

Supporting Information

**Rhodium(I)/Bisoxazolinephosphine-Catalyzed Regio- and
Enantioselective Amination of Allylic Carbonates: A
Computational Study**

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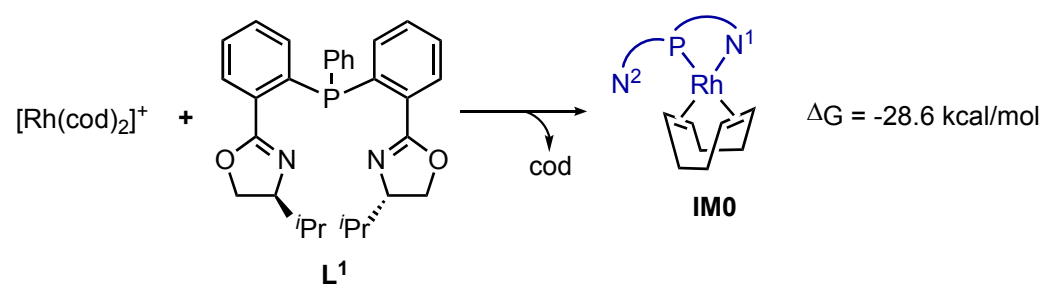
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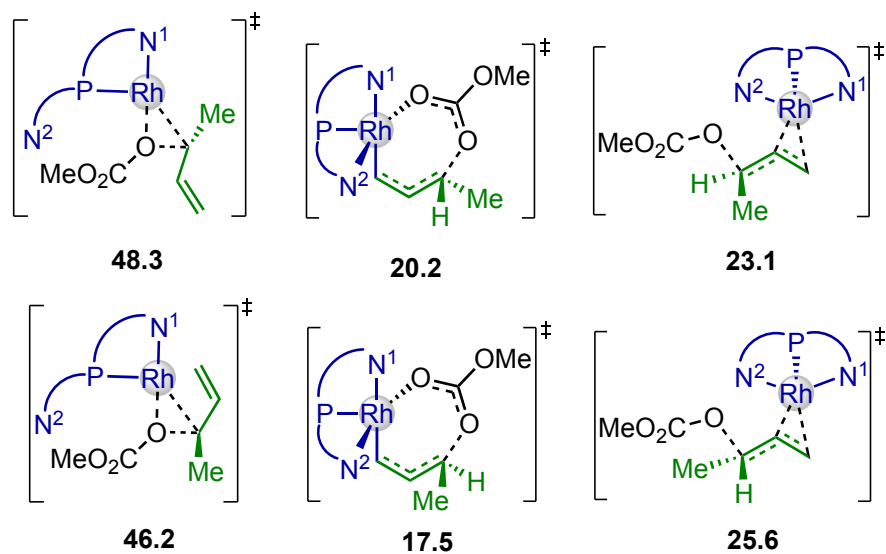
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1. Formation of IM0



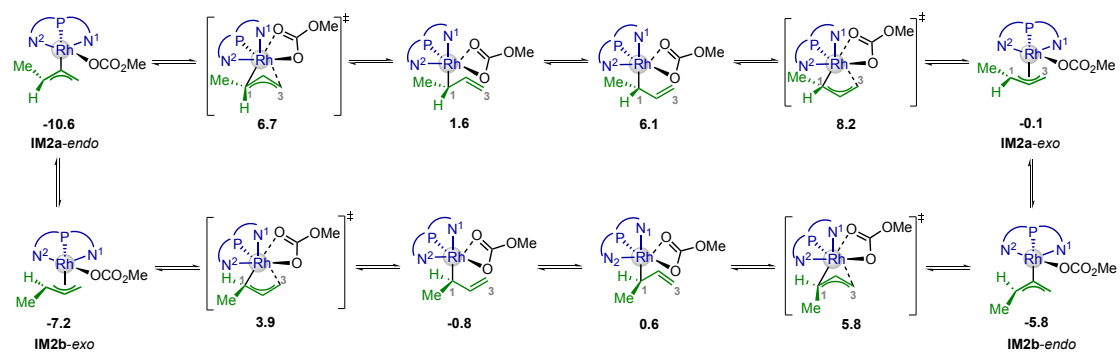
Scheme S1. Ligand exchange between $[\text{Rh}(\text{cod})_2]^+$ and L^1 to form intermediate **IM0**.

2. Other possibilities for the C-O oxidative addition



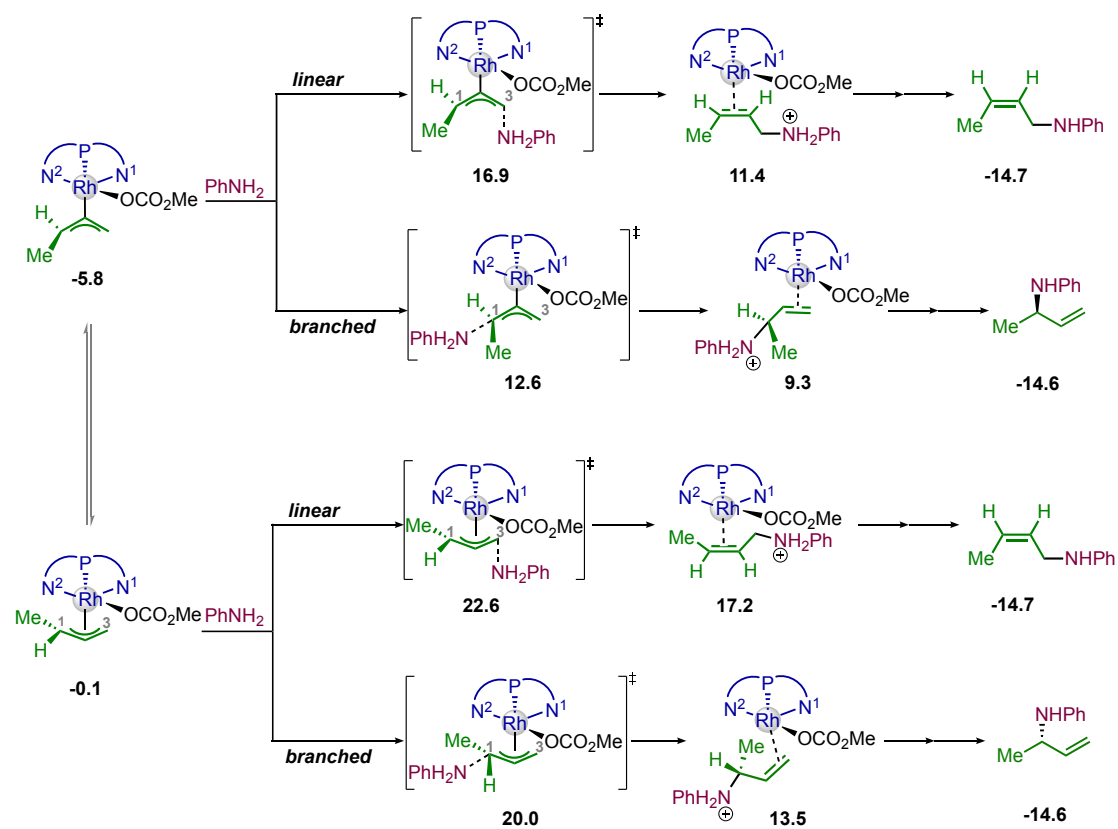
Scheme S2. C-O oxidative addition via three- and seven-membered cyclic transition states and S_N2 front-side attack transition state. Energies are given in kcal/mol.

3. Allylic isomerization

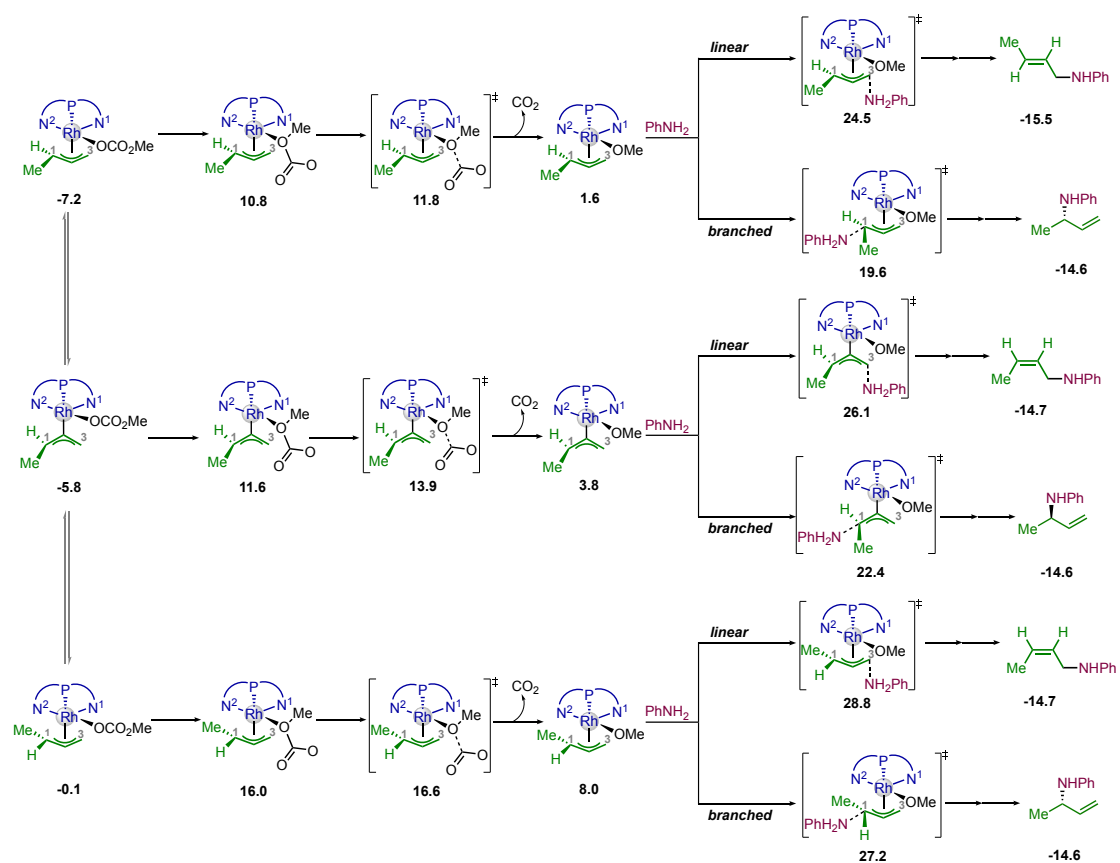


Scheme S3. Allylic isomerization of the other species. Energies are given in kcal/mol.

4. C-N bond formation

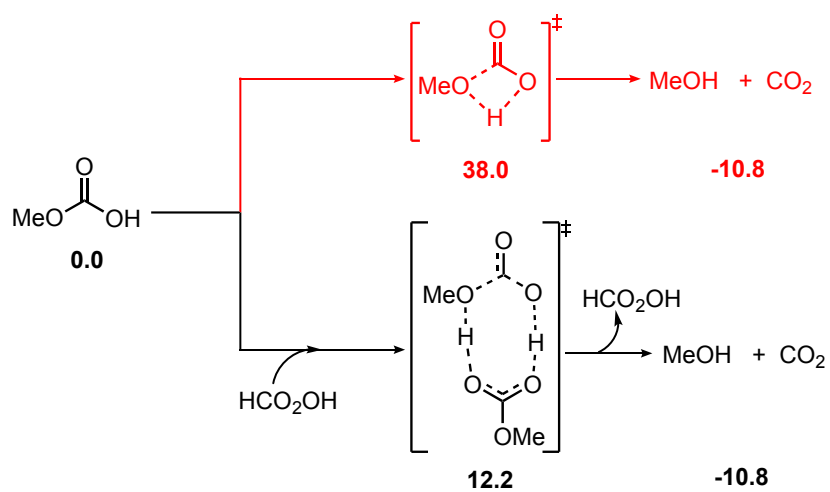
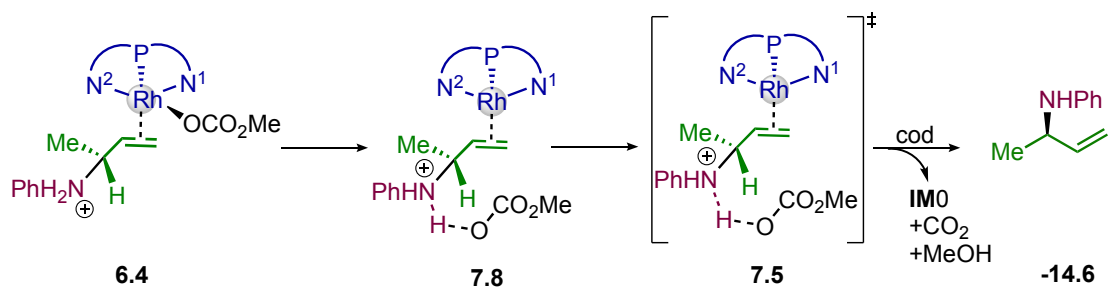


Scheme S4. C-N bond formation via the nucleophilic attack from **IM2a-exo** and **IM2b-endo**. Energies are given in kcal/mol.



