77561100
C	-1.39057300	0.10415500	1.32371500
C	-1.27571700	0.94230900	2.39640700
C	-0.96724500	2.31678400	2.20558900
C	-0.82831300	2.75578100	0.85801600
C	-0.95840000	1.86017200	-0.16452600
N	-1.24145200	0.55387100	0.05280900
H	-1.57424600	-0.95431700	1.42943200

H	-1.39430300	0.51714000	3.38304700
H	-0.59957300	3.78251600	0.60755400
H	-0.84866800	2.16801100	-1.19664600
N	-0.80946800	3.15608300	3.24094200
C	-0.94638700	2.66311900	4.60580100
H	-1.94145400	2.23689100	4.76940000
H	-0.19015400	1.90167100	4.82597300
H	-0.81234400	3.49306300	5.29673800
C	-0.45056000	4.54972900	3.00782200
H	0.48840300	4.62322600	2.44947900
H	-1.23893700	5.07104600	2.45427200
H	-0.31863000	5.04628900	3.96757400
C	1.65307100	-1.46753000	0.11397600
N	1.15040200	0.22267100	-1.36955600
N	2.11550000	-0.63536600	-0.79523700
O	0.45919100	-1.60302900	0.51463800
C	2.70953100	-2.37822600	0.70046400
C	2.33361700	-3.25628900	1.71999800
C	4.04224500	-2.37092700	0.27010900
C	3.26843300	-4.10787000	2.30772200
H	1.29539000	-3.25445000	2.03645400
C	4.97679100	-3.22149200	0.85580500
H	4.33153100	-1.69709300	-0.52980600
C	4.59415400	-4.09299300	1.87751300
H	2.96104300	-4.78455400	3.10041100

H	6.00751400	-3.20822800	0.51234800
H	5.32432500	-4.75761100	2.33066200
C	1.70535300	1.37610200	-1.92952100
C	1.02933600	2.20998900	-2.84922100
C	2.99479900	1.79060000	-1.52141200
C	1.61678900	3.37839800	-3.33216600
H	0.03727300	1.97436700	-3.21679000
C	3.56304700	2.95845000	-2.01315300
H	3.53344900	1.17164400	-0.81669700
C	2.88743300	3.77176000	-2.92514000
H	1.05944500	3.98175400	-4.04398900
H	4.55800700	3.23572600	-1.67476000
H	3.33889600	4.68100500	-3.30827400

γ -TS2/3(SR)

C	2.39180000	0.27628300	-1.47468400
H	2.62048300	0.68582300	-2.44908300
C	1.07077900	0.14086000	-1.12228800
C	-0.02143600	0.04662500	-2.19201800
H	0.10644700	-0.92820300	-2.66624400
C	3.52170000	0.02606800	-0.60850400
O	4.68773500	0.28740800	-1.25369300
O	3.51975200	-0.38380600	0.54639900
C	5.88508400	0.07051100	-0.50046300
C	7.05237100	0.44629600	-1.38602200
H	5.93257600	-0.97977700	-0.19447600

H	5.85398500	0.68097700	0.40773000
H	7.99135900	0.29346600	-0.84587100
H	7.06986100	-0.16885300	-2.28993700
H	6.99295900	1.49705700	-1.68308400
C	0.10307100	1.11585700	-3.27696500
H	1.01854500	0.98469200	-3.85842500
H	-0.74865300	1.02684300	-3.95728200
H	0.10534800	2.11444900	-2.83523400
C	0.90927300	-0.16318900	1.32633800
C	0.61857000	-0.91020400	2.43624200
C	0.16041000	-2.24708900	2.30379100
C	0.04441000	-2.74515400	0.97556700
C	0.34593600	-1.93719100	-0.08425400
N	0.75592000	-0.65639500	0.07562500
H	1.26007400	0.85627600	1.38511500
H	0.75805900	-0.44828200	3.40368600
H	-0.28869900	-3.75263500	0.76736700
H	0.26510100	-2.29875600	-1.10181100
N	-0.14547500	-3.00405200	3.37114800
C	0.01388100	-2.46496200	4.71540300
H	-0.31254900	-3.21176500	5.43679300
H	1.06167800	-2.21842700	4.91960700
H	-0.59722900	-1.56637200	4.85076500
C	-0.60796300	-4.37367600	3.18936200
H	-1.52899000	-4.40060900	2.59782300

H	0.15383800	-4.98566200	2.69394400
H	-0.81510300	-4.81001600	4.16500400
C	-0.87522800	1.90790000	-0.30893900
N	-1.33373600	0.03449700	-1.56283800
N	-1.77060300	1.10788500	-0.80313900
O	0.41933200	1.80576500	-0.42215500
C	-1.38880900	3.06707100	0.48806300
C	-0.47596600	3.90833300	1.13073400
C	-2.76059000	3.31982700	0.61936000
C	-0.92526200	4.97904000	1.90337900
H	0.58524000	3.71423400	1.01188200
C	-3.20631000	4.38691300	1.39216700
H	-3.46588900	2.67364100	0.10709800
C	-2.29060800	5.22028900	2.03908300
H	-0.20616500	5.62664500	2.39686100
H	-4.27204400	4.57427700	1.48746200
H	-2.64075200	6.05452500	2.64000000
C	-2.28931300	-0.93741100	-1.83189600
C	-2.14712200	-1.88313400	-2.86905900
C	-3.44641300	-1.01293000	-1.02590000
C	-3.10723400	-2.87609200	-3.05897500
H	-1.31284900	-1.83903100	-3.56028600
C	-4.39542700	-2.00387100	-1.23880200
H	-3.57540600	-0.28637300	-0.23441100
C	-4.23708500	-2.95510800	-2.24904900

H	-2.96885200	-3.58667000	-3.86923100
H	-5.27226600	-2.03395300	-0.59765100
H	-4.98249900	-3.72719000	-2.40811200

γ -3(SR)