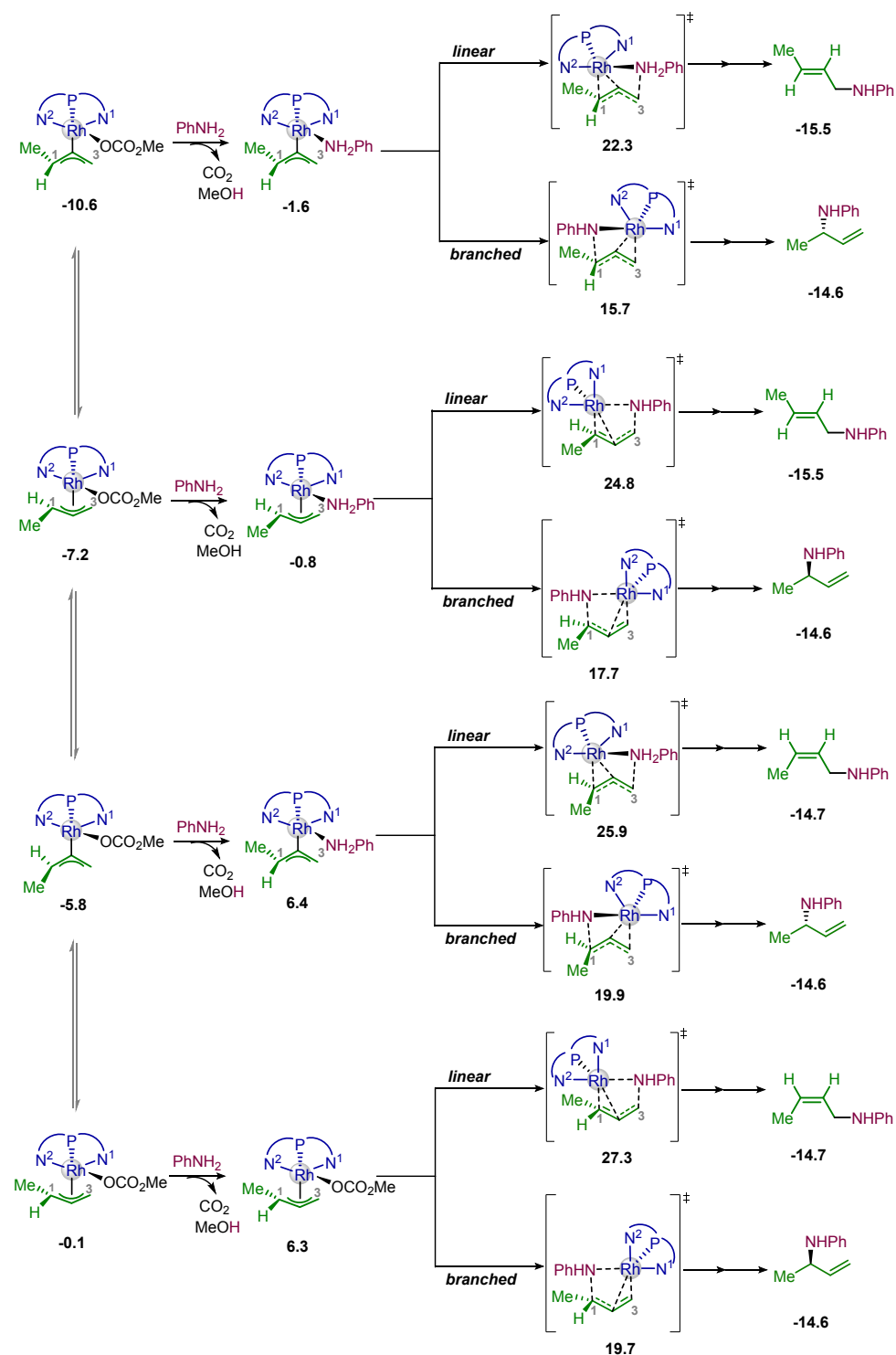
Scheme S5. C-N bond formation via the decarboxylation/nucleophilic attack from **IM2a-exo**, **IM2b-exo** and **IM2b-endo**. Energies are given in kcal/mol.

5. Deprotonation and off-cycle decarboxylation



Scheme S6. Calculated energies of the deprotonation and off-cycle decarboxylation. Energies are given in kcal/mol.

6. C-N bond formation via the deprotonation/C-N reductive elimination



Scheme S7. C-N bond formation via the deprotonation/C-N reductive elimination. Energies are given in kcal/mol.

7. AIM analysis

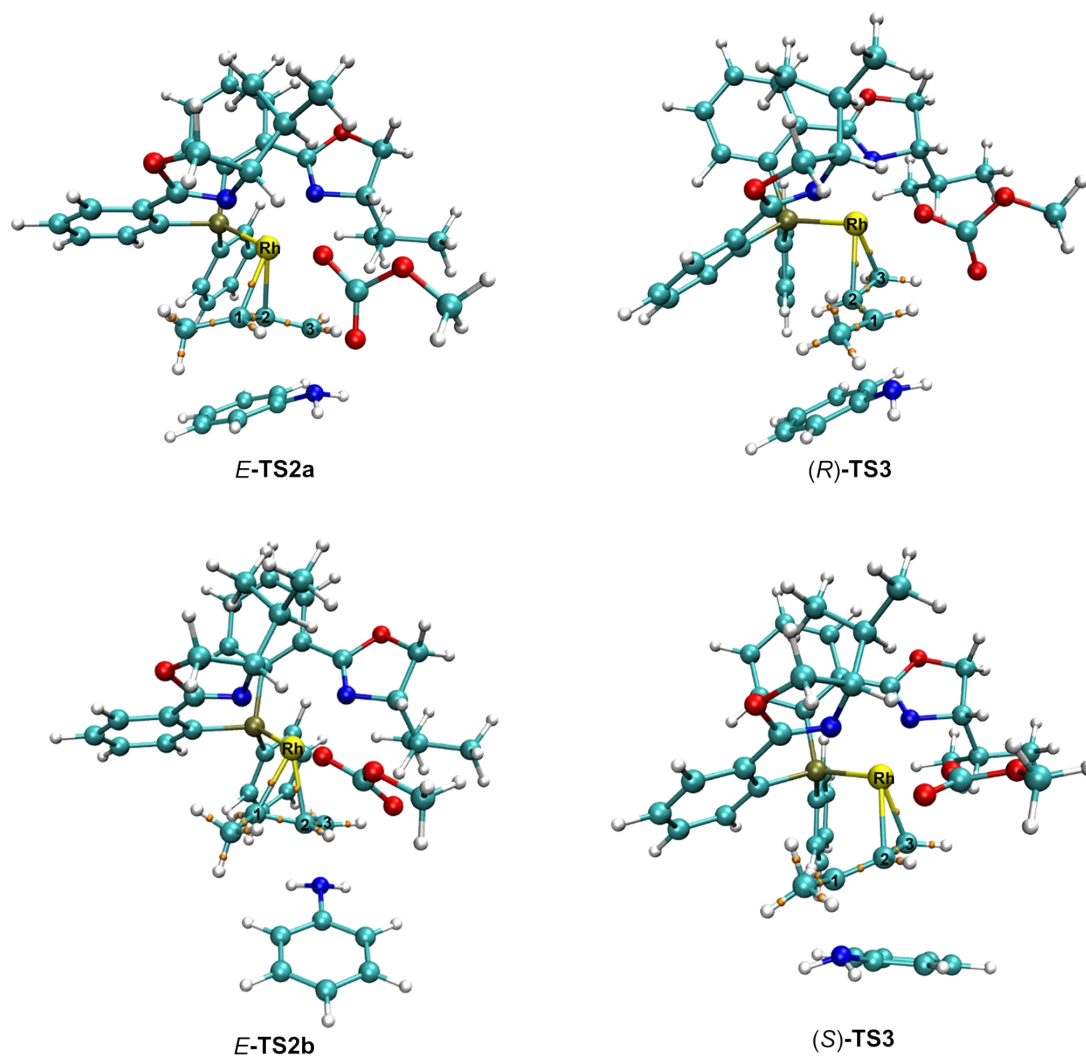


Figure S1. AIM analysis of the outer-sphere nucleophilic attack transition states.

8. Table of calculated energies and energy corrections

Stationary point	Single-point energy- B3LYPP-D3(BJ) 6-311+G(d,p), SDD (a.u.)	Thermal correction to Gibbs free energy at 298.15 K (a.u.)
(<i>R</i>)-1a	-460.4945574	0.120277
(<i>S</i>)-1a	-460.4945619	0.120322
cod	-312.1607657	0.148958
PhNH ₂	-287.7244832	0.088047
IM0	-2187.7106286	0.684671
IM1a-exo	-2336.0218054	0.655746
IM1a-endo	-2336.03240170	0.653115
IM1b-exo	-2336.0289003	0.654079
IM1b-endo	-2336.0289003	0.654079
TS1a-exo	-2336.0028738	0.650666
TS1a-endo	-2336.01722402	0.649988
TS1b-exo	-2336.0143074	0.651910
TS1b-endo	-2336.0175141	0.652064
IM2a-exo	-2336.0459382	0.657395
IM2a-endo	-2336.0549898	0.657250
IM2b-exo	-2336.0578962	0.657073
IM2b-endo	-2336.0549898	0.657250
TS-iso-1	-2336.0373402	0.654078
IM-iso-1	-2336.0471273	0.654007
IM-iso-2	-2336.0448234	0.654304
TS-iso-2	-2336.034491	0.654521
<i>E</i> -TS2a	-2623.7638285	0.765241
(<i>R</i>)-TS3	-2623.7754207	0.765256
<i>E</i> -TS2b	-2623.7632460	0.764321
(<i>S</i>)-TS3	-2623.7716371	0.766019
<i>E</i> -IM3a	-2623.7753414	0.767567
(<i>R</i>)-IM4	-2623.7849569	0.770263
<i>E</i> -IM3b	-2623.7742245	0.769107
(<i>S</i>)-IM4	-2623.7814454	0.770659
<i>E</i> -3a	-443.8019888	0.169920

(R)-2a	-443.8005761	0.170007
(S)-2a	-443.8005761	0.170007
IM2a'-endo	-2336.0406299	0.659433
TS4a-endo	-2336.0346923	0.655806
IM5a-endo	-2147.3845741	0.647669
E-TS5a	-2435.0843362	0.754762
(R)-TS6	-2435.0925796	0.753781

9. Cartesian coordinates

(R)-1a

C	-0.16152000	2.84378900	0.29621700
H	0.17071100	1.83555100	0.06385200
H	-0.61944700	2.99920400	1.27040900
C	-0.01040900	3.84618800	-0.56794400
H	0.44761800	3.67904600	-1.54267300
C	-0.41044300	5.26433000	-0.28047900
H	-0.89348700	5.33626200	0.69559500
C	0.75693200	6.23417600	-0.37396500
H	1.23123100	6.17711800	-1.35865100
H	1.50220100	5.98206600	0.38573600
O	-1.36149800	5.71437900	-1.30795200
C	-2.64488900	5.34055500	-1.26512800
O	-3.41644700	5.61588900	-2.16032400
O	-2.96342000	4.66978100	-0.14857800
C	-4.33694600	4.24303300	-0.06130900
H	-4.58511800	3.58194300	-0.89464400
H	-4.41415500	3.70602800	0.88381000
H	-5.00719200	5.10559700	-0.06387600
H	0.41718400	7.26021500	-0.20498100

(S)-1a

C	-0.16408800	2.84744200	-1.04117000
H	0.16407000	1.83781300	-0.80905500
H	-0.61688400	3.00588600	-2.01728000
C	-0.01434200	3.84789300	-0.17450900
H	0.43840400	3.67775400	0.80215900
C	-0.40899100	5.26763800	-0.46158000
C	0.76064200	6.23403300	-0.36111400
H	1.50892800	5.98084800	-1.11748900
H	1.22999100	6.17432200	0.62579800
H	-0.88728400	5.34238700	-1.43978600
O	-1.36350800	5.71885500	0.56214400
C	-2.64783400	5.34913000	0.51276700
O	-3.42269800	5.62579100	1.40468600
O	-2.96318700	4.68062500	-0.60601900
C	-4.33771000	4.25860000	-0.70046900
H	-4.41229500	3.72366700	-1.64697400
H	-4.59187200	3.59673600	0.13045400
H	-5.00512300	5.12335700	-0.69929700
H	0.42464600	7.26127200	-0.53035200

cod

C	-0.64207500	5.12498900	-0.45324000
H	-1.11942100	5.71116500	0.33241900

C	0.74278300	4.62342000	-0.11412100
H	1.41359800	4.69185300	-0.97204700
H	1.16908600	5.28083900	0.65195800
C	0.75460900	3.18945300	0.45358700
H	1.78362600	2.93520600	0.75028500
H	0.18004600	3.18229900	1.39031600
C	0.21282700	2.08339700	-0.41598300
H	-0.00224600	1.16773600	0.13690200
C	-0.03722100	2.05641300	-1.73158500
H	-0.45710500	1.13104300	-2.12673700
C	0.14965800	3.15319400	-2.75449200
H	0.23746800	2.69032800	-3.74389300
H	1.08416100	3.69318300	-2.59416000
C	-1.03063500	4.14397600	-2.81391500
H	-1.93391100	3.59055600	-3.10630900
H	-0.85517300	4.85481000	-3.63580400
C	-1.36174800	4.91965100	-1.56405400
H	-2.35062600	5.37969500	-1.59264900

PhNH₂

N	0.73018900	6.30681300	-1.67661900
H	0.23033000	6.57750800	-0.83817800
C	2.10943700	6.49435700	-1.61840200
C	2.97006800	5.75784500	-2.45496300
C	2.66862200	7.46578800	-0.76683700
C	4.34352000	5.99250500	-2.43837100
H	2.54904500	5.00335200	-3.11477100
C	4.04420300	7.69151000	-0.75909200
H	2.01426200	8.03843700	-0.11428000
C	4.89511500	6.95975200	-1.59246100
H	4.98871000	5.41000700	-3.09078900
H	4.45344700	8.44479000	-0.09102200
H	5.96597300	7.13764600	-1.58185100
H	0.44136400	5.39222900	-2.00273000

IMO

Rh	4.89036300	12.52648100	3.96148700
P	4.65857100	10.24521200	4.18949200
O	1.30181200	10.37380500	1.05088000
C	3.20750200	12.94335600	5.26162400
H	2.95129300	12.02765400	5.79337000
N	6.91174700	12.04273000	3.44091800
O	8.75385200	11.10611800	2.58073800
C	2.77996600	13.03407700	3.92764000
H	2.26682400	12.16477800	3.53490400
N	3.46082500	10.78952100	1.58461500

C	2.49506700	14.32587500	3.17119100
H	2.10568800	15.07962700	3.86108800
H	1.69728400	14.13239500	2.44775000
C	3.72320000	14.87444400	2.41183100
H	3.76009300	14.42382500	1.41624500
H	3.61588000	15.95757300	2.25599700
C	4.30621000	15.23698100	5.46736100
H	3.60477900	15.92429200	4.98897400
H	4.85094600	15.82126100	6.21533700
C	5.29711000	14.71325100	4.44588200
H	6.33118100	14.71083200	4.77097900
C	5.04089700	14.57747100	3.09063300
H	5.89287200	14.48976900	2.41805600
C	3.54707300	14.09913400	6.17564900
H	4.16765000	13.70872400	6.98995800
H	2.63155700	14.48786600	6.64589000
C	5.46172600	9.71769000	5.75878400
C	5.51023000	10.63367500	6.82052700
H	5.07431700	11.61783100	6.69352100
C	6.72791000	9.03658300	8.16603800
H	7.22385000	8.77358300	9.09558100
C	6.13464700	10.29239900	8.02015600
H	6.16945400	11.01144100	8.83320600
C	6.05602800	8.45662200	5.91351600
H	6.02989900	7.73700700	5.10257700
C	6.68812800	8.12110100	7.11149000
H	7.14980200	7.14429900	7.22016300
C	5.59710300	9.27375300	2.94891800
C	5.85542500	7.23557000	1.64650000
H	5.47234000	6.26336300	1.35269300
C	5.13635300	8.01451600	2.55353500
H	4.20404000	7.63537800	2.95514800
C	7.53545100	8.95466300	1.51297600
H	8.46922000	9.32622900	1.11035800
C	7.05637600	7.70926000	1.12024300
H	7.61869000	7.11476300	0.40786500
C	6.82165200	9.74625000	2.42928000
C	7.43708900	11.01710900	2.84300200
C	9.16624700	12.46127600	2.92326400
H	9.24534300	13.02875500	1.99210900
H	10.14023300	12.40090300	3.40697000
C	8.02854800	12.95290000	3.82113900
H	7.76384400	13.97724100	3.56178200
C	8.29961500	12.86753800	5.33950500

H	7.32996400	13.03379600	5.82417900
C	8.81734700	11.49645700	5.78732900
H	8.14647100	10.68718200	5.48799200
H	8.89531800	11.46769000	6.87824400
H	9.81369900	11.28991900	5.38180000
C	9.24986600	13.99301800	5.76012200
H	10.22919000	13.88724100	5.27885900
H	9.40984200	13.97643700	6.84289500
H	8.84659800	14.97547200	5.49041300
C	2.99519400	9.46031200	4.23869400
C	2.60708700	8.80478900	5.41512500
H	3.29843100	8.74134700	6.24589300
C	1.34621700	8.22066900	5.54190400
H	1.07959600	7.71840400	6.46652600
C	0.44346500	8.27919000	4.48290300
H	-0.53764800	7.82322500	4.56833200
C	0.80452100	8.93171500	3.30751900
H	0.10664100	8.98787700	2.48114100
C	2.06535600	9.53108900	3.16741000
C	2.35211500	10.24236100	1.91192200
C	1.83740700	11.03502300	-0.12993900
H	1.15945200	11.84469400	-0.40189700
H	1.87569800	10.30180500	-0.94130400
C	3.23145300	11.51984300	0.32052400
H	3.18748900	12.58642100	0.57198400
C	4.36006000	11.32668600	-0.70525400
H	3.99472000	11.76281800	-1.64564400
C	4.68331600	9.84951900	-0.94559700
H	3.80425800	9.28194600	-1.26879100
H	5.06369500	9.38498000	-0.03357700
H	5.44813800	9.74595300	-1.72236500
C	5.60534600	12.10710200	-0.26946500
H	6.42586200	11.97009300	-0.98196100
H	5.94928200	11.76845300	0.71101300
H	5.39394600	13.17976600	-0.19751300
IM1a-exo			
Rh	9.86639400	5.16304200	25.05805400
C	10.40729700	6.62761300	28.17505100
O	9.01031400	0.96985000	25.91681500
N	9.86090100	2.95630900	25.31564300
P	10.18567500	5.09727800	27.20341000
N	12.02375700	5.44784500	24.88704000
O	14.24657900	5.29872000	25.12289600
C	10.69784100	6.58179400	29.54970500

H	10.74553100	5.63262700	30.07193900
C	10.93512600	7.76233200	30.25026400
H	11.15149100	7.72049500	31.31324600
C	7.22372600	3.69074700	29.70835500
H	6.69171300	4.05512200	30.58121600
C	8.19643400	4.49418400	29.11001400
H	8.40446100	5.46940500	29.53124500
C	8.89817800	4.05734700	27.98364800
C	10.39704000	7.86064200	27.51100600
H	10.21871200	7.88869400	26.44435500
C	10.64363400	9.03937100	28.21701100
H	10.63866100	9.98969700	27.69223600
C	10.90473700	8.99262100	29.58656600
H	11.09621300	9.90955300	30.13568600
C	6.94568500	2.42966300	29.18744100
H	6.19510500	1.79702000	29.64963700
C	7.62336100	1.98324500	28.05496400
H	7.39407600	1.01259400	27.63243300
C	9.20018000	2.27819500	26.19246400
C	8.58933400	2.78502200	27.43106700
C	9.46365200	0.76894700	24.54310600
H	8.57550200	0.68765400	23.91118200
H	10.02638800	-0.16327900	24.51130800
C	11.82400300	1.83352100	24.24866800
H	12.25594400	2.83963900	24.21099900
C	10.29466000	2.03223900	24.24142400
H	10.00485900	2.46533500	23.28030500
C	12.32975200	1.13724900	25.51621400
H	12.00851000	0.09043500	25.55278600
H	11.97944500	1.63493800	26.42314600
H	13.42353800	1.14321500	25.53679400
C	11.73593100	4.17572000	27.60922200
C	12.25811000	1.07916600	22.98734300
H	11.94440400	1.60600000	22.07921700
H	11.82726000	0.07134100	22.95816800
H	13.34740800	0.97334900	22.95906900
C	11.74092700	3.38046100	28.76139300
H	10.83316400	3.26704000	29.34184900
C	12.90017300	2.72906200	29.18604100
H	12.87235800	2.11717300	30.08203200
C	14.08285900	2.86995100	28.46343100
H	14.98902500	2.36802300	28.78622000
C	14.09619800	3.65069900	27.31150900
H	15.00547600	3.74771900	26.73099700

C	12.93407400	4.30046300	26.86747800
C	13.01190200	5.04307000	25.60674300
C	14.05457200	5.80945500	23.76775200
H	14.28143500	4.99642400	23.07292800
H	14.75452200	6.63076900	23.61951200
C	12.56974500	6.21500700	23.74146900
H	12.08449300	5.86683100	22.82591400
C	12.29881700	7.72617700	23.90332000
H	11.21807500	7.81802200	24.05807500
C	12.66669900	8.46638300	22.61317700
H	12.12335900	8.06124700	21.75216900
H	13.73965100	8.39129200	22.40022300
H	12.42163700	9.53003400	22.69816700
C	13.00665300	8.33311500	25.11914500
H	14.09517300	8.33303200	24.99433400
H	12.76664500	7.79647000	26.04070600
H	12.69290800	9.37320600	25.25459500
C	8.67021800	6.83439200	24.59924000
C	7.84177200	5.66746100	24.77758900
C	6.78543500	5.53485700	25.85066800
C	6.74477200	6.64182000	26.89235000
H	5.99992400	6.40902000	27.65708900
H	6.48403000	7.59423500	26.42208800
H	7.71106200	6.76148100	27.38357800
O	5.48935000	5.55177800	25.13822400
C	4.49477300	4.87005600	25.70982800
O	4.55176900	4.21686400	26.73485800
O	3.40023300	5.02044700	24.94926000
C	2.22954800	4.33367700	25.43147500
H	1.95161600	4.69497500	26.42461400
H	1.44189600	4.56239900	24.71375500
H	2.40297800	3.25543600	25.47040100
H	6.84625200	4.55980400	26.33476300
H	8.92427600	7.14684700	23.58388000
H	8.57855000	7.66696300	25.28941800
H	7.55607800	5.11071200	23.88068700

IM1a-endo

Rh	10.28290400	4.96603100	25.39904700
C	11.39717700	6.91207300	27.97699500
O	9.32449800	1.07860100	27.09650200
N	10.14501900	2.84788200	25.99040800
P	11.08930800	5.21725900	27.38583600
N	12.31935400	4.88031100	24.57870400
O	14.55261500	4.74888300	24.41219900

C	12.70776000	7.40204900	28.07232900
H	13.55247200	6.75167800	27.87692200
C	12.93147200	8.73496400	28.42131000
H	13.94927700	9.10543300	28.49461600
C	8.94136100	4.38475900	30.80406800
H	8.75463700	4.88178900	31.75064800
C	9.74959400	5.00394800	29.84846600
H	10.18927600	5.96700500	30.07519900
C	10.00785800	4.39435100	28.61655800
C	10.31524200	7.77310300	28.23077100
H	9.29704300	7.40651900	28.16076900
C	10.54659000	9.10001300	28.58643700
H	9.70528700	9.75540800	28.78932200
C	11.85460600	9.58418500	28.67905200
H	12.03184200	10.61978300	28.95274400
C	8.38682700	3.13449100	30.54124600
H	7.75704900	2.64586100	31.27744800
C	8.64612500	2.50451100	29.32634800
H	8.22193300	1.52966100	29.11947300
C	9.66998600	2.38439400	27.09652100
C	9.44760500	3.11740200	28.35205000
C	9.43275600	0.62369300	25.71291500
H	8.41978500	0.54898700	25.30946300
H	9.90024800	-0.36033800	25.72228600
C	11.74535200	1.37251700	24.77468900
H	12.21809600	2.30282800	24.44417700
C	10.26534100	1.72578400	25.03025500
H	9.80889900	2.02775800	24.08384000
C	12.46991500	0.88839400	26.03514000
H	12.08554600	-0.08081700	26.37279200
H	12.37599100	1.60062500	26.85880000
H	13.53705600	0.76216600	25.82844400
C	12.69705200	4.34592100	27.58625000
C	11.85364700	0.35038100	23.63854700
H	11.37166600	0.71642900	22.72503400
H	11.38222100	-0.60121700	23.91068500
H	12.90389200	0.14383600	23.40820700
C	12.99800600	3.85078300	28.86181600
H	12.28269500	3.97038200	29.66679700
C	14.20676600	3.20625900	29.12232000
H	14.40959100	2.82889100	30.11944800
C	15.14430500	3.05396400	28.10292000
H	16.08730500	2.55166500	28.29239600
C	14.86644800	3.54563700	26.83150500

H	15.58800600	3.42219300	26.03364200
C	13.64836800	4.18654900	26.55110000
C	13.43716000	4.63027500	25.16573500
C	14.10788100	4.98923400	23.04557600
H	14.27925500	4.07325000	22.47472900
H	14.71610400	5.79650100	22.63845400
C	12.61040400	5.32811000	23.19484200
H	12.00882200	4.73016300	22.50435900
C	12.25039800	6.81461800	22.99300600
H	11.17427200	6.88615800	23.17662300
C	12.51517800	7.23270000	21.54302900
H	11.99891100	6.57246500	20.83694400
H	13.58450400	7.21165800	21.30385000
H	12.16038100	8.25403000	21.37128500
C	12.95772200	7.73452100	23.99238200
H	14.04728700	7.70024200	23.87558000
H	12.71433400	7.46534900	25.02438900
H	12.64487000	8.77210900	23.83575700
C	9.33146200	6.80436200	25.13122200
H	9.69677400	7.66232900	25.69018900
H	9.19256300	7.01059300	24.06983300
C	8.43298500	5.86870800	25.77284500
H	8.15491700	6.03814600	26.81348300
C	7.38092500	5.14532500	24.97203200
C	6.61393000	4.10521800	25.76769200
H	5.84138600	3.63535200	25.15249500
H	6.13859300	4.55731100	26.64441100
H	7.30166900	3.32975600	26.11292600
O	6.36947400	6.11060600	24.48178400
C	6.52891400	6.56559000	23.23988200
O	7.36919100	6.21552400	22.42916300
O	5.58345300	7.48836800	23.01362500
C	5.61026300	8.07919800	21.70000500
H	5.46032800	7.31823600	20.93038700
H	4.78794600	8.79448000	21.68709400
H	6.55963000	8.59218100	21.52757400
H	7.82495600	4.69554800	24.07958300

IM1b-exo

Rh	9.91836800	5.08773900	24.83370300
C	10.08391500	6.85859600	27.77742900
O	8.97259600	0.96625900	25.96802300
N	9.86498800	2.89543600	25.25357500
P	10.07118800	5.20999500	26.99699300
N	12.08312100	5.26677400	24.75324900

O	14.28130900	5.15275000	25.17424900
C	11.29289800	7.39088700	28.25247500
H	12.19905500	6.79712600	28.23624600
C	11.33662700	8.69257800	28.75337500
H	12.27707500	9.09308500	29.11901200
C	7.09387600	3.90350300	29.53140300
H	6.56136400	4.30425300	30.38786400
C	8.06924200	4.67918300	28.90224700
H	8.28950400	5.66490700	29.29140400
C	8.76848400	4.19678100	27.79152000
C	8.92207800	7.64938100	27.80874600
H	7.97322700	7.26148000	27.46060000
C	8.97278300	8.94492000	28.32007100
H	8.06528200	9.54031300	28.35039700
C	10.17906800	9.47145100	28.78897400
H	10.21547500	10.48276900	29.18235200
C	6.81720900	2.62120800	29.06368300
H	6.06203900	2.01015000	29.54704200
C	7.51538900	2.11798100	27.96863700
H	7.30197700	1.12159600	27.60184200
C	9.15251600	2.29370000	26.14457300
C	8.48719700	2.88934400	27.31493900
C	9.50535500	0.65057000	24.64606800
H	8.65581900	0.52424800	23.96990500
H	10.05744400	-0.28531700	24.72447100
C	11.88817700	1.68621400	24.43099800
H	12.32521800	2.68423200	24.31917200
C	10.36403900	1.88108100	24.29508500
H	10.14714300	2.22814200	23.28138600
C	12.29993900	1.12935400	25.79797100
H	11.97010700	0.09199700	25.92351600
H	11.89155100	1.72141400	26.62076800
H	13.38984300	1.13888900	25.89427500
C	11.61176800	4.40878700	27.62410800
C	12.40846000	0.80750800	23.28839000
H	12.15680700	1.23445600	22.31108000
H	11.98319000	-0.20203000	23.33481000
H	13.49745800	0.70961400	23.34500000
C	11.55197600	3.82561900	28.89631100
H	10.62113200	3.83607100	29.45004000
C	12.67396300	3.23200600	29.47477300
H	12.59465500	2.78422400	30.46015600
C	13.88624500	3.22054300	28.78792100
H	14.76436700	2.75906300	29.22750600

C	13.96837000	3.80328300	27.52751900
H	14.90469400	3.79224800	26.98357800
C	12.84331400	4.39431300	26.93078200
C	13.01153700	4.95811300	25.58896200
C	14.20298600	5.51816000	23.76414600
H	14.51552900	4.64971100	23.17859000
H	14.89400900	6.34400000	23.59879600
C	12.71719300	5.87247300	23.55631600
H	12.32220300	5.37814600	22.66456100
C	12.40893300	7.38181200	23.46085200
H	11.31932400	7.45922700	23.39749700
C	13.00313300	7.96413300	22.17398100
H	12.66742000	7.40709600	21.29193300
H	14.09900200	7.94508600	22.18753500
H	12.69500000	9.00746200	22.05143500
C	12.86198300	8.15737900	24.70108000
H	13.94842800	8.10855500	24.83766900
H	12.38375400	7.77565200	25.60772700
H	12.59151400	9.21395100	24.60391100
C	8.85736300	6.83928200	24.41344600
C	7.96184800	5.70388500	24.41053300
C	6.80856600	5.55590700	25.36235600
C	6.03575200	4.25928300	25.18930500
H	5.22945700	4.18465800	25.92480400
H	6.70250900	3.40467800	25.32114800
H	5.60293500	4.20547900	24.18487700
O	5.85758800	6.66287900	25.09147200
C	5.41212000	7.34494800	26.14268900
O	5.67856100	7.14394400	27.31617900
O	4.60478200	8.31798800	25.69875100
C	4.05033200	9.16228700	26.72635900
H	4.84535900	9.67492600	27.27360400
H	3.42665400	9.88611000	26.20199700
H	3.44574500	8.57683900	27.42320000
H	7.11619300	5.67128300	26.39774400
H	9.14998900	7.27022600	23.45444500
H	8.78141400	7.58211000	25.20531400
H	7.73640300	5.28031300	23.42451900
IM1b-endo			
Rh	9.75259300	5.55956600	25.45609400
C	11.01917300	7.50032900	27.98056400
O	9.14865500	1.59662500	27.13106200
N	9.79811500	3.42690000	26.01057800
P	10.72367300	5.80982900	27.37272500