C	1.80450500	0.15525400	-1.97209000
H	1.74347100	0.07074000	-3.04702700
C	0.58414900	0.28463600	-1.19444100
C	-0.71263500	0.12156800	-2.02034300
H	-0.70441500	-0.86181900	-2.48991900
C	3.04445600	0.21370400	-1.32387100
O	4.11526700	0.08861800	-2.18500600
O	3.25017200	0.34549200	-0.10335900
C	5.40376200	0.16071900	-1.58669000
C	6.42760600	-0.00248200	-2.69080500
H	5.50731000	-0.62536200	-0.83021700
H	5.52211500	1.12359300	-1.07632300
H	7.43899800	0.05124900	-2.27589800
H	6.30916100	-0.96862000	-3.19035900
H	6.31982800	0.78745500	-3.43985200
C	-0.83849300	1.19919600	-3.09867100
H	-0.04802000	1.10748300	-3.84532100
H	-1.80714500	1.09721900	-3.59692300
H	-0.77951900	2.19794800	-2.65826500
C	0.92569100	-0.41565300	1.21890400
C	1.01030000	-1.34353200	2.22910600

C	0.71895000	-2.70555500	1.97445800
C	0.36256600	-3.03080300	0.63535600
C	0.30795700	-2.04775000	-0.31397800
N	0.55201900	-0.75002400	-0.03225700
H	1.17771200	0.62198600	1.38331200
H	1.32339700	-0.99910900	3.20486800
H	0.14997600	-4.04647500	0.33156400
H	0.08807700	-2.28729700	-1.34656700
N	0.78845400	-3.64475300	2.93698300
C	1.21951300	-3.27736100	4.27813400
H	1.24755200	-4.17174000	4.89819200
H	2.22268200	-2.83760300	4.26109300
H	0.52517700	-2.56207200	4.73262800
C	0.47609900	-5.03363000	2.63134700
H	-0.53672600	-5.12816400	2.22602900
H	1.18841200	-5.45354500	1.91185400
H	0.52968400	-5.61652100	3.54927800
C	-0.73564000	1.81460500	0.06227200
N	-1.82077300	0.16996200	-1.07939900
N	-1.82478200	1.17544800	-0.15612000
O	0.46960000	1.54757900	-0.51185200
C	-0.70353500	2.94960500	1.00812600
C	0.51995100	3.52896800	1.36150600
C	-1.89268900	3.45328600	1.55230700
C	0.55095100	4.59722500	2.25704800

H	1.44006400	3.14509500	0.93189400
C	-1.85331100	4.51617400	2.44634700
H	-2.83840700	3.00819800	1.26030300
C	-0.63143300	5.09256500	2.80178700
H	1.50392300	5.04310900	2.52528200
H	-2.77884500	4.90344400	2.86166400
H	-0.60457900	5.92688400	3.49627200
C	-3.03248900	-0.49403200	-1.28675300
C	-3.25927700	-1.25985200	-2.44284900
C	-4.05036500	-0.41465100	-0.31887800
C	-4.46554900	-1.93844700	-2.60897500
H	-2.51733100	-1.31658200	-3.23118500
C	-5.24884200	-1.09102200	-0.50743200
H	-3.88303000	0.17481200	0.57388200
C	-5.47136300	-1.86166500	-1.64980900
H	-4.61884200	-2.51917400	-3.51416600
H	-6.01933300	-1.01399800	0.25459400
H	-6.41109700	-2.38550000	-1.79006500

γ -TS3/P(SR)

C	-1.72671600	-0.22162700	-2.01619700
H	-1.59355000	0.14593100	-3.02520400
C	-0.57650700	-0.48252600	-1.24289300
C	0.74436300	-0.64691000	-1.99838800
H	0.89929900	0.24451800	-2.61152200
C	-3.03479600	-0.29804100	-1.47191600

O	-3.99907300	-0.04483400	-2.41446300
O	-3.36050900	-0.54764600	-0.30710500
C	-5.34740900	-0.10014400	-1.95360000
C	-6.24764300	0.15450200	-3.14382600
H	-5.49806000	0.65200800	-1.17102800
H	-5.54172300	-1.08166600	-1.50848500
H	-7.29617800	0.12529700	-2.83193500
H	-6.04626400	1.13606800	-3.58269000
H	-6.09595800	-0.60613800	-3.91503600
C	0.70382800	-1.89167100	-2.89009600
H	-0.04811200	-1.78585600	-3.67388300
H	1.68429100	-2.04622800	-3.34985900
H	0.45787100	-2.77569800	-2.29461400
C	-1.02506600	0.96162800	0.97475200
C	-1.05754200	2.07740200	1.78217400
C	-0.25704100	3.20305100	1.46555900
C	0.55235700	3.09253100	0.30532800
C	0.52314100	1.93352700	-0.43753000
N	-0.24323200	0.88130100	-0.11583800
H	-1.65366200	0.09889000	1.17028000
H	-1.70962300	2.06719700	2.64520600
H	1.20553300	3.89388000	-0.01326700
H	1.14534800	1.83987600	-1.32192100
N	-0.26216600	4.32149400	2.22720900
C	-1.11023400	4.39200600	3.40606100

H	-0.84608500	3.61397200	4.13149100
H	-0.97484900	5.36218200	3.88160200
H	-2.16863000	4.28221900	3.14211000
C	0.56310100	5.45914200	1.85599300
H	1.62615100	5.19230500	1.84356800
H	0.28483700	5.84691500	0.86904100
H	0.42050000	6.25345000	2.58735100
C	0.40428400	-1.77516300	0.44025900
N	1.81416500	-0.73204000	-1.01525200
N	1.59609400	-1.42314100	0.13652800
O	-0.71220600	-1.48867200	-0.29011500
C	0.11029100	-2.54174300	1.66610500
C	-1.22046900	-2.77159200	2.03516300
C	1.14998200	-3.02734200	2.46917200
C	-1.50308800	-3.48025400	3.20216200
H	-2.02343700	-2.39406900	1.40780700
C	0.85872200	-3.72830700	3.63326000
H	2.17838300	-2.85263900	2.16921900
C	-0.46872700	-3.95717000	4.00399800
H	-2.53697000	-3.65763400	3.48256000
H	1.66849400	-4.10222000	4.25258100
H	-0.69267200	-4.50899000	4.91199500
C	3.13055500	-0.35927100	-1.29120300
C	3.49548000	0.12458400	-2.55976300
C	4.11667900	-0.44323800	-0.29095500

C	4.80825500	0.52200700	-2.80755200
H	2.77574800	0.17266700	-3.36898200
C	5.42091800	-0.04957600	-0.56132700
H	3.84313900	-0.81162100	0.68956500
C	5.78333300	0.43884100	-1.81793200
H	5.06622600	0.88654100	-3.79775200
H	6.16481600	-0.12523300	0.22678600
H	6.80511300	0.74210400	-2.02089300

γ -P(S)

C	-1.92143900	-1.56557700	0.17967200
H	-1.85875400	-2.63417000	0.34517600
C	-0.79438400	-0.84415200	0.27505200
C	0.54492800	-1.41908200	0.65068400
H	0.52804900	-2.48698200	0.43350800
C	-3.25072100	-1.00115200	-0.10440700
O	-4.17947200	-1.97681100	-0.09647400
O	-3.51817300	0.16353400	-0.31237900
C	-5.53328200	-1.56087200	-0.33998000
C	-6.40957800	-2.78625800	-0.21488300
H	-5.59110100	-1.11645200	-1.33853600
H	-5.80121800	-0.79012500	0.38900200
H	-7.45259800	-2.51457300	-0.39981200
H	-6.11785800	-3.54882200	-0.94210400
H	-6.33659000	-3.21505900	0.78830600
C	0.85388200	-1.18757400	2.13556000

H	0.10859100	-1.68988800	2.75733900
H	1.84179400	-1.59301700	2.37214500
H	0.84841000	-0.12175200	2.38262500
C	0.38229800	1.16327900	-0.04311400
N	1.53273600	-0.77897400	-0.23035400
N	1.50881800	0.59333700	-0.21643900
O	-0.80874700	0.49903600	0.11721900
C	0.22064000	2.62829200	-0.05843100
C	-1.05798000	3.19550400	-0.05049100
C	1.35218700	3.45303200	-0.08629400
C	-1.19780600	4.58210900	-0.07147100
H	-1.93184300	2.55161600	-0.03837600
C	1.20273500	4.83408900	-0.10712000
H	2.33915000	3.00178600	-0.09020600
C	-0.07274900	5.40329700	-0.09881400
H	-2.19160400	5.01905800	-0.06868400
H	2.08270300	5.46952900	-0.12704900
H	-0.18682300	6.48289900	-0.11403500
C	2.83549200	-1.34436800	-0.26848600
C	2.97084000	-2.70917500	-0.55265600
C	3.97913400	-0.57165500	-0.04450800
C	4.23309200	-3.29209800	-0.59354000
H	2.09294900	-3.31026800	-0.76816500
C	5.23852400	-1.16597800	-0.09829800
H	3.87419800	0.48555600	0.16645700

C	5.37624900	-2.52615500	-0.36563100
H	4.32158200	-4.35039900	-0.82038200
H	6.11897800	-0.55557200	0.08030700
H	6.35987200	-2.98300800	-0.40394900

γ -TS2/4(SR)

C	0.22717500	0.49694600	1.66999800
H	0.97145700	0.85188700	2.37266700
C	-0.24134900	-0.80967500	1.85228900
C	0.93288500	-1.72835800	1.71820900
H	0.58694100	-2.75224900	1.54069200
C	-0.66677500	1.59922700	1.16981500
O	-0.38071500	2.75599100	1.77332600
O	-1.52031800	1.47160300	0.32041900
C	-1.07710500	3.92064600	1.28812200
C	-2.44790200	4.04405300	1.92368200
H	-1.13841200	3.85983800	0.19750900
H	-0.43204100	4.75650800	1.56505100
H	-2.92900300	4.96370700	1.57741000
H	-3.08223000	3.19833500	1.64742200
H	-2.36529400	4.08803700	3.01346800
C	1.88174500	-1.70570900	2.91834900
H	2.26389900	-0.69622100	3.09568200
H	1.35862900	-2.04504500	3.81607600
H	2.74363100	-2.35614300	2.74951700
C	-1.28472800	-1.50949500	-0.27866500

C	-2.37675400	-1.82291900	-1.04591200
C	-3.67969800	-1.80904200	-0.48302800
C	-3.76396000	-1.48309300	0.89721500
C	-2.62409900	-1.19435900	1.60304400
N	-1.39740300	-1.20103300	1.03880500
H	-0.27996200	-1.48143000	-0.69395500
H	-2.20819000	-2.05580100	-2.08871300
H	-4.71047500	-1.44857500	1.41950300
H	-2.64263300	-0.93784300	2.65534900
N	-4.77473200	-2.08862300	-1.21655800
C	-4.64812600	-2.34439400	-2.64454800
H	-4.17301600	-1.49939600	-3.15422700
H	-4.06105700	-3.24944300	-2.83604800
H	-5.64132100	-2.48318400	-3.06798600
C	-6.09023700	-2.08679900	-0.59491700
H	-6.83115500	-2.39401200	-1.33137800
H	-6.12866300	-2.79333000	0.24133600
H	-6.35741800	-1.08838400	-0.22913800
C	1.28482300	0.55678600	-0.97283800
N	1.61994800	-1.25476100	0.44620000
N	1.54142300	0.14972700	0.30635000
O	1.13124700	-0.17956000	-1.95308200
C	1.29168800	2.05351400	-1.14545700
C	0.64621500	2.59666200	-2.26070200
C	1.94919400	2.90364800	-0.25060600

C	0.64622000	3.97210100	-2.47311400
H	0.15095700	1.92155600	-2.95175000
C	1.95843100	4.28111600	-0.46957900
H	2.46207800	2.47723900	0.60613700
C	1.30534800	4.81782900	-1.57804800
H	0.14003700	4.38721400	-3.33981800
H	2.48204700	4.93354900	0.22350000
H	1.31573200	5.89037500	-1.75011400
C	2.81975400	-1.85657500	0.06269300
C	3.00432200	-3.24010900	0.26865300
C	3.84790000	-1.14609100	-0.58309800
C	4.17090000	-3.87350500	-0.14158900
H	2.22725300	-3.82674700	0.74775400
C	5.01158700	-1.79560600	-0.98760700
H	3.73446000	-0.08519500	-0.76897900
C	5.19101500	-3.16003800	-0.77272100
H	4.27968900	-4.94047100	0.03350800
H	5.78702600	-1.21804500	-1.48349700
H	6.09984000	-3.65874600	-1.09368900