N	11.70397300	5.64702500	24.47112100
O	13.92013900	5.67502600	24.11584100
C	12.31744700	8.03023700	27.99182800
H	13.16422900	7.41247300	27.71607400
C	12.52595800	9.36026200	28.36025500
H	13.53459400	9.76166500	28.36788000
C	8.90279800	4.80971100	30.93346500
H	8.77012100	5.27916500	31.90294500
C	9.60167500	5.48517000	29.93080800
H	10.01303100	6.46406900	30.14298200
C	9.78785000	4.91220000	28.66910500
C	9.93320000	8.31803500	28.33935900
H	8.92449700	7.91977900	28.33854000
C	10.15013600	9.64239000	28.71323300
H	9.30688000	10.26429000	28.99725100
C	11.44593200	10.16676700	28.72110400
H	11.61140300	11.20028100	29.00962400
C	8.38696500	3.53983900	30.68718300
H	7.84208000	3.00774500	31.46004900
C	8.57635300	2.94606200	29.44146700
H	8.18297500	1.95572100	29.24713500
C	9.42697600	2.91804800	27.13630700
C	9.26722600	3.61511700	28.42098000
C	9.17586000	1.17534800	25.73297200
H	8.14041400	1.05733400	25.40331200
H	9.69080500	0.21645500	25.68487200
C	11.36945100	2.05993900	24.63756900
H	11.77184700	3.02256700	24.30549300
C	9.89920000	2.33212400	25.01705100
H	9.35621200	2.63064800	24.11651200
C	12.21127000	1.56979700	25.82014600
H	11.89923400	0.57204300	26.14851700
H	12.14799200	2.24793200	26.67474800
H	13.26380900	1.50327700	25.52869300
C	12.37373200	4.99780900	27.39885200
C	11.43384200	1.08236500	23.45936100
H	10.87097500	1.45898500	22.59787300
H	11.02106100	0.10325000	23.72923600
H	12.47112700	0.92789800	23.14499600
C	12.80566500	4.45750800	28.61711800
H	12.16265300	4.51135100	29.48758600
C	14.05525300	3.84975100	28.73653500
H	14.36109900	3.43528500	29.69174400
C	14.90192500	3.78160600	27.63201100

H	15.87529500	3.30893700	27.71255700
C	14.49384200	4.32078100	26.41612900
H	15.14405700	4.26428500	25.55189500
C	13.23350600	4.92428800	26.27814000
C	12.88153300	5.43307900	24.94568900
C	13.34624600	5.98125700	22.81131400
H	13.51855700	5.11957600	22.16138800
H	13.87041300	6.85089900	22.41613600
C	11.85151900	6.21633300	23.10882300
H	11.22524800	5.64057400	22.42166800
C	11.39823000	7.69087600	23.06275000
H	10.34020900	7.68414300	23.34058000
C	11.51085700	8.23797300	21.63595400
H	10.96339100	7.61003300	20.92386800
H	12.55336700	8.29436900	21.30222800
H	11.09462500	9.24920400	21.58325900
C	12.14143100	8.56854600	24.07398500
H	13.21706400	8.60760600	23.86544300
H	12.00331600	8.20412700	25.09590800
H	11.76275600	9.59514000	24.03246100
C	8.62694500	7.32444200	25.33720300
C	7.90570000	6.30883900	26.07077300
H	7.78497100	6.44284800	27.14391100
C	6.78867900	5.48845200	25.48016500
C	6.87563500	5.26529700	23.98157800
H	6.08205200	4.59462700	23.64120800
H	6.80179400	6.20573900	23.42885000
H	7.84345800	4.80255800	23.74592200
O	5.45298900	5.37580500	27.85378700
C	4.97985100	6.02075100	26.93575100
O	5.48634600	6.15498200	25.70936100
O	3.83775000	6.72125600	26.99339200
C	3.15975900	6.67204100	28.26340700
H	3.78980200	7.08784300	29.05361400
H	2.26361500	7.27951100	28.13796400
H	2.88672700	5.64466400	28.51645600
H	6.73251100	4.52967500	26.00099800
H	8.99355900	8.20186200	25.86503000
H	8.35584300	7.53325200	24.30182200
TS1a-exo			
Rh	9.88320700	5.05221000	25.21112700
C	10.63867500	6.68096300	28.17241700
O	8.87107400	0.99202400	26.31870900
N	9.83288200	2.88503800	25.61469000

P	10.37696500	5.08523900	27.34721100
N	11.91027800	5.47451400	24.94371900
O	14.13091400	5.26101100	24.90909700
C	11.84911600	6.95621200	28.82714000
H	12.63051100	6.20781600	28.87899200
C	12.05058200	8.20429700	29.41679600
H	12.98917000	8.41207200	29.92086400
C	7.68615600	3.90094000	30.21308500
H	7.30670400	4.30368300	31.14638800
C	8.63298500	4.62495100	29.48384300
H	8.98109400	5.57998600	29.85897600
C	9.13062500	4.13089200	28.27600300
C	9.63660100	7.66299200	28.11645500
H	8.69872900	7.45394500	27.61992200
C	9.84463700	8.90478800	28.71179800
H	9.06386300	9.65770100	28.66944500
C	11.05319100	9.17868700	29.35828700
H	11.21510400	10.14921300	29.81713100
C	7.23569400	2.67115800	29.74051200
H	6.49761800	2.10559200	30.29941000
C	7.73480900	2.15904400	28.54297900
H	7.38883500	1.20027200	28.17610300
C	9.16380200	2.28563600	26.53973900
C	8.67820900	2.87488700	27.79680100
C	9.25509800	0.70975900	24.93448900
H	8.33653500	0.65420100	24.34586900
H	9.76210700	-0.25400000	24.92189300
C	11.65571000	1.62093900	24.46753400
H	12.14102200	2.59954400	24.37486000
C	10.14358700	1.90906500	24.54468200
H	9.82024300	2.33471300	23.59095900
C	12.19510200	0.93062700	25.72365700
H	11.80956100	-0.09077700	25.81511800
H	11.93594400	1.47684000	26.63350700
H	13.28578600	0.86403600	25.67642000
C	11.92471100	4.14282000	27.63359300
C	11.96770400	0.81018700	23.20528200
H	11.63369600	1.33306500	22.30223500
H	11.47366700	-0.16820600	23.23078300
H	13.04470700	0.63476000	23.11793600
C	12.03859200	3.38085200	28.80023200
H	11.21098200	3.33157800	29.49788300
C	13.21692300	2.68835300	29.08739500
H	13.28353900	2.10269000	29.99844900

C	14.29810600	2.75253800	28.21052800
H	15.21435600	2.21411800	28.42856900
C	14.20004600	3.50729100	27.04448100
H	15.03232700	3.55590700	26.35272800
C	13.01977800	4.20054300	26.74446200
C	12.96611600	4.98602100	25.51261800
C	13.79383800	5.91177500	23.63983200
H	13.86661700	5.15514800	22.85448200
H	14.52355200	6.70182900	23.47180700
C	12.35570700	6.39911900	23.86563200
H	11.73937700	6.23617600	22.97962400
C	12.23539100	7.87334600	24.31175700
H	11.19731900	8.01071400	24.62439400
C	12.50163600	8.79551400	23.11698300
H	11.82338000	8.57613600	22.28500900
H	13.52962900	8.69158100	22.75100300
H	12.35782700	9.84174400	23.40456200
C	13.12953000	8.22590200	25.50524000
H	14.19361500	8.15787500	25.25427200
H	12.93519500	7.58172300	26.36667200
H	12.93212500	9.25502700	25.82180900
C	8.92335600	6.85875000	24.65340900
C	7.95186200	5.81138300	24.46598200
C	7.01307100	5.35843000	25.38957500
C	6.66097100	6.02542000	26.67667900
H	5.62136900	5.79803500	26.91575100
H	6.79291100	7.10825600	26.62404200
H	7.27279300	5.64220900	27.49673900
O	5.02544400	6.01096700	24.37715900
C	4.17227400	5.10814600	24.60863000
O	4.30859100	4.01618700	25.19393300
O	2.90662100	5.44371200	24.11342100
C	1.88808600	4.47496300	24.33583100
H	1.72747900	4.28850100	25.40379800
H	0.97316000	4.88542500	23.89846800
H	2.12145000	3.51788300	23.85533900
H	6.55422400	4.39263300	25.21774000
H	9.35780300	7.29364400	23.75550600
H	8.79631900	7.56555800	25.46809600
H	7.95509400	5.29390800	23.50432500
TS1a-endo			
Rh	10.20818800	4.95359900	25.42145900
C	11.44860100	6.90636500	27.96129100
O	9.34237300	1.07770600	27.13589700

N	10.14417000	2.84557000	26.02026200
P	11.06982800	5.21748700	27.40269400
N	12.17745300	5.01614100	24.62597900
O	14.37350100	4.74462700	24.31246300
C	12.78517600	7.32308900	28.06194700
H	13.59439500	6.62789300	27.87403400
C	13.08065400	8.64246500	28.40624800
H	14.11721600	8.95549600	28.48190700
C	8.90235400	4.42667000	30.80721200
H	8.70066800	4.93619800	31.74385700
C	9.71141400	5.04147600	29.84898200
H	10.13803200	6.01366400	30.06169300
C	9.98476300	4.41264800	28.63137400
C	10.41522000	7.82636100	28.20974200
H	9.37805600	7.51967100	28.14603100
C	10.71930300	9.13977000	28.55971100
H	9.91464600	9.84085300	28.75738000
C	12.05149800	9.55140700	28.65430600
H	12.28472000	10.57705900	28.92303800
C	8.36646900	3.16564000	30.55950600
H	7.73667100	2.68127200	31.29833700
C	8.64204100	2.51819500	29.35644700
H	8.22882300	1.53624200	29.16156000
C	9.67672400	2.38274800	27.13058700
C	9.44297900	3.12488300	28.37978500
C	9.43427500	0.62144900	25.74947300
H	8.41556200	0.54237000	25.36243900
H	9.90627600	-0.36007900	25.75395900
C	11.72598400	1.37576800	24.76648900
H	12.19557300	2.30919100	24.43903200
C	10.25210100	1.72682100	25.05375800
H	9.77454300	2.03186800	24.11894600
C	12.47057400	0.86814500	26.00535400
H	12.09520800	-0.11044500	26.32498100
H	12.38432000	1.56006200	26.84668600
H	13.53492200	0.75180900	25.78101000
C	12.65099000	4.30267700	27.54875000
C	11.80964200	0.37152200	23.61234800
H	11.31549300	0.75517400	22.71277800
H	11.33606300	-0.58082900	23.87765400
H	12.85469200	0.16203300	23.36250300
C	12.97293900	3.76702200	28.80071500
H	12.28164100	3.87595900	29.62806800
C	14.17950000	3.09657000	29.00522600

H	14.40458000	2.68582300	29.98410300
C	15.08695700	2.96119900	27.95661800
H	16.02653100	2.43996600	28.10687900
C	14.78402500	3.49306200	26.70658400
H	15.48063300	3.38188800	25.88499700
C	13.56974700	4.15984000	26.48468600
C	13.31091400	4.66347500	25.13247200
C	13.85120500	5.04889900	22.98257400
H	13.87868700	4.12516000	22.39931800
H	14.50855600	5.79231000	22.53406100
C	12.41742400	5.53912900	23.25501600
H	11.70754000	5.06559400	22.57237400
C	12.22660500	7.06866400	23.18858400
H	11.18775400	7.25296100	23.47234600
C	12.41629500	7.55817500	21.74863000
H	11.76380200	7.01678900	21.05437000
H	13.45047700	7.43071200	21.40929700
H	12.17617100	8.62366800	21.67631000
C	13.12463100	7.82482200	24.17196400
H	14.18786700	7.66766900	23.95736600
H	12.93415700	7.52219600	25.20566300
H	12.93236800	8.90041700	24.10315400
C	9.29442400	6.80270200	25.09233100
H	9.70802700	7.69801800	25.54844300
H	9.10781000	6.88699400	24.02177200
C	8.34729300	6.02152700	25.85594900
H	8.14832300	6.26338800	26.89690500
C	7.56061100	5.00229600	25.28129300
C	6.72994400	4.08008800	26.11203100
H	5.78665000	3.87326800	25.60288300
H	6.52461400	4.49734000	27.10149900
H	7.24802900	3.12384300	26.24157500
O	5.99021500	6.05865500	24.32012800
C	6.37175900	6.36100100	23.14310600
O	7.34044500	5.92588700	22.49352700
O	5.54516900	7.31162400	22.56843600
C	5.89238900	7.70402400	21.24080100
H	5.86735900	6.85607300	20.54831800
H	5.14626600	8.44349800	20.93917500
H	6.89008400	8.15390000	21.20124500
H	7.79394100	4.69700200	24.26654000
TS1b-exo			
Rh	9.91247700	5.02920600	24.77450000
C	10.05739400	6.91049900	27.64570600

O	8.94591500	0.96810400	26.03445400
N	9.84599600	2.86973400	25.26984800
P	10.03986200	5.23152000	26.95148900
N	12.00071500	5.30223800	24.74391200
O	14.19323500	5.07332200	25.09341700
C	11.26533100	7.44568200	28.12084100
H	12.16459500	6.84200700	28.14639900
C	11.31475100	8.76646800	28.56656500
H	12.25274300	9.17247400	28.93203200
C	6.99393600	4.04348700	29.44429300
H	6.44338300	4.48068900	30.27077700
C	7.98403500	4.79250000	28.80535600
H	8.19577000	5.79406400	29.15545600
C	8.70639800	4.25952100	27.73457400
C	8.89978500	7.70866600	27.62250100
H	7.94406800	7.31769000	27.28495500
C	8.96059900	9.02402200	28.08030100
H	8.05996500	9.63032900	28.07180200
C	10.16493100	9.55749700	28.54637100
H	10.20597100	10.58448200	28.89634000
C	6.72234500	2.74501000	29.02255900
H	5.95450600	2.15660700	29.51380300
C	7.43949200	2.19540900	27.96157800
H	7.22773500	1.18678100	27.62881700
C	9.11686000	2.29785500	26.16842800
C	8.42898900	2.93617200	27.30181400
C	9.49761700	0.61102000	24.72856100
H	8.65666600	0.47374100	24.04422200
H	10.03993600	-0.32653600	24.84248200
C	11.88967900	1.62590200	24.54808700
H	12.33647700	2.61853900	24.42930000
C	10.37186300	1.82420200	24.35907900
H	10.18485700	2.13856800	23.32915400
C	12.25654000	1.09360700	25.93717700
H	11.91898700	0.06006600	26.07136300
H	11.82659500	1.70160900	26.73692800
H	13.34284200	1.10105200	26.06564000
C	11.56051500	4.43041200	27.59979300
C	12.44107100	0.72278700	23.43953500
H	12.22734100	1.13429700	22.44684200
H	12.00484800	-0.28178500	23.48966900
H	13.52635100	0.61689700	23.53650800
C	11.49577400	3.87604300	28.88309100
H	10.56700000	3.90912700	29.43983800