γ -4(SR)

C	0.26982100	0.36552900	0.28697200
H	0.16708600	0.80865500	1.28939200
C	-0.59678800	-0.82229400	0.04938600
C	0.21328500	-2.05555500	-0.15157700
H	-0.13626600	-2.65639500	-1.00289100

C	0.02341500	1.49231800	-0.74707400
O	-0.43300100	2.60193400	-0.15453300
O	0.21951100	1.37766500	-1.93148100
C	-0.72281200	3.72092700	-1.01772400
C	-2.10279400	3.58367400	-1.62990000
H	0.05498900	3.78057900	-1.78305000
H	-0.65443900	4.59296600	-0.36502500
H	-2.31161000	4.45056300	-2.26390800
H	-2.16804500	2.68367200	-2.24690200
H	-2.86946900	3.53738000	-0.85070400
C	0.26377200	-2.92520800	1.11846600
H	0.78269100	-2.38622700	1.91771900
H	-0.75155900	-3.14520700	1.46414300
H	0.78009600	-3.87419800	0.94636900
C	-2.70480100	-1.94539900	-0.02839400
C	-4.08256500	-1.92995600	0.05836500
C	-4.79728400	-0.77789600	0.40683100
C	-4.00187000	0.34899600	0.67059400
C	-2.63324400	0.32769400	0.56528000
N	-1.93124900	-0.81496200	0.19043800
H	-2.16848000	-2.83912300	-0.30885800
H	-4.58481700	-2.86652200	-0.15422900
H	-4.45162300	1.28263500	0.99351500
H	-2.03896300	1.20367100	0.78092200
N	-6.20204300	-0.72506300	0.55179300

C	-6.89120900	-1.99412400	0.41633700
H	-6.82845700	-2.41119100	-0.60460400
H	-6.48185400	-2.72351500	1.12015300
H	-7.94670100	-1.84630100	0.65697200
C	-6.86166100	0.32546100	-0.21762300
H	-6.84532800	0.11374800	-1.30029000
H	-7.90221500	0.40591300	0.10811100
H	-6.38344600	1.29106500	-0.04943400
C	2.65294900	0.61004700	-0.32909300
N	1.52536600	-1.47974900	-0.54370800
N	1.62158100	-0.20901200	0.12031500
O	3.50779100	0.22885800	-1.10517100
C	2.67945800	1.98083000	0.28021900
C	2.98000500	3.06432300	-0.54936900
C	2.43401700	2.18682100	1.64025500
C	3.00123000	4.35361700	-0.02434600
H	3.18361100	2.88369400	-1.60088800
C	2.47367900	3.47617300	2.16584100
H	2.22396400	1.33822100	2.28625300
C	2.74578700	4.56028400	1.33222300
H	3.22304200	5.19718200	-0.67105800
H	2.29362000	3.63470200	3.22459400
H	2.76888100	5.56601900	1.74113900
C	2.62887300	-2.35533700	-0.31661000
C	2.71878900	-3.46207500	-1.16666000

C	3.57359200	-2.18688100	0.69734900
C	3.72583500	-4.40425200	-0.98822400
H	1.99900200	-3.56544800	-1.97354300
C	4.59084900	-3.12709600	0.85889700
H	3.52131400	-1.32428600	1.35382300
C	4.66986600	-4.24164600	0.02669600
H	3.78296100	-5.25899800	-1.65562600
H	5.32714000	-2.98338800	1.64419700
H	5.46374000	-4.96986600	0.15861800

γ -TS2/5(SR)

C	0.86692400	-1.30016600	-0.89066000
H	1.73733600	-1.18641200	-1.53417500
C	-0.28992000	-0.69600700	-1.42761300
C	-0.12898700	0.75622800	-1.81509100
H	-1.08666000	1.11707600	-2.19804800
C	0.75890400	-2.71222700	-0.37301200
O	1.71933200	-3.48697100	-0.89148300
O	-0.07959700	-3.11897400	0.40026800
C	0.90962600	1.01593700	-2.90840300
H	0.62314000	0.47963200	-3.81676000
H	0.95473300	2.08758400	-3.12836400
H	1.91532700	0.69972000	-2.62248100
C	-1.59055800	-0.62284800	0.67674400
C	-2.76671500	-0.70882900	1.37996800
C	-3.97452800	-1.04531900	0.71714500

C	-3.88106400	-1.27516800	-0.68234000
C	-2.66452100	-1.18594200	-1.31042000
N	-1.52688000	-0.86504700	-0.65629500
H	-0.64802700	-0.36584700	1.14322400
H	-2.73713300	-0.51009900	2.44263100
H	-4.74475300	-1.54123700	-1.27637400
H	-2.54237600	-1.37346700	-2.37100300
N	-5.14660400	-1.14735600	1.37654700
C	-5.19768100	-0.91066600	2.81225400
H	-4.54320700	-1.60568800	3.34982600
H	-4.90108000	0.11601800	3.05474700
H	-6.21858000	-1.06363700	3.15884000
C	-6.36095800	-1.50013700	0.65699300
H	-6.59153000	-0.76166000	-0.11908300
H	-6.27182000	-2.48818100	0.19140400
H	-7.19178200	-1.52723400	1.35989000
C	2.03253000	0.61758200	0.31615900
N	0.14058400	1.59038800	-0.59979400
N	1.48829100	1.66528500	-0.19991600
O	1.48522300	-0.57846900	0.50771500
C	3.44852400	0.75112600	0.78443400
C	4.10106400	-0.35787700	1.33062800
C	4.13571700	1.96860700	0.68877400
C	5.41854700	-0.25234700	1.77668000
H	3.56578200	-1.29857400	1.40282800

C	5.44889900	2.07141700	1.13421200
H	3.62999000	2.82487300	0.25559100
C	6.09568400	0.96079400	1.68116600
H	5.91417900	-1.12094000	2.20038900
H	5.97154400	3.02007000	1.05292400
H	7.12184500	1.04281800	2.02739600
C	-0.51332600	2.83904300	-0.52649500
C	-1.90665000	2.89499800	-0.72113500
C	0.15995800	4.02745300	-0.20204300
C	-2.58888600	4.10358900	-0.63750900
H	-2.46172900	1.97978300	-0.91104700
C	-0.53709300	5.23094700	-0.11667600
H	1.22536800	3.99460300	-0.01627500
C	-1.91112400	5.28669200	-0.33972300
H	-3.66438700	4.11562000	-0.79185300
H	0.00981600	6.13761700	0.12754200
H	-2.44633400	6.22831400	-0.26983200
C	1.69754200	-4.87024100	-0.49722200
C	2.85974000	-5.55392600	-1.17981400
H	0.73679000	-5.30205500	-0.79457500
H	1.77195500	-4.92565400	0.59290500
H	2.87081900	-6.61383400	-0.91029600
H	2.77425400	-5.47437900	-2.26685300
H	3.80922700	-5.10870400	-0.87091500

γ -5(SR)

C	0.82422300	-1.40675500	-0.74732200
H	1.63909200	-1.46556400	-1.47409200
C	-0.31485700	-0.72261800	-1.36598700
C	-0.00071200	0.69016900	-1.77569800
H	-0.91589600	1.14751300	-2.16146800
C	0.47168100	-2.80989700	-0.29617200
O	0.91788100	-3.73083700	-1.15812400
O	-0.16127700	-3.07922700	0.70064100
C	0.53845000	-5.09036300	-0.88267900
C	1.11396000	-5.95256600	-1.98256000
H	-0.55395300	-5.14835100	-0.84733000
H	0.92498300	-5.37171400	0.10177500
H	0.84498800	-6.99826200	-1.80811200
H	0.72279700	-5.65087400	-2.95786300
H	2.20445700	-5.87656100	-2.00579400
C	1.06075600	0.81622200	-2.87060300
H	0.71511300	0.30527900	-3.77247800
H	1.23307100	1.87271800	-3.10320500
H	2.02201300	0.38354200	-2.58013200
C	-1.53670500	-0.42096900	0.80022500
C	-2.69387000	-0.34341000	1.53755300
C	-3.95311300	-0.53402900	0.91687300
C	-3.92669200	-0.82100700	-0.47401600
C	-2.72556800	-0.90574700	-1.13387900
N	-1.53398400	-0.70412000	-0.52713800

H	-0.56535500	-0.27263100	1.24915900
H	-2.60748900	-0.12844200	2.59398600
H	-4.83297300	-1.00091200	-1.03656500
H	-2.65703500	-1.14828900	-2.18779800
N	-5.11025900	-0.45221900	1.60794500
C	-5.08517700	-0.18090500	3.03752600
H	-4.54916600	-0.96702200	3.58175500
H	-4.60837500	0.78277800	3.24753300
H	-6.10864500	-0.14333200	3.40730600
C	-6.37940800	-0.68363700	0.93661600
H	-6.53441100	0.03594700	0.12490200
H	-6.43405600	-1.69862900	0.52592200
H	-7.18621900	-0.56204400	1.65763800
C	2.11708500	0.37001200	0.33989800
N	0.36704200	1.56659200	-0.59242100
N	1.68090600	1.47239500	-0.14077800
O	1.44204300	-0.79482400	0.48398900
C	3.49872100	0.33422200	0.89798700
C	4.01341100	-0.86254400	1.40690600
C	4.29602300	1.48723800	0.92503400
C	5.30333700	-0.90621200	1.93485900
H	3.39558000	-1.75351700	1.39109400
C	5.58071000	1.44001600	1.45286700
H	3.89512200	2.41336400	0.52721600
C	6.09074000	0.24210000	1.95991400

H	5.69108400	-1.84159600	2.32723900
H	6.18865200	2.33965300	1.46825200
H	7.09550300	0.20695200	2.37035700
C	-0.06917700	2.91269000	-0.67933300
C	-1.44630000	3.15522600	-0.81848900
C	0.80026600	4.00875000	-0.59658800
C	-1.93270400	4.45461800	-0.90842000
H	-2.13663300	2.31505700	-0.82977300
C	0.30039100	5.30768900	-0.67978900
H	1.86043000	3.83289900	-0.46447100
C	-1.06284700	5.54416300	-0.84298200
H	-3.00181100	4.61635700	-1.01412400
H	0.99239900	6.14321000	-0.61965600
H	-1.44413900	6.55831400	-0.90701300

α -TS1/2(R)

C	-0.80652700	-0.72005100	1.03586000
H	-1.71654200	-0.37010700	1.50587700
C	0.36308200	0.04119700	1.35382200
C	0.37630200	1.25546800	1.95312400
H	1.31609200	1.80665900	1.93272000
C	-0.77990900	-2.16748000	0.83137100
O	-1.96154300	-2.71839500	1.17800600
O	0.13294400	-2.83093700	0.36121500
C	-2.13104300	-4.10265100	0.85778700
C	-3.53840500	-4.47907900	1.26733900

H	-1.37194000	-4.68813700	1.38664600
H	-1.97037300	-4.23557800	-0.21762700
H	-4.26128300	-3.85145800	0.73907200
H	-3.73370900	-5.52702400	1.02308700
H	-3.67727200	-4.33979100	2.34272200
C	-0.75340800	1.90917900	2.68623000
H	-1.67469600	1.32721800	2.64666400
H	-0.48393300	2.06353300	3.73846900
H	-0.96099400	2.89387600	2.25442300
C	1.72907100	-0.78512800	-0.49022700
C	2.92236900	-1.20959300	-1.01835600
C	4.07598000	-1.30814800	-0.20764300
C	3.92334000	-0.96576600	1.16392300
C	2.70461200	-0.54742200	1.62578500
N	1.62865800	-0.43853000	0.81575900
H	0.82457700	-0.66576700	-1.07514700
H	2.94150200	-1.45748200	-2.06996700
H	4.74111600	-1.03721600	1.86704600
H	2.53339700	-0.29237000	2.66434100
N	5.26598100	-1.71497900	-0.70479000
C	5.37836400	-2.07184100	-2.11131100
H	4.72676100	-2.91739700	-2.35833000
H	5.11641600	-1.22389500	-2.75308500
H	6.40766500	-2.35685300	-2.32268400
C	6.42487900	-1.82021800	0.16694700