C	12.61684200	3.28340400	29.46593700
H	12.54008800	2.85892900	30.46163500
C	13.82430400	3.24136200	28.77161300
H	14.69899100	2.77940900	29.21707800
C	13.90713200	3.79209800	27.49636500
H	14.83936000	3.75626800	26.94643000
C	12.78494500	4.38425400	26.89842700
C	12.93830500	4.93403800	25.55213400
C	14.07892900	5.43457700	23.68071400
H	14.26544100	4.53166200	23.09380100
H	14.84133800	6.18229000	23.46942200
C	12.63264700	5.93897800	23.55679800
H	12.15736700	5.55112700	22.65281100
C	12.47706200	7.47435300	23.59467900
H	11.40240000	7.66590200	23.63528900
C	13.02070000	8.08714000	22.29941600
H	12.54239600	7.64506800	21.41820300
H	14.10278700	7.94103200	22.20485400
H	12.83152200	9.16506800	22.28193600
C	13.10932400	8.11183400	24.83569000
H	14.19528100	7.96832600	24.86259500
H	12.68342200	7.70506300	25.75724100
H	12.92057000	9.19017700	24.83654700
C	9.02653400	6.85158500	24.22176800
C	8.00528100	5.84506700	24.04592200
C	7.14092700	5.39148100	25.04695000
C	6.28332800	4.18054200	24.86380000
H	5.46997900	4.17301200	25.59015000
H	6.87530900	3.27084500	25.01046300
H	5.86734700	4.14340700	23.85299300
O	5.43235800	6.78964200	24.98691200
C	5.26003600	7.27955600	26.14165900
O	5.83886200	7.00028300	27.21213700
O	4.27585900	8.25920000	26.15427700
C	4.03440700	8.86759800	27.42126100
H	4.92525800	9.38029700	27.80044100
H	3.23561300	9.59664000	27.26115000
H	3.71558100	8.13436700	28.16961900
H	7.22753800	5.78362100	26.04947200
H	9.42836500	7.29141000	23.31064400
H	8.93734100	7.55838300	25.04289200
H	7.85858000	5.43377500	23.04566400
TS1b-endo			
Rh	9.72811200	5.53496000	25.36728900

C	10.98153300	7.51994700	27.88354800
O	9.13313700	1.61064900	27.04542800
N	9.85687900	3.42143400	25.94817100
P	10.65809600	5.82279800	27.31840700
N	11.65482100	5.74264100	24.48586200
O	13.85785500	5.64863900	24.11455100
C	12.30377800	7.97483700	28.00511700
H	13.13506400	7.30564700	27.82001900
C	12.55548500	9.29865800	28.36637700
H	13.58124400	9.64148600	28.45829900
C	8.61104700	4.90407000	30.76177000
H	8.39872500	5.39834600	31.70417900
C	9.37095100	5.56432300	29.79332600
H	9.74966600	6.55722700	30.00170800
C	9.65338300	4.95475100	28.56873800
C	9.91782700	8.40621400	28.12766600
H	8.89126500	8.06985700	28.04616200
C	10.17844900	9.72415300	28.49460500
H	9.35104400	10.39903400	28.68937200
C	11.49669700	10.17378900	28.61053700
H	11.69600800	11.20296300	28.89273700
C	8.13552400	3.61893700	30.51605500
H	7.54395900	3.10003200	31.26296000
C	8.42020700	2.99191100	29.30401300
H	8.05230200	1.99167000	29.11081800
C	9.41608400	2.92620400	27.05579300
C	9.17007000	3.64397200	28.31673600
C	9.22752100	1.17695200	25.65133000
H	8.20817100	1.05967900	25.27598100
H	9.74109800	0.21666100	25.63688000
C	11.46625300	2.03739600	24.62954400
H	11.89300000	2.99595700	24.31544500
C	9.98822900	2.32531900	24.95989200
H	9.47656300	2.62855600	24.04265100
C	12.25930800	1.52715000	25.83638300
H	11.92834200	0.52753400	26.13932600
H	12.16782300	2.19392700	26.69708500
H	13.32135900	1.45602300	25.58422300
C	12.27984800	4.97677400	27.37687800
C	11.55595800	1.06655400	23.44739400
H	11.03234100	1.45911100	22.56851400
H	11.11470400	0.09436100	23.69614100
H	12.60106600	0.89422100	23.17098900
C	12.67419400	4.41456300	28.59594800

H	12.01245100	4.46517200	29.45274400
C	13.91580800	3.79154600	28.72861200
H	14.19833800	3.35827000	29.68252500
C	14.78371100	3.73114000	27.64036500
H	15.74963500	3.24620500	27.73433600
C	14.40740200	4.29055100	26.42242400
H	15.07347900	4.23629800	25.57029000
C	13.15808400	4.91066600	26.27253200
C	12.82403200	5.45202800	24.95026800
C	13.28844400	5.99537500	22.81533700
H	13.38605300	5.12030100	22.16835600
H	13.87247600	6.82187700	22.41326500
C	11.82147000	6.34228100	23.13548700
H	11.14342400	5.83524400	22.44455500
C	11.49253000	7.85024700	23.13511300
H	10.43969000	7.92798500	23.41800400
C	11.64087900	8.42226700	21.72095600
H	11.04480900	7.85621400	20.99638200
H	12.68358300	8.40912100	21.38421600
H	11.30192200	9.46279700	21.69769200
C	12.31496400	8.63722100	24.15898100
H	13.38747000	8.60096800	23.93497800
H	12.16249300	8.25683800	25.17257900
H	12.01514700	9.69011200	24.15185200
C	8.62823700	7.31876500	25.09008200
C	7.85550600	6.46084500	25.95002000
H	7.77653200	6.67948000	27.00962600
C	7.15951900	5.30925800	25.53200100
C	6.97365200	4.87303500	24.10956100
H	6.15074900	4.16032400	24.04437200
H	6.77164000	5.72085600	23.44998800
H	7.88139300	4.37207600	23.73889400
O	5.51645600	5.43008800	27.97847300
C	4.85461700	5.92611400	27.05029200
O	5.07745700	5.90736500	25.79954100
O	3.68625500	6.62044600	27.35267800
C	3.35478600	6.68061100	28.73743800
H	4.13283700	7.18672300	29.31950700
H	2.42316100	7.24927400	28.80353000
H	3.20323900	5.68266300	29.16339200
H	6.92061500	4.60135200	26.31338600
H	9.00045300	8.25564800	25.49480800
H	8.37613300	7.36453300	24.02983900

IM2a-exo

Rh	9.82310800	5.10250500	25.34987100
C	10.48079200	6.67121100	28.48653500
O	8.98458800	1.02651400	26.31169600
N	9.81010000	2.98573900	25.62696100
P	10.28102900	5.09538500	27.57964400
N	11.97383400	5.26337200	25.02822700
O	14.19718100	5.05572100	25.19321700
C	11.77288600	7.21255600	28.59052000
H	12.63250700	6.66012500	28.23084900
C	11.96643800	8.46995600	29.16156400
H	12.97172500	8.87284800	29.23503500
C	7.65025100	3.55205100	30.35392200
H	7.27044700	3.84137000	31.32841900
C	8.58734200	4.36425000	29.71123600
H	8.93087600	5.26404900	30.20446100
C	9.08498200	4.02647400	28.45160400
C	9.38896100	7.41675800	28.96205500
H	8.38185700	7.02790400	28.89237500
C	9.59086700	8.66878200	29.54177500
H	8.73767700	9.22708900	29.91403800
C	10.87796900	9.20050800	29.64013400
H	11.03118600	10.17728800	30.08839200
C	7.21189600	2.37956900	29.74494500
H	6.47919400	1.74596800	30.23351300
C	7.72731300	2.00933600	28.50425500
H	7.40252800	1.08849700	28.03607300
C	9.17961200	2.33376500	26.55167500
C	8.66207000	2.81860600	27.84312400
C	9.37351300	0.79615500	24.92137400
H	8.45802100	0.76536200	24.32566700
H	9.88433500	-0.16415300	24.87593000
C	11.76780400	1.75670100	24.64128700
H	12.23901700	2.74045000	24.57020500
C	10.24901300	2.00998600	24.59024300
H	9.99074100	2.40469800	23.61296000
C	12.22837300	1.08532200	25.93888300
H	11.85609300	0.05741400	26.01048500
H	11.89646100	1.63263600	26.82460700
H	13.32086400	1.03985000	25.97063500
C	11.86732100	4.22943100	27.92550800
C	12.19099100	0.94737200	23.41000000
H	11.90653500	1.45862500	22.48357400
H	11.72728300	-0.04604800	23.40376400
H	13.27640400	0.80530100	23.40048600

C	11.97616800	3.56298600	29.15271300
H	11.13131500	3.53572600	29.82947100
C	13.15863500	2.92705200	29.52839800
H	13.21004200	2.41273200	30.48257100
C	14.26286000	2.95836300	28.67998300
H	15.18785900	2.46503800	28.95955000
C	14.17537600	3.62297200	27.46167700
H	15.02683700	3.64147600	26.79399600
C	12.98577200	4.25832500	27.06749000
C	12.98078200	4.89482300	25.74352300
C	13.99614700	5.49559600	23.82020800
H	14.30516800	4.67871900	23.16431900
H	14.63920600	6.36044000	23.65764200
C	12.48807200	5.79915600	23.73569000
H	12.01522300	5.22704200	22.93884300
C	12.13502800	7.28211800	23.53029900
H	11.04485800	7.31802600	23.46756600
C	12.68305000	7.77467800	22.18585000
H	12.34866500	7.13412700	21.36205100
H	13.77869000	7.79704600	22.17305400
H	12.33304800	8.79242500	21.98521000
C	12.59271000	8.16467400	24.69413500
H	13.68442200	8.16252500	24.79553400
H	12.16328400	7.82985600	25.64317800
H	12.28207400	9.20211800	24.53214100
C	9.20341200	7.29620700	25.42081900
C	8.24715000	6.49110900	24.79294800
C	7.61822900	5.39654400	25.45892900
C	6.89256300	5.55172200	26.76943300
H	5.87291200	5.89652200	26.54835100
H	7.34792600	6.29553300	27.42170500
H	6.79958500	4.60931800	27.30938000
O	7.92896900	3.60992100	22.92295000
C	8.92989500	4.22046100	22.54165600
O	9.80616800	4.85998600	23.23911800
O	9.25978200	4.27743100	21.21313600
C	8.37297600	3.57898500	20.33147300
H	7.36057800	3.99088100	20.37933500
H	8.78102500	3.71771000	19.32862900
H	8.33477000	2.51231700	20.57146400
H	7.16868700	4.67173200	24.78573900
H	9.75265300	8.01560700	24.82717500
H	9.15292500	7.50992100	26.48013700
H	8.21176800	6.52243300	23.70900400

IM2a-endo

Rh	9.80354000	5.08396000	25.58233600
C	11.29482100	6.92051700	28.13223200
O	9.23403000	1.10095600	27.11846800
N	9.83256400	2.96341500	26.03882100
P	10.89159600	5.24317700	27.53761700
N	11.70671200	5.11959600	24.61464300
O	13.85767800	4.80018300	24.09306500
C	12.53206100	7.46442500	27.74766900
H	13.25794400	6.85993400	27.21667000
C	12.83956600	8.79165900	28.04385700
H	13.79912500	9.19784800	27.73976300
C	9.19123400	4.06592600	31.10088200
H	9.10916300	4.46928800	32.10489900
C	9.86957300	4.79296400	30.11987300
H	10.32326300	5.73844300	30.38662300
C	9.98429000	4.30715900	28.81493400
C	10.37430500	7.73026900	28.81827800
H	9.41587700	7.33835500	29.13647700
C	10.69276500	9.05430400	29.11848700
H	9.97573300	9.66515100	29.65784100
C	11.92175500	9.58964700	28.72873800
H	12.16347500	10.62229600	28.96037800
C	8.63465500	2.82923000	30.78806200
H	8.10479000	2.25744300	31.54262700
C	8.76646500	2.31645100	29.49919600
H	8.34209400	1.35060400	29.25547900
C	9.52349800	2.41428900	27.16666200
C	9.43292800	3.03817400	28.49961100
C	9.15100600	0.74636500	25.70154700
H	8.09079500	0.68352300	25.44273600
H	9.62259100	-0.22728800	25.57713700
C	11.31678700	1.60255500	24.55453600
H	11.73852200	2.55993700	24.23642800
C	9.87064800	1.90563200	24.99643000
H	9.30900200	2.26722900	24.13568500
C	12.18757500	1.03765700	25.68180000
H	11.85639400	0.03638000	25.97917000
H	12.17954400	1.67797400	26.56750900
H	13.22590700	0.95241800	25.34727400
C	12.50900700	4.38268700	27.49536000
C	11.30262200	0.67040800	23.33813800
H	10.71901000	1.09926000	22.51615200
H	10.87024000	-0.30592100	23.58634700

H	12.32162700	0.49766600	22.97698100
C	12.98994900	3.85396800	28.69927900
H	12.39591000	3.93810000	29.60125500
C	14.22821400	3.21618400	28.76134100
H	14.57508900	2.80975900	29.70578800
C	15.00977900	3.10573400	27.61317500
H	15.97331400	2.60842200	27.64873600
C	14.54946000	3.63261600	26.41111800
H	15.14923800	3.54029200	25.51510700
C	13.30012000	4.27031700	26.33406400
C	12.88184200	4.76418700	25.01587300
C	13.22650200	5.07466400	22.80919400
H	13.24709100	4.14882200	22.22956300
H	13.82107300	5.83685400	22.30673800
C	11.80105800	5.51748600	23.18045100
H	11.06338200	4.93517000	22.63212800
C	11.50910700	7.01324800	22.96365100
H	10.48625800	7.17507400	23.30697200
C	11.54349000	7.33121900	21.46464300
H	10.86250000	6.67650800	20.90982800
H	12.54845000	7.20870000	21.04497200
H	11.23670400	8.36712600	21.28816500
C	12.43438500	7.92462900	23.77323500
H	13.48083400	7.81925800	23.46410000
H	12.37276000	7.70864100	24.84398900
H	12.15472400	8.97324200	23.62837800
C	9.15073800	7.13255100	25.42830700
H	9.82325300	7.91588700	25.76582600
H	8.76114500	7.22159800	24.42014500
C	8.33456200	6.48737700	26.40410500
H	8.44478200	6.73205200	27.45587700
C	7.59826300	5.33957500	26.08075500
C	6.85318300	4.54436400	27.10916800
H	5.79251600	4.82736400	27.08390500
H	7.23087300	4.71841700	28.11872200
H	6.89795700	3.47237400	26.89409200
O	9.06269400	4.50497400	23.65164700
C	8.46292000	5.18034600	22.73747900
O	7.75652100	6.18719900	22.84929900
O	8.68984800	4.61907600	21.50430000
C	8.04247500	5.26825300	20.40353800
H	8.37867700	6.30380600	20.30039000
H	8.32317700	4.69858200	19.51565500
H	6.95502200	5.25722100	20.52193200