H	6.66087900	-0.85460800	0.62794400
H	6.26263400	-2.56091800	0.95858400
H	7.28452400	-2.13361700	-0.42291000
C	-0.19848300	2.09300400	-0.79961800
N	-1.27475900	0.12676500	-0.80752100
N	-1.36930600	1.41183500	-0.53702000
O	0.84544200	1.63089700	-1.27241000
C	-0.28698600	3.56521100	-0.48777800
C	-1.47437700	4.17651900	-0.07027900
C	0.87088600	4.33671500	-0.61875500
C	-1.49721400	5.54022100	0.21576400
H	-2.36899300	3.57006700	0.02204400
C	0.84885200	5.69812200	-0.32766500
H	1.77744800	3.84264600	-0.95451300
C	-0.33630300	6.30332500	0.09148700
H	-2.42339000	6.00902500	0.53532900
H	1.75440100	6.28936400	-0.42897400
H	-0.35580600	7.36547300	0.31745400
C	-2.55339400	-0.49972100	-0.95568400
C	-2.56414000	-1.71922400	-1.63773700
C	-3.75345100	0.04700400	-0.49023200
C	-3.76222800	-2.39732200	-1.84239700
H	-1.61968900	-2.11816800	-2.00000000
C	-4.94774100	-0.63760000	-0.69474600
H	-3.72745900	1.00528800	0.01753600

C	-4.95947400	-1.85990900	-1.36957800
H	-3.76293700	-3.34227400	-2.37882900
H	-5.87869600	-0.21329300	-0.32983600
H	-5.89638300	-2.38424100	-1.53213500

α -2(R)

C	0.30705000	1.15738100	1.22601600
H	1.22810200	1.51449200	1.69957600
C	-0.25785900	0.05586300	2.09868500
C	0.20864900	-0.37307900	3.27069600
H	-0.29340300	-1.23263100	3.71481900
C	-0.60337800	2.38803300	1.19800300
O	-0.13770600	3.30910700	0.37040700
O	-1.59700500	2.51559900	1.88358100
C	-0.95909900	4.47454300	0.16293100
C	-0.35865200	5.23930100	-0.99330900
H	-0.97424000	5.05968600	1.08761200
H	-1.97927300	4.14198700	-0.05288600
H	-0.35531900	4.62493500	-1.89786600
H	-0.94850700	6.14037700	-1.18427100
H	0.66895400	5.53780900	-0.77037800
C	1.35658700	0.18816600	4.04717700
H	2.09898100	-0.59648100	4.22400500
H	1.85637000	1.01877000	3.54717300
H	1.01133700	0.53411000	5.02735800
C	-1.15492100	-1.58937900	0.55536900

C	-2.19560200	-2.22405600	-0.06956100
C	-3.54079900	-1.90694600	0.25850400
C	-3.73443600	-0.93688800	1.28598200
C	-2.65433700	-0.33784900	1.87474000
N	-1.38516600	-0.65138100	1.51304600
H	-0.10245200	-1.75876400	0.29656200
H	-1.95225000	-2.94864000	-0.83458700
H	-4.72212300	-0.63935200	1.61071700
H	-2.74944900	0.42885800	2.63376800
N	-4.57683200	-2.48538600	-0.37092900
C	-4.33301000	-3.43085200	-1.45442600
H	-3.75349200	-2.96375100	-2.25768800
H	-3.79514600	-4.31351600	-1.09241300
H	-5.28925700	-3.75471800	-1.86098800
C	-5.94392400	-2.12867200	-0.01610600
H	-6.14182400	-2.33738900	1.04050900
H	-6.13953400	-1.06889100	-0.21481300
H	-6.63031800	-2.72443100	-0.61512300
C	2.46197500	-0.81729700	-0.20028600
N	0.73018100	0.66770100	-0.06560600
N	2.13463700	0.46944200	-0.13189100
O	1.70312400	-1.82038200	-0.22827400
C	3.95736800	-1.05824500	-0.26877200
C	4.88770100	-0.01741500	-0.37111700
C	4.41504900	-2.37734000	-0.23382100

C	6.25162000	-0.29714400	-0.43156800
H	4.52745700	1.00545400	-0.40625200
C	5.77930500	-2.65817800	-0.29113600
H	3.67826700	-3.17116800	-0.16320400
C	6.70208500	-1.61762500	-0.39048400
H	6.96643900	0.51697300	-0.51392200
H	6.12223800	-3.68873200	-0.26149500
H	7.76588500	-1.83305200	-0.43799900
C	-0.00585300	0.76467400	-1.23128600
C	-1.39291000	1.03761800	-1.24202800
C	0.62118000	0.54013900	-2.47593200
C	-2.09906400	1.11251100	-2.43908500
H	-1.94790200	1.16667100	-0.31799600
C	-0.10166500	0.61591800	-3.65983300
H	1.67939700	0.31190400	-2.49311600
C	-1.46759700	0.90645700	-3.66431000
H	-3.16425000	1.32838600	-2.40222300
H	0.41829100	0.44221400	-4.59830000
H	-2.02280800	0.96384100	-4.59489200

α -TS2/P(R)

C	0.27250100	0.92448200	0.88185200
H	1.10151700	1.47804000	1.34735000
C	0.18390000	-0.43032000	1.58094400
C	0.04901600	-0.41069300	2.96159200
H	0.09407200	-1.36837500	3.47329900