H	7.26882900	5.22369700	25.05335000
IM2b-exo			
Rh	9.90895300	5.17540600	24.70821700
C	9.90165500	7.05306400	27.69987600
O	8.81930500	1.18854100	25.87447700
N	9.79294800	3.07509900	25.17787700
P	9.95541700	5.39038000	26.95884300
N	12.05724800	5.23878600	24.71959700
O	14.20678600	4.97334200	25.27962200
C	11.09344100	7.64570800	28.14332000
H	12.02163000	7.08599400	28.13548700
C	11.08971400	8.96368300	28.60128000
H	12.01615500	9.41278000	28.94525700
C	6.86596100	4.10931100	29.37259400
H	6.32511100	4.50035700	30.22826900
C	7.88920400	4.86850100	28.80004300
H	8.13384300	5.83054300	29.23169900
C	8.60197700	4.39865600	27.69385100
C	8.71091600	7.80081500	27.70845900
H	7.78487600	7.36300900	27.35168900
C	8.71426200	9.11356600	28.17635600
H	7.78846200	9.68003700	28.18774100
C	9.90281600	9.69750300	28.62196200
H	9.90278100	10.72152300	28.98232700
C	6.55045200	2.85908600	28.84833500
H	5.75535000	2.26349200	29.28430100
C	7.26603300	2.36571600	27.75979100
H	7.03011700	1.38996000	27.35396500
C	9.00939500	2.50927300	26.03746700
C	8.29139300	3.11886400	27.16955800
C	9.41609600	0.84017000	24.58531300
H	8.60151600	0.75829000	23.86089600
H	9.91086300	-0.12285500	24.70036200
C	11.84357700	1.74897400	24.60379300
H	12.34917700	2.71180100	24.49720600
C	10.35650400	2.01685700	24.29474900
H	10.26381000	2.36139300	23.26632900
C	12.08542600	1.22831300	26.02437700
H	11.67346800	0.22171800	26.15848300
H	11.64466000	1.88218700	26.78111700
H	13.15953000	1.17127600	26.22546300
C	11.44386700	4.61591200	27.69265000
C	12.42633600	0.79910100	23.55132900
H	12.29654100	1.19958500	22.53988000

H	11.94621200	-0.18575900	23.58873700
H	13.49738500	0.65055300	23.72271000
C	11.33583600	4.14934500	29.00906300
H	10.39251400	4.23443700	29.53481300
C	12.42389600	3.57395300	29.66262400
H	12.31055300	3.21667200	30.68098400
C	13.64632800	3.46146200	29.00357900
H	14.50000400	3.01077000	29.49869400
C	13.77210600	3.92596200	27.69898100
H	14.71771600	3.83047800	27.18200800
C	12.68123200	4.50395500	27.02642200
C	12.91144900	4.93588700	25.64039600
C	14.24540900	5.18046900	23.83998400
H	14.51907000	4.22948700	23.37644800
H	15.01290000	5.92569800	23.63594200
C	12.81569900	5.62703600	23.49504100
H	12.42978500	5.04485700	22.65967700
C	12.66745100	7.12530700	23.17514700
H	11.60916400	7.27548800	22.96625300
C	13.42868500	7.46079300	21.88850100
H	13.11212300	6.80971000	21.06648500
H	14.51275700	7.35401600	22.00901100
H	13.23181500	8.49625000	21.59226700
C	13.07490200	8.02503700	24.34433500
H	14.13578100	7.91265300	24.59800900
H	12.48567300	7.80676500	25.24083200
H	12.91041800	9.07640800	24.08646200
C	9.35179500	7.28963300	24.37019300
C	8.31781000	6.44029600	23.91407300
C	7.68213100	5.49879300	24.74642500
C	6.78544600	4.43700200	24.17274400
H	5.75589700	4.81079300	24.09551000
H	6.75514600	3.55335500	24.81590800
H	7.11809700	4.13184800	23.17695900
O	10.01381000	4.50313100	22.69273000
C	10.15030100	5.18148100	21.60523000
O	10.02674700	6.39482600	21.42391000
O	10.47213900	4.34346100	20.56846800
C	10.63459400	4.97869400	19.29507900
H	11.45284100	5.70462300	19.31570400
H	10.86966900	4.17781200	18.59166800
H	9.71675300	5.48656800	18.98473100
H	7.47600700	5.77028400	25.77738100
H	9.89704300	7.83846700	23.61341600

H	9.31255200	7.75201500	25.34758700
H	8.23699400	6.30281600	22.84099700
IM2b-endo			
Rh	9.77442700	5.12236300	25.54632400
C	11.36706600	6.93951300	28.08358300
O	9.14011500	1.18126900	27.10060800
N	9.82265600	3.01219900	26.01802600
P	10.88705600	5.28135100	27.49118800
N	11.69293300	5.20773600	24.57031000
O	13.85787700	4.92414400	24.07504700
C	12.65233700	7.40617200	27.75876600
H	13.36463500	6.75837300	27.26198600
C	13.02747900	8.71138600	28.07448900
H	14.02340300	9.05724200	27.81618500
C	9.14117000	4.18223800	31.05976200
H	9.06644300	4.59460700	32.06068300
C	9.84296400	4.88393100	30.07626600
H	10.31937700	5.82052300	30.33615700
C	9.95197400	4.38346000	28.77707500
C	10.46986700	7.80348300	28.73450200
H	9.47800400	7.47089000	29.01494000
C	10.85555000	9.10478400	29.05399300
H	10.15507700	9.75733400	29.56542500
C	12.13124900	9.56371400	28.72069500
H	12.42614700	10.57881200	28.96781000
C	8.55065200	2.95992600	30.75336600
H	8.00254100	2.40864500	31.51013700
C	8.67129900	2.43408700	29.46813700
H	8.22296500	1.47740400	29.23069600
C	9.46549900	2.48516000	27.14311700
C	9.36418000	3.12830300	28.46699200
C	9.08358300	0.81380600	25.68460900
H	8.02890400	0.77891600	25.39948600
H	9.52962100	-0.17438500	25.58279700
C	11.29978300	1.59619700	24.57975700
H	11.76210200	2.54048100	24.27724700
C	9.85383300	1.94415700	24.98600000
H	9.32137600	2.31573600	24.11140800
C	12.12271100	0.99946200	25.72589500
H	11.74805000	0.01132600	26.01543000
H	12.11777500	1.64088100	26.61076400
H	13.16430800	0.87547300	25.41523600
C	12.46525200	4.35499300	27.42846200
C	11.28315600	0.66864100	23.35978300

H	10.74050900	1.12246200	22.52328300
H	10.80428000	-0.28961500	23.59277200
H	12.30401000	0.45507200	23.02689600
C	12.92040700	3.76366600	28.61260200
H	12.32895100	3.84070200	29.51674600
C	14.13083700	3.07195800	28.65022100
H	14.45926800	2.61647000	29.57876700
C	14.90846900	2.97049600	27.49861700
H	15.84927100	2.43051700	27.51557200
C	14.47361000	3.56154300	26.31662900
H	15.07067900	3.47787100	25.41777200
C	13.25271500	4.25313200	26.26407300
C	12.86044900	4.82611800	24.96941800
C	13.26413100	5.31901000	22.80544500
H	13.32133400	4.45969200	22.13362300
H	13.86018900	6.13889000	22.40567200
C	11.81723300	5.70183800	23.16953300
H	11.11725500	5.13566400	22.55780000
C	11.49044300	7.19985000	23.04030200
H	10.45038400	7.30734900	23.34902800
C	11.57046200	7.61951300	21.56843900
H	10.92631900	6.98885000	20.94598300
H	12.59235800	7.55200900	21.17789100
H	11.24131400	8.65706600	21.45149700
C	12.36009700	8.07882800	23.94159100
H	13.42025700	8.02280900	23.66758100
H	12.26564100	7.79256100	24.99286600
H	12.05603000	9.12707100	23.85363900
C	8.98907800	7.15799400	25.35944500
H	9.63833600	7.98825800	25.62133900
H	8.57372200	7.15025600	24.35646700
C	8.32887500	6.48865000	26.41935400
H	8.56153900	6.77642800	27.43755100
C	7.65043100	5.26081000	26.24046400
O	9.05648800	4.51341700	23.62437400
C	8.64243600	5.15113200	22.59190200
O	8.20417500	6.30369100	22.50163800
O	8.72847600	4.35361700	21.47581200
C	8.26435400	4.94572000	20.25744100
H	8.85353800	5.82941800	19.99516100
H	8.38736000	4.17992300	19.48917300
H	7.21059200	5.23049800	20.33027700
H	7.47621500	4.70921800	27.16251600
C	6.66083500	4.94899600	25.15141500

H	5.65434400	5.10625300	25.56276500
H	6.78237100	5.58649700	24.27677600
H	6.72525200	3.90341700	24.83900600
TS-iso-1			
Rh	10.39559300	5.05116700	25.18076700
C	11.00526500	7.12188800	27.96873900
O	9.61453300	1.12330200	26.71346600
N	10.63202200	2.92197100	25.85352600
P	10.91469900	5.42141900	27.32799000
N	12.33457000	5.35933900	24.71474900
O	14.51676100	4.94231400	24.61038400
C	12.25861700	7.73034800	28.13574700
H	13.16952000	7.16295800	27.98268200
C	12.33995200	9.07443900	28.50141100
H	13.31412000	9.53594000	28.62957700
C	8.35258900	4.27228900	30.34354200
H	7.96974800	4.71788900	31.25594600
C	9.24638400	4.99212100	29.54737000
H	9.55044800	5.98286900	29.86033300
C	9.75553200	4.45195400	28.36300000
C	9.83767400	7.87686200	28.16745500
H	8.86255400	7.41990700	28.04504900
C	9.92667200	9.21622900	28.54188500
H	9.01848600	9.78829000	28.70421200
C	11.17686400	9.81822600	28.70641300
H	11.24282900	10.86278900	28.99482000
C	7.96201100	2.99174200	29.96369500
H	7.26421400	2.42545500	30.57166800
C	8.47931200	2.42699200	28.79943900
H	8.19060900	1.42380700	28.51186100
C	9.91194000	2.43389500	26.80393400
C	9.37637200	3.13469700	27.98696300
C	10.06945800	0.68403000	25.39628200
H	9.18601200	0.57511800	24.76336100
H	10.55726200	-0.28191500	25.52224200
C	12.50708300	1.51051600	25.00273100
H	13.01800700	2.45292800	24.77982000
C	10.99803300	1.82176000	24.93315300
H	10.76037300	2.12925600	23.91374400
C	12.95796800	1.03543700	26.38705100
H	12.52284000	0.06140200	26.63691400
H	12.68129300	1.74641200	27.16998100
H	14.04599300	0.92237200	26.41103900
C	12.54198400	4.68329000	27.71459400

C	12.88542600	0.50740700	23.90792600
H	12.60306700	0.87803600	22.91612700
H	12.38993000	-0.45833800	24.06035100
H	13.96540100	0.32816400	23.90842700
C	12.78677000	4.26584700	29.02586800
H	12.01515600	4.38219000	29.77884400
C	14.00934400	3.69314100	29.37824500
H	14.17606600	3.36875500	30.40031300
C	15.00566200	3.53656900	28.41602700
H	15.95700600	3.08610500	28.67869600
C	14.77902100	3.95385100	27.10801500
H	15.54894700	3.82630300	26.35797600
C	13.55163100	4.52987900	26.74144800
C	13.39698600	4.95883100	25.34804600
C	14.11056600	5.16876500	23.22339000
H	14.04653200	4.19141300	22.73800800
H	14.88194200	5.77504600	22.75334900
C	12.75063000	5.85554100	23.36648200
H	12.03539200	5.48880000	22.63123700
C	12.81725200	7.39840500	23.30668000
H	11.81196500	7.76466400	23.51457000
C	13.17715100	7.83885000	21.88205700
H	12.48696400	7.40865800	21.14785200
H	14.19447600	7.54117500	21.60449600
H	13.12077500	8.92889100	21.80055100
C	13.75996800	8.01214300	24.34685700
H	14.80008500	7.70617000	24.19017500
H	13.47007600	7.74039000	25.36670600
H	13.72502700	9.10413800	24.27826000
C	9.79371400	6.96096900	24.65616100
H	10.39054800	7.71094300	25.17739200
H	9.91679100	7.03399700	23.57398000
C	8.38164200	6.93913200	25.06273200
H	8.15451600	7.16637600	26.10294400
C	7.35767900	6.59916200	24.25324500
O	9.95686700	4.43707000	23.18736600
C	8.83995200	3.81254800	23.31750600
O	8.23905100	3.65214800	24.39546000
O	8.36075600	3.32744500	22.14926300
C	7.10604400	2.63205400	22.22795900
H	6.88199500	2.31301300	21.20920000
H	7.18148400	1.76011700	22.88309100
H	6.31529800	3.29292100	22.59315300
H	7.57300200	6.36613500	23.20992700

C	5.92745200	6.50501900	24.67558100
H	5.29188800	7.17730300	24.08427200
H	5.54133900	5.49060700	24.51067200
H	5.80179400	6.75279000	25.73439500
IM-iso-1			
Rh	10.44772900	4.89672500	25.15039600
C	10.71325500	6.93797200	27.93758300
O	9.96544800	0.86587100	26.52115800
N	10.79811400	2.77779500	25.71187600
P	10.86860200	5.25005800	27.28973400
N	12.42587000	5.26245800	24.73128600
O	14.60969500	4.81875400	24.68852800
C	11.86054100	7.69203700	28.22181800
H	12.84421500	7.23984900	28.16156000
C	11.73750200	9.03364200	28.58655100
H	12.62888400	9.61239400	28.80776300
C	8.35686400	3.79367300	30.20495900
H	7.91078400	4.18311800	31.11432300
C	9.18527800	4.61506700	29.43703600
H	9.37647400	5.62804200	29.76838100
C	9.77344100	4.14779300	28.25812400
C	9.44594300	7.53889700	28.01426800
H	8.55503900	6.96284700	27.78902400
C	9.33106100	8.87576800	28.38808200
H	8.34841500	9.33216600	28.45413700
C	10.47633300	9.62557100	28.67119000
H	10.38438700	10.66880300	28.95738700
C	8.11183300	2.48466700	29.80110700
H	7.46746400	1.83859600	30.38813000
C	8.70251700	1.99691400	28.63708100
H	8.51893300	0.97608900	28.32615100
C	10.13272400	2.19576800	26.65163200
C	9.53426400	2.80784600	27.85201400
C	10.43521200	0.51983600	25.18073000
H	9.55260400	0.37898000	24.55154900
H	10.99079000	-0.41383200	25.25609200
C	12.80046200	1.54836900	24.85845800
H	13.24229100	2.53197100	24.67637300
C	11.27309900	1.74202900	24.76380000
H	11.01856100	2.06332800	23.75188800
C	13.25985000	1.06895500	26.23909000
H	12.90676300	0.05343400	26.44996000
H	12.90730000	1.72872800	27.03648200
H	14.35303700	1.05133700	26.28508400

C	12.54562300	4.68831600	27.75473400
C	13.28120300	0.61277200	23.74437100
H	12.98571800	0.98642500	22.75767300
H	12.86789900	-0.39571500	23.86093100
H	14.37237100	0.52637300	23.76196600
C	12.77241800	4.35982100	29.09564900
H	11.96662000	4.45256200	29.81525600
C	14.01931600	3.90309200	29.52191400
H	14.17015500	3.64801400	30.56582400
C	15.05951100	3.77048300	28.60381900
H	16.03136700	3.40912600	28.92306500
C	14.85134400	4.09794500	27.26778200
H	15.65709000	3.98978800	26.55338500
C	13.60052400	4.56083700	26.82570300
C	13.47447700	4.89767800	25.40314500
C	14.22962400	4.95607900	23.28400900
H	14.16065000	3.94982100	22.86238000
H	15.01446700	5.52167500	22.78608000
C	12.87748600	5.66785700	23.36439100
H	12.17044500	5.27479300	22.63213000
C	12.97816700	7.20377900	23.21243400
H	11.98435100	7.60713000	23.40802300
C	13.33981300	7.54868600	21.76229600
H	12.62830100	7.10185000	21.05905200
H	14.34317900	7.19734800	21.49686800
H	13.32258100	8.63337000	21.61728300
C	13.94334100	7.85626200	24.20786800
H	14.97470200	7.51645200	24.06564600
H	13.65365400	7.65602100	25.24437600
H	13.93349400	8.94218200	24.07054700
C	9.89053700	6.83693200	24.59245600
H	10.46344800	7.53416400	25.20941200
H	10.21916400	6.90074100	23.55241100
C	8.43432200	7.07652000	24.67609600
H	8.00160400	7.17850700	25.67084800
C	7.60924000	7.14383900	23.61843300
O	9.46711600	4.21491700	23.23957800
C	8.41852900	4.06277000	23.93336600
O	8.42529600	4.29790300	25.19169000
O	7.31225300	3.64559500	23.32450900
C	6.13460600	3.49461200	24.14922000
H	5.33569500	3.21487100	23.46307200
H	6.28705900	2.70603600	24.89005900
H	5.89269200	4.43381400	24.64919300

H	8.03205200	7.03149400	22.61847800
C	6.12560100	7.34910700	23.69488400
H	5.81447100	8.25723100	23.16105400
H	5.58652900	6.51540700	23.22535000
H	5.78453800	7.43164200	24.73232000

IM-iso-2

Rh	10.44585300	4.83641600	24.98562800
C	10.40617600	6.86329100	27.82894900
O	10.02332200	0.77707500	26.28472300
N	10.83330400	2.72721300	25.54829700
P	10.70847300	5.20608300	27.15147200
N	12.43028000	5.21331100	24.65978500
O	14.62737500	4.85942700	24.76657600
C	11.49664400	7.71729200	28.05970700
H	12.51041100	7.36775200	27.89695500
C	11.27972200	9.01710100	28.51458800
H	12.12737800	9.67132800	28.69308700
C	8.21253100	3.54270600	29.98084600
H	7.74472700	3.88552200	30.89803300
C	9.02359100	4.41695900	29.25465000
H	9.17719400	5.41904800	29.63244000
C	9.64254300	4.01813900	28.06476100
C	9.09958400	7.33224100	28.03622100
H	8.24843000	6.69356400	27.83275700
C	8.89310400	8.62358500	28.52085000
H	7.88070400	8.97228200	28.69746700
C	9.97936600	9.46799900	28.75570600
H	9.81399300	10.47577200	29.12426200
C	8.01118200	2.24365500	29.52560600
H	7.37702800	1.55718500	30.07677200
C	8.64087400	1.81758800	28.35884200
H	8.50265100	0.80125300	28.01215400
C	10.13380700	2.11025000	26.43883600
C	9.46177600	2.68125500	27.61883400
C	10.59825800	0.46366500	24.97785000
H	9.76842200	0.30408700	24.28456300
H	11.17741300	-0.45246700	25.08383700
C	12.94259500	1.57164400	24.87003100
H	13.36833100	2.56605700	24.71817100
C	11.42404500	1.71587000	24.63822400
H	11.24937500	2.03264300	23.60844500
C	13.29615800	1.12040700	26.29066500
H	12.94058600	0.10378800	26.49127400
H	12.87343900	1.78891700	27.04576700

H	14.38251400	1.11975400	26.42323300
C	12.39509300	4.77205000	27.71738500
C	13.54792200	0.64433900	23.81109600
H	13.32435500	0.99906200	22.79883200
H	13.16109200	-0.37703600	23.90311300
H	14.63593700	0.59683200	23.92168800
C	12.56833400	4.51992500	29.08310000
H	11.72085100	4.59562900	29.75488700
C	13.81368200	4.16251000	29.59729400
H	13.92067800	3.96521600	30.65899500
C	14.90947900	4.05282400	28.74280300
H	15.88198200	3.76679100	29.12934400
C	14.75671000	4.30860800	27.38453400
H	15.60718300	4.22140000	26.72123000
C	13.50723700	4.67480800	26.85351000
C	13.45031000	4.93512700	25.41007800
C	14.33056800	4.87639700	23.33742300
H	14.35772700	3.84269000	22.98348300
H	15.10825000	5.45998000	22.84943900
C	12.93024500	5.49656900	23.27703200
H	12.29022200	4.96903800	22.56770000
C	12.93556900	7.00432100	22.94072800
H	11.90131100	7.34282100	22.99586900
C	13.40398900	7.20755600	21.49429100
H	12.80754400	6.60953400	20.79625800
H	14.45653600	6.93526800	21.35978000
H	13.29938100	8.25972600	21.21140400
C	13.75631100	7.83932900	23.92837700
H	14.81594500	7.56108100	23.91880000
H	13.38376700	7.73483400	24.95236900
H	13.69257600	8.89892800	23.66111900
C	9.90932000	6.75693600	24.36627000
H	10.60511500	7.49027700	24.78218900
H	10.09096900	6.64297900	23.29123900
C	8.50481600	7.15584300	24.60500900
H	7.72808600	6.50365900	24.20650200
C	8.12571100	8.26890200	25.25178800
O	9.63223700	4.06430400	23.01902900
C	8.55375300	3.85489600	23.64868500
O	8.43474400	4.18970700	24.87950300
O	7.54648800	3.27472300	23.00228100
C	6.33889200	3.03135700	23.76047500
H	5.65532300	2.54524400	23.06509400
H	6.54644500	2.37439700	24.60811600

H	5.91171900	3.97254200	24.11316100
H	8.89592800	8.93072900	25.64685600
C	6.70609100	8.68618200	25.48945900
H	6.49815000	8.78218100	26.56367300
H	6.49512600	9.66854100	25.04630500
H	5.99835100	7.96362900	25.06953100

TS-iso-2

Rh	10.37491200	5.02991300	25.07309400
C	10.96242100	7.13923700	27.86718400
O	9.57824600	1.13489800	26.62753600
N	10.63366900	2.92355500	25.79293200
P	10.85669700	5.43734900	27.23048500
N	12.31718500	5.38793800	24.65605000
O	14.49531200	4.95157500	24.56165200
C	12.22203000	7.74691800	27.98489100
H	13.12581600	7.17830800	27.79858500
C	12.31958000	9.09174800	28.34306900
H	13.29889000	9.55152500	28.43186000
C	8.26801800	4.29364900	30.22940200
H	7.87726500	4.74045000	31.13783900
C	9.17135500	5.01162000	29.44215500
H	9.47497300	6.00066200	29.76007200
C	9.69099900	4.47119800	28.26266900
C	9.80591300	7.89684100	28.11151400
H	8.82751600	7.44034700	28.03101700
C	9.91057400	9.23714200	28.47916400
H	9.00973400	9.80967000	28.67688100
C	11.16664300	9.83824800	28.59161000
H	11.24547200	10.88344500	28.87439700
C	7.87816300	3.01405200	29.84610400
H	7.17226100	2.44977300	30.44650100
C	8.40941400	2.44667100	28.68951300
H	8.12527300	1.44232800	28.40139300
C	9.87885200	2.44380600	26.72168700
C	9.31711700	3.15216000	27.88711200
C	10.07064600	0.68911000	25.32578500
H	9.20735000	0.59687300	24.66280700
H	10.53708600	-0.28527100	25.46618600
C	12.53247800	1.48386500	25.03887100
H	13.06620100	2.41662100	24.82833300
C	11.03206600	1.81199000	24.89735500
H	10.84678200	2.11220900	23.86530200
C	12.91595600	1.01829000	26.44617500
H	12.45269900	0.05552700	26.68889500

H	12.62137100	1.74359200	27.20895000
H	13.99968300	0.88566800	26.51643200
C	12.47975700	4.69068300	27.63914200
C	12.94633900	0.46302000	23.97354200
H	12.70910200	0.82221100	22.96588000
H	12.43717400	-0.49670500	24.11826800
H	14.02380400	0.27520800	24.02157900
C	12.70797600	4.28552800	28.95705400
H	11.93048300	4.41647000	29.70151300
C	13.92194000	3.70557300	29.32813200
H	14.07524400	3.39206900	30.35569500
C	14.92644300	3.52709100	28.37839600
H	15.87039200	3.07022300	28.65618200
C	14.71714900	3.93232800	27.06369600
H	15.49355100	3.79156200	26.32251400
C	13.49966500	4.51690500	26.67970100
C	13.36869800	4.95869100	25.28905700
C	14.10136600	5.23758100	23.17951500
H	14.00588200	4.27960700	22.66149400
H	14.89236400	5.83493200	22.73083700
C	12.76503800	5.95951400	23.35095300
H	12.04878200	5.67403000	22.58125900
C	12.88947300	7.50019700	23.41784600
H	11.91496000	7.88120500	23.72633500
C	13.18164300	8.04661500	22.01552200
H	12.41846300	7.72555200	21.29815700
H	14.15695100	7.71150600	21.64469600
H	13.19351000	9.14093700	22.03121400
C	13.91694900	7.99504000	24.44211900
H	14.93569500	7.68255500	24.18999000
H	13.68679100	7.64313500	25.45215300
H	13.90617600	9.08935700	24.47039600
C	9.73059300	6.90222000	24.44435300
H	10.07843400	7.67913100	25.12792200
H	10.11775800	7.05316400	23.43680700
C	8.27655200	6.68588200	24.45496600
H	7.85322700	6.17877500	23.58955100
C	7.44033800	6.99923800	25.46621000
O	10.00522000	4.33936500	23.09111900
C	8.89654400	3.69909100	23.21870900
O	8.23941300	3.62803400	24.27516700
O	8.49562500	3.08909800	22.08202800
C	7.26030500	2.35849200	22.16429300
H	7.09237100	1.95242300	21.16604000

H	7.33569800	1.54396100	22.88971500
H	6.43418500	3.01802300	22.44286200
H	7.84020300	7.52320100	26.33067200
C	5.97774200	6.68890400	25.48917800
H	5.72695900	6.05742900	26.35265000
H	5.37671500	7.60205200	25.59209000
H	5.66194800	6.16723800	24.58036000

E-TS2a

Rh	9.96421500	5.05385100	25.62901400
C	11.12437100	6.65781800	28.50753100
O	9.10889600	0.97228000	26.83529700
N	9.77343800	2.90865400	25.92639800
P	10.82135000	5.05061900	27.68142300
N	12.04494400	4.99105200	24.85415800
O	14.23044700	4.57466000	24.55679300
C	12.39089400	7.24853700	28.37629000
H	13.19742400	6.71229200	27.88904700
C	12.62506200	8.53161100	28.87251300
H	13.61018700	8.97511200	28.76449700
C	8.87599400	3.60093700	31.02650700
H	8.74424500	3.91882200	32.05584100
C	9.63499900	4.38365500	30.15531500
H	10.09350300	5.28885300	30.53122800
C	9.82009100	4.01396200	28.81887700
C	10.09583300	7.37970500	29.13670400
H	9.10412700	6.95398600	29.23405400
C	10.33941200	8.65582500	29.64270100
H	9.53636600	9.19719400	30.13086800
C	11.60230700	9.23650000	29.50920000
H	11.78694500	10.23304200	29.89862300
C	8.30069100	2.41721600	30.57216700
H	7.70575300	1.80147800	31.23874500
C	8.50011100	2.01571300	29.25415900
H	8.06603900	1.08911100	28.90017900
C	9.40667000	2.28021500	26.99170000
C	9.25185400	2.79792100	28.36324600
C	9.11728300	0.70781900	25.40071400
H	8.07768700	0.60641100	25.07829600
H	9.64436600	-0.23274600	25.24079400
C	11.25273400	1.71332800	24.30473500
H	11.62690200	2.70354100	24.03699000
C	9.81242000	1.94171500	24.79972600
H	9.23501200	2.36900100	23.98083400
C	12.17126300	1.12372800	25.37915400

H	11.89875100	0.08956300	25.61926900
H	12.14051500	1.70754500	26.30236200
H	13.20826800	1.11647200	25.02808800
C	12.47414100	4.23313100	27.80343700
C	11.24101600	0.85387900	23.03659700
H	10.62026100	1.30773600	22.25603300
H	10.85248800	-0.15196500	23.23548100
H	12.25570900	0.74241800	22.64014100
C	12.83302500	3.72884900	29.06166700
H	12.13543400	3.79688900	29.88706700
C	14.07422000	3.13695000	29.28536800
H	14.31627400	2.75376400	30.27155500
C	14.99258500	3.04279100	28.24184700
H	15.96209100	2.58132500	28.39902800
C	14.65993900	3.54214700	26.98826900
H	15.36637000	3.46418700	26.17220600
C	13.40896500	4.13922500	26.74801300
C	13.15455100	4.60459700	25.37677200
C	13.74918100	4.87046200	23.21592100
H	13.82016600	3.95191700	22.62827100
H	14.40669700	5.62792100	22.78806800
C	12.29618500	5.33441700	23.43072600
H	11.60090100	4.75039600	22.82799100
C	12.03430800	6.82302400	23.14443200
H	10.98357400	6.98457100	23.38931600
C	12.20782500	7.10901000	21.64937000
H	11.56926300	6.45025100	21.05045000
H	13.24465000	6.96474800	21.32372700
H	11.93333300	8.14468900	21.42306700
C	12.87449600	7.75573000	24.01977500
H	13.94739900	7.63602200	23.82829300
H	12.69703000	7.56854300	25.08374200
H	12.62154300	8.80164200	23.81616900
C	9.16269600	7.71224500	24.89510900
H	10.00950600	8.38492300	24.98111600
H	8.91623300	7.34435800	23.90690200
C	8.86118200	6.89639000	26.01794100
H	9.11624200	7.32346300	26.97967900
C	8.00522300	5.73630300	26.00552100
C	7.21053600	5.34151000	27.22628900
H	6.23434700	5.84557300	27.23166200
H	7.72429100	5.60658800	28.15293800
H	7.01909600	4.26362500	27.24867900
O	7.92892300	6.03915300	22.65323000