C	-0.99063600	1.76376200	1.05317000
O	-0.67190800	3.03602300	1.28780400
O	-2.12611400	1.35765100	0.96003300
C	-1.76793300	3.96685000	1.34841800
C	-1.17340700	5.34979900	1.47837400
H	-2.40018200	3.70577400	2.20305200
H	-2.36147800	3.86053100	0.43476800
H	-0.53290400	5.57406100	0.62080100
H	-1.97538400	6.09258400	1.51607000
H	-0.57976000	5.43460700	2.39257700
C	0.10643400	0.85068500	3.79205000
H	0.14554700	0.57606500	4.85097900
H	0.98994000	1.48541300	3.61292200
H	-0.77261000	1.51048600	3.69315700
C	-0.81519600	-1.84260700	-0.43498200
C	-1.83412700	-2.50078600	-1.08042100
C	-3.08659500	-2.67894400	-0.43629200
C	-3.19881700	-2.14343900	0.87130000
C	-2.13228500	-1.48337900	1.43358300
N	-0.95578600	-1.33860200	0.80838100
H	0.14478000	-1.71627100	-0.91578600
H	-1.64708000	-2.88077700	-2.07591400
H	-4.11548300	-2.21737100	1.44080900
H	-2.16008100	-1.02759800	2.42016200
N	-4.11147200	-3.32015500	-1.03956600

C	-3.96858600	-3.79575500	-2.40699300
H	-3.74195000	-2.97119900	-3.09285200
H	-3.17489400	-4.54716100	-2.48385500
H	-4.90406000	-4.25576100	-2.72197500
C	-5.38741600	-3.45562700	-0.35451100
H	-5.26506800	-3.97224500	0.60339100
H	-5.84934000	-2.47765100	-0.17265500
H	-6.06079100	-4.04667900	-0.97357100
C	2.15603000	-0.76428100	0.07273400
N	0.56995800	0.73694800	-0.55236300
N	1.84162300	0.18698700	-0.73650000
O	1.38698400	-1.25566000	1.04236200
C	3.48064600	-1.42442200	-0.06776600
C	4.27694100	-1.17498000	-1.19218000
C	3.93890700	-2.29599300	0.92399400
C	5.51680000	-1.79127000	-1.31936000
H	3.91272900	-0.49617200	-1.95646200
C	5.18538500	-2.90777600	0.79367200
H	3.31710700	-2.48550000	1.79261200
C	5.97605200	-2.65880300	-0.32601000
H	6.12754400	-1.59326200	-2.19523800
H	5.53762700	-3.58005900	1.57032700
H	6.94561600	-3.13749500	-0.42703600
C	0.39300100	1.91214600	-1.35892100
C	-0.87800600	2.16690400	-1.87671700

C	1.44207200	2.79853300	-1.61186400
C	-1.10818800	3.32514300	-2.61664100
H	-1.67400600	1.45109800	-1.69446700
C	1.20814600	3.94681600	-2.36496800
H	2.42954300	2.57751700	-1.21994100
C	-0.06686600	4.21978400	-2.86146600
H	-2.09983900	3.51857900	-3.01538500
H	2.02539000	4.63535100	-2.55909700
H	-0.24508400	5.11813200	-3.44482300

α -P(R)

C	-1.07563800	-0.43710600	0.59084600
H	-1.95258600	-0.36747400	1.23619600
C	-0.12721800	-1.44643200	1.18654200
C	-0.42258400	-2.42077400	2.04453300
H	0.40612900	-3.06031000	2.34179100
C	-1.52645000	-0.92310500	-0.79638900
O	-2.48393300	-1.84510400	-0.67808500
O	-1.06126700	-0.53838600	-1.83940100
C	-2.94796000	-2.44328700	-1.90802600
C	-3.99798700	-3.46513800	-1.54221700
H	-2.09101900	-2.89662900	-2.41472600
H	-3.34699600	-1.65163000	-2.54873400
H	-4.83864200	-2.99333300	-1.02645800
H	-4.37518500	-3.94271100	-2.45062800
H	-3.57807800	-4.23922000	-0.89421700

C	-1.77414800	-2.74598900	2.59942400
H	-2.52897100	-1.99228400	2.36697200
H	-2.13039400	-3.70124400	2.19705700
H	-1.72270500	-2.85310800	3.68730500
C	1.61271900	-0.14094700	0.29497900
N	-0.42564400	0.84816900	0.52939100
N	0.90147100	0.91427000	0.22044500
O	1.15882300	-1.36633900	0.69374400
C	3.04614500	-0.12872600	-0.05548700
C	3.61416500	1.01399400	-0.63322200
C	3.84594100	-1.24918000	0.19012600
C	4.96700200	1.03418900	-0.94990100
H	2.98407000	1.87361200	-0.83679200
C	5.20147700	-1.22321300	-0.13317200
H	3.40820400	-2.13640300	0.63391800
C	5.76626800	-0.08374500	-0.70051000
H	5.39980800	1.92301800	-1.39871100
H	5.81520400	-2.09715700	0.06313400
H	6.82238200	-0.06563300	-0.95192400
C	-1.17018300	2.02372100	0.35099800
C	-0.51968200	3.26788600	0.32584800
C	-2.56641800	1.98292900	0.22344100
C	-1.25809100	4.43553900	0.18394000
H	0.55843000	3.30318800	0.42085900
C	-3.29128800	3.16625100	0.09037300

H	-3.10587700	1.04202600	0.21143200
C	-2.64910100	4.39986300	0.06891900
H	-0.73632700	5.38809900	0.16769300
H	-4.37136000	3.11082800	-0.00924700
H	-3.21767800	5.31752600	-0.04013600

α -TS1/2(S)

C	-0.21198200	0.40083500	1.70898000
H	-1.27586000	0.40591700	1.91205800
C	0.50862300	-0.81288600	2.03871100
C	0.14404600	-1.77882900	2.89674200
H	0.73171400	-2.69441500	2.91813000
C	0.44964300	1.66543000	1.68426900
O	-0.42627700	2.70131700	1.58404800
O	1.66907300	1.85943100	1.70481700
C	0.15194100	3.99281100	1.38724600
C	-0.98649600	4.97670700	1.23054700
H	0.78981500	3.96987800	0.49658600
H	0.78350500	4.24322900	2.24696800
H	-0.58885900	5.98153500	1.05760600
H	-1.61755500	4.70102500	0.38070300
H	-1.60837700	5.00040700	2.13023700
C	-1.09582200	-1.71026400	3.72965800
H	-1.29383900	-0.69207700	4.07797200
H	-1.96285200	-2.03186400	3.13549100
H	-1.02555900	-2.36658800	4.60078000

C	2.91781100	-0.68110000	1.52505700
C	4.00259600	-0.98401400	0.74158700
C	3.83715300	-1.76176500	-0.43716500
C	2.51687400	-2.19880500	-0.73281600
C	1.47783300	-1.85812300	0.09444200
N	1.67897200	-1.11403300	1.20915700
H	2.99037500	-0.07437800	2.41753100
H	4.96937900	-0.60649500	1.04421100
H	2.29384000	-2.79207100	-1.60891200
H	0.44344600	-2.13516700	-0.08428900
N	4.87918800	-2.06614100	-1.23451600
C	6.22023700	-1.62134000	-0.88297200
H	6.27997900	-0.52764600	-0.85457800
H	6.52378300	-2.01893200	0.09179600
H	6.92143200	-1.98440000	-1.63249200
C	4.66822300	-2.84067500	-2.44980900
H	4.27489300	-3.83763400	-2.22159400
H	3.97314000	-2.33090800	-3.12560700
H	5.62101700	-2.95772800	-2.96315800
C	-2.40989300	-1.12298900	-0.29385900
N	-0.61953500	0.16919400	-0.60423900
N	-1.90337500	0.09614500	-0.72722800
O	-1.77167000	-1.96920800	0.33094200
C	-3.86339100	-1.32519900	-0.59754200
C	-4.62700000	-0.36549700	-1.27226600

C	-4.46386500	-2.52293000	-0.19466100
C	-5.97282200	-0.60600800	-1.54000600
H	-4.15999200	0.56388300	-1.57860800
C	-5.80883600	-2.76043100	-0.46093600
H	-3.85794700	-3.25662700	0.32785300
C	-6.56631900	-1.80161200	-1.13509300
H	-6.56003100	0.14261400	-2.06347000
H	-6.26772900	-3.69207900	-0.14323900
H	-7.61611400	-1.98626200	-1.34369100
C	-0.08959300	1.38494800	-1.12606200
C	1.30248000	1.46115100	-1.25016000
C	-0.88253000	2.45294000	-1.57278200
C	1.89647900	2.57631000	-1.83524700
H	1.90909600	0.63888000	-0.88374700
C	-0.28354200	3.56377400	-2.15488700
H	-1.95874500	2.38797200	-1.46147900
C	1.10632300	3.62953800	-2.29308100
H	2.97750300	2.62413200	-1.92608300
H	-0.90201200	4.38650500	-2.50296400
H	1.56777400	4.49895500	-2.75206900
α-2(S)			
C	1.33637400	0.04913400	0.99768500
H	1.61773800	1.06761400	1.28857900
C	0.22297200	-0.40358600	1.92580000
C	0.13320700	-0.10615600	3.22264700

H	-0.70444800	-0.52542000	3.77868100
C	2.56653900	-0.84104400	1.15318200
O	3.68565400	-0.14062300	1.01562900
O	2.54036600	-2.03623800	1.36936700
C	4.91521200	-0.88983400	0.97492400
C	6.01497700	0.07474400	0.59910000
H	4.80400400	-1.69055200	0.23715200
H	5.07758200	-1.34593100	1.95651600
H	6.96754800	-0.46003000	0.54472200
H	5.81159900	0.52554100	-0.37618000
H	6.10711100	0.87243200	1.34087400
C	1.10676200	0.72540600	3.99780700
H	0.57215700	1.40661000	4.66606600
H	1.73460200	0.08185500	4.62531300
H	1.76048600	1.31985400	3.35693800
C	-0.53854800	-2.32692500	0.65011100
C	-1.50201900	-3.03379200	-0.01932100
C	-2.84710900	-2.57302100	-0.03465800
C	-3.11811500	-1.37672300	0.68553700
C	-2.09980900	-0.71207000	1.30985700
N	-0.83314700	-1.19253100	1.32725300
H	0.49898900	-2.63820900	0.69012400
H	-1.20178300	-3.93089500	-0.54287200
H	-4.10368500	-0.93238200	0.70844600
H	-2.24894400	0.24069500	1.80342400

N	-3.81289500	-3.22647200	-0.70321500
C	-3.48939200	-4.41798500	-1.47645000
H	-2.77043500	-4.19010400	-2.27113500
H	-3.07500100	-5.20055800	-0.83256700
H	-4.40060600	-4.79993700	-1.93358900
C	-5.16527100	-2.68658200	-0.74356700
H	-5.58248300	-2.59915100	0.26481600
H	-5.18364200	-1.70165500	-1.22389400
H	-5.79725800	-3.36169400	-1.31747800
C	-0.34896600	2.03392800	-0.10455900
N	0.85052600	0.03276500	-0.39310500
N	-0.34710800	0.79088600	-0.57836100
O	0.58946300	2.68808700	0.41687300
C	-1.71166600	2.70021000	-0.22102200
C	-2.80008400	2.08554600	-0.85376400
C	-1.88121200	3.97242600	0.33101100
C	-4.03223300	2.73196000	-0.92609800
H	-2.65822200	1.10275300	-1.29176900
C	-3.11558800	4.61850600	0.26397900
H	-1.02459800	4.43844400	0.80846900
C	-4.19620000	3.99974000	-0.36355500
H	-4.86691800	2.24971300	-1.42844100
H	-3.23351000	5.60705300	0.69915700
H	-5.15729300	4.50306300	-0.42141200
C	1.81956800	0.15422500	-1.43063300

C	2.58731900	-0.96683200	-1.77921900
C	1.99136200	1.34123500	-2.15131200
C	3.53438400	-0.88946700	-2.79773100
H	2.42174200	-1.90635700	-1.25825600
C	2.92539100	1.40642700	-3.18278800
H	1.40283800	2.21047800	-1.88137400
C	3.70901400	0.29865200	-3.50710000
H	4.11965100	-1.76884700	-3.05311100
H	3.04813400	2.33720000	-3.72951000
H	4.43792600	0.35734700	-4.30984100