C	8.80862600	5.16820500	22.62714600
O	9.43399200	4.61116800	23.59021900
O	9.23358000	4.65497600	21.41851400
C	8.60377800	5.20644100	20.25885900
H	8.77351200	6.28505700	20.18884500
H	9.06142900	4.70563600	19.40322100
H	7.52574000	5.01805000	20.26219600
H	7.48853700	5.54781300	25.06514400
C	8.02453900	10.89300200	28.11710100
C	8.28817400	10.57117100	26.78680700
C	7.50833100	9.60381000	26.14434900
C	6.48450100	8.94696100	26.83402700
C	6.23330900	9.27186500	28.16745600
C	6.99931100	10.24486000	28.81309100
H	8.62591800	11.64882600	28.61271300
H	9.09088800	11.06262700	26.24442300
H	5.89298400	8.19150500	26.32624700
H	5.43565800	8.76238200	28.69945600
H	6.80076600	10.49690200	29.85006100
N	7.84180300	9.18730600	24.82903400
H	7.05507400	8.78026400	24.32761100
H	8.27153300	9.91826500	24.26504900

(R)-TS3

Rh	9.85302200	5.18753200	25.38282600
C	11.46532000	7.03276300	27.86523000
O	9.12899700	1.26087400	27.13486000
N	9.79439000	3.04049000	25.94563700
P	11.00423700	5.36955300	27.26385800
N	11.69516000	5.10084400	24.30079500
O	13.84861300	4.86341400	23.73052500
C	12.78120900	7.48854400	27.69179900
H	13.54413900	6.82428300	27.30239400
C	13.12060000	8.80184800	28.02037900
H	14.14304100	9.14029700	27.88315900
C	9.34726800	4.46445900	30.93430600
H	9.30837700	4.93473300	31.91167700
C	10.04066400	5.08937700	29.89557600
H	10.54030900	6.03026800	30.08837100
C	10.10536300	4.51908100	28.62081200
C	10.49451600	7.91707600	28.36819300
H	9.47021300	7.59326500	28.51036100
C	10.84216200	9.22458800	28.70285000
H	10.08322800	9.89208800	29.09785500
C	12.15404900	9.67144800	28.52722800

H	12.42056900	10.69173200	28.78578500
C	8.71733700	3.24306900	30.71156500
H	8.17453200	2.74899700	31.51072300
C	8.79040000	2.64758400	29.45423200
H	8.30809600	1.69391700	29.27877700
C	9.49261100	2.56275300	27.10330400
C	9.47320300	3.26748100	28.39750800
C	8.99988800	0.83770400	25.74249000
H	7.93233500	0.78492000	25.51223600
H	9.44537800	-0.15275900	25.65529500
C	11.13120300	1.56945200	24.43939100
H	11.56465200	2.50004400	24.05958100
C	9.72575100	1.94293000	24.95437700
H	9.12969800	2.29565500	24.11159300
C	12.04867700	1.02343900	25.53845800
H	11.70115800	0.05004300	25.90309200
H	12.11538300	1.70460600	26.39070700
H	13.06173000	0.88333000	25.14878200
C	12.59497700	4.45791900	27.18201900
C	11.01466100	0.58778800	23.26846900
H	10.39848700	1.00192300	22.46262400
H	10.56354000	-0.36049000	23.58415800
H	12.00365900	0.36120100	22.85676500
C	13.10765000	3.92804900	28.37250200
H	12.55484000	4.05265300	29.29625200
C	14.32136200	3.24211700	28.39549100
H	14.69200000	2.83597900	29.33115400
C	15.04996600	3.08529500	27.21774000
H	15.99392000	2.55021300	27.22146700
C	14.56159900	3.61473000	26.02758300
H	15.12053800	3.48784700	25.10909200
C	13.33442300	4.29810400	25.98837200
C	12.88723300	4.78557100	24.67536800
C	13.17644900	5.14042800	22.46701600
H	13.21180800	4.22732600	21.86743000
H	13.73150400	5.93204400	21.96373700
C	11.74422400	5.52798500	22.87973600
H	11.00639400	4.94298300	22.33102200
C	11.39405000	7.01998500	22.72301800
H	10.38120000	7.12907400	23.11805800
C	11.36044000	7.39427100	21.23779100
H	10.68140000	6.73741200	20.68352600
H	12.35249300	7.32182800	20.77648900
H	11.01314300	8.42489000	21.11075700

C	12.31696700	7.93633800	23.53072400
H	13.35327900	7.88493000	23.17671400
H	12.30647100	7.67829400	24.59421400
H	11.99155900	8.97784600	23.43785800
C	9.08146900	7.12416200	25.39514800
H	9.69474900	7.89505400	25.85466500
H	8.67192600	7.38709700	24.42420000
C	8.24683500	6.31582600	26.26327400
H	8.34297400	6.40267400	27.34181100
C	7.04895000	5.67929600	25.82898300
C	6.43327500	4.58667300	26.65193300
H	5.38449700	4.42271600	26.39215200
H	6.51745800	4.79374100	27.72243600
H	6.96951000	3.65303200	26.44767200
O	7.64591900	6.31359000	22.72891100
C	8.34112800	5.29584500	22.61878700
O	8.91699000	4.60209900	23.52729000
O	8.56360200	4.74548100	21.37346800
C	7.92013000	5.41009600	20.28211900
H	8.26493600	6.44365400	20.18506300
H	8.19112200	4.84654100	19.38687800
H	6.83249900	5.41000400	20.40287300
H	6.88350500	5.64706500	24.75683400
C	7.23816500	9.81257900	28.06521800
C	6.77792300	9.07861400	26.97207100
C	5.96911400	7.95617900	27.18090300
C	5.62888300	7.56547500	28.48194500
C	6.09615300	8.30452300	29.56804500
C	6.90431300	9.42766100	29.36593700
H	7.86226000	10.68477400	27.89755000
H	7.04479700	9.36513900	25.95964800
H	5.00507500	6.68980900	28.63430400
H	5.82715500	8.00134200	30.57539700
H	7.26600800	9.99973400	30.21458800
N	5.61429900	7.13583600	26.08296700
H	4.72991400	6.64683200	26.20067800
H	5.62750100	7.62756800	25.19241800
E-TS2b			
Rh	9.77021000	5.04450100	25.49892600
C	11.19620100	6.98366900	28.11973900
O	9.21157200	1.13502200	27.20064800
N	9.87532700	2.95701600	26.08009200
P	10.85117400	5.32188800	27.43641900
N	11.71932400	5.07101200	24.45772100

O	13.91299400	4.92016300	24.00908400
C	12.45009100	7.57253500	27.90189800
H	13.24694900	7.00583500	27.43351600
C	12.68213000	8.89507400	28.28447800
H	13.65787100	9.33859300	28.11148000
C	9.24214500	4.21223800	31.08771200
H	9.19661800	4.63936400	32.08444700
C	9.90852100	4.90313700	30.07330600
H	10.38008000	5.84741800	30.31117200
C	9.98529900	4.39327800	28.77308500
C	10.17659000	7.74418300	28.72062900
H	9.19292000	7.31486900	28.87508200
C	10.41677500	9.06099700	29.10921100
H	9.62334200	9.63403300	29.57911700
C	11.66941300	9.64042900	28.88984800
H	11.85353000	10.66755200	29.18950700
C	8.64723600	2.98285200	30.81796500
H	8.12285900	2.44019700	31.59764600
C	8.74125000	2.44049200	29.53903900
H	8.30100700	1.47419000	29.32597000
C	9.51052100	2.45098500	27.20929500
C	9.40412300	3.12630800	28.51017000
C	9.20733500	0.72509300	25.79782400
H	8.16350500	0.64877100	25.48108200
H	9.68478000	-0.25232200	25.73763300
C	11.43089800	1.54361300	24.73064100
H	11.86061600	2.49096800	24.39369000
C	9.96339200	1.85694700	25.08564500
H	9.44194800	2.18437900	24.18731900
C	12.24972400	1.03791600	25.92270700
H	11.90595000	0.05211800	26.25611900
H	12.19992400	1.72363700	26.77243700
H	13.30263700	0.93879700	25.64144500
C	12.50914600	4.51746400	27.40845900
C	11.48248800	0.55939000	23.55706700
H	10.93846500	0.94788600	22.68886300
H	11.04181200	-0.40803300	23.82504700
H	12.51874300	0.37686800	23.25397900
C	13.01045000	4.04441300	28.62875600
H	12.41560000	4.14889100	29.52813100
C	14.26179800	3.43712800	28.71658700
H	14.61826000	3.07628500	29.67608000
C	15.04390900	3.29922300	27.57183300
H	16.01829300	2.82445300	27.62304200

C	14.56909600	3.77183000	26.35336700
H	15.17046200	3.66063400	25.46029400
C	13.30558300	4.37992800	26.24820100
C	12.90045100	4.81709500	24.90179700
C	13.29665400	5.12617100	22.70620000
H	13.37330000	4.18746100	22.15063700
H	13.86047600	5.90467000	22.19256300
C	11.84335500	5.50401700	23.04309900
H	11.14045500	4.92391600	22.44323100
C	11.50090000	6.99697100	22.87985100
H	10.46092700	7.08469100	23.19903600
C	11.55423800	7.38861300	21.40014100
H	10.89008400	6.75183700	20.80736800
H	12.56758900	7.30791100	20.98929400
H	11.22961900	8.42660000	21.26956400
C	12.37514200	7.90823100	23.74523700
H	13.43078100	7.85881300	23.45291600
H	12.30368500	7.64831000	24.80574400
H	12.05676900	8.95076700	23.63778900
C	9.11899400	7.84361600	25.56720800
C	8.35089700	6.66996500	25.33682600
H	7.91273900	6.59405500	24.34782400
C	7.94538700	5.70390500	26.32799700
C	6.73003500	4.83447300	26.10066900
H	6.78540900	3.91984900	26.70260800
H	6.64840700	4.54226200	25.05035900
H	5.80567400	5.35673100	26.38472300
H	8.06989100	5.99674600	27.37168000
C	4.46683600	8.17342500	25.32988800
C	5.65959100	8.45029100	25.99911400
C	6.66625000	9.16597600	25.34534500
C	6.49392100	9.58844800	24.02367300
C	5.29851800	9.30663900	23.36380800
C	4.28217000	8.59856700	24.01244300
H	3.68283700	7.62319000	25.84111900
H	5.81293700	8.11840000	27.02152900
H	7.29130100	10.13042500	23.52329300
H	5.16217600	9.64023700	22.33962100
H	3.35395000	8.38014000	23.49377000
N	7.92383300	9.34394100	25.98191100
O	8.83514200	4.26225200	23.74713200
C	8.49309200	4.80655700	22.63839900
O	8.53772900	5.99136700	22.29107700
O	8.01287400	3.84868900	21.77054200

C	7.60419000	4.33424000	20.48990500
H	8.43609000	4.80535800	19.95689800
H	7.26048600	3.45955200	19.93355500
H	6.78788300	5.05799800	20.57817100
H	8.41959800	10.17951300	25.67607400
H	7.86143900	9.33572100	26.99810600
H	9.55376000	8.32216700	24.69692500
H	9.68385200	7.95475400	26.47844900

(S)-TS3

Rh	9.57867500	4.86647400	25.42379700
C	10.96838200	7.13562500	27.75723000
O	9.64284800	1.02534400	27.57517800
N	9.91919400	2.78072500	26.20409600
P	10.68214000	5.38756300	27.29334800
N	11.44628900	5.04889900	24.39096300
O	13.61722800	5.05318100	23.83430300
C	12.25205400	7.69132100	27.63649500
H	13.09355900	7.07123600	27.35214100
C	12.45928700	9.04961700	27.88160300
H	13.45824600	9.46339200	27.78331800
C	9.17517800	4.55926200	31.04526000
H	9.02150800	5.10662600	31.96987000
C	9.73888600	5.20764500	29.94458000
H	10.02926400	6.24702100	30.03466900
C	9.94234400	4.53424500	28.73692100
C	9.89793100	7.96975600	28.12291100
H	8.89557500	7.57240000	28.21644100
C	10.11269000	9.32287600	28.37828900
H	9.27618800	9.95028000	28.66687200
C	11.39276400	9.86774800	28.25544000
H	11.55635000	10.92334100	28.44986200
C	8.82561600	3.21404700	30.95435500
H	8.39035300	2.69971100	31.80488600
C	9.03679200	2.52325000	29.76331500
H	8.76366200	1.47806100	29.68835500
C	9.73639200	2.36528200	27.41095800
C	9.58316300	3.16500200	28.64164500
C	9.57107000	0.45396400	26.23457500
H	8.52777400	0.18746200	26.04499600
H	10.18945100	-0.44290300	26.22100100
C	11.50934800	1.44897300	24.81472600
H	11.76256400	2.41360300	24.36334900
C	10.06315000	1.59427800	25.32724800
H	9.39180000	1.72114700	24.48001300

C	12.51563000	1.15748400	25.93278900
H	12.36236400	0.15926200	26.35827300
H	12.44784300	1.88847500	26.74209200
H	13.53655900	1.19207500	25.54099000
C	12.38353900	4.68462000	27.28765800
C	11.56732600	0.38054900	23.71778000
H	10.88373700	0.61843800	22.89500600
H	11.29382300	-0.60701300	24.10829900
H	12.57947400	0.30381500	23.30705000
C	12.94695200	4.31353700	28.51459700
H	12.36749300	4.41478200	29.42443900
C	14.24864900	3.81927200	28.59328200
H	14.65705000	3.53349100	29.55739900
C	15.01708600	3.70077400	27.43658100
H	16.03081900	3.31695300	27.48557100
C	14.47785000	4.07435700	26.21009700
H	15.06562700	3.97625200	25.30622300
C	13.16325800	4.56066600	26.11795400
C	12.66692400	4.90364200	24.78018400
C	12.92287700	5.18251300	22.55970900
H	13.05357000	4.24387500	22.01496200
H	13.39520500	5.99625200	22.01028200
C	11.46013900	5.44504700	22.95707300
H	10.77519000	4.78694700	22.42390600
C	10.98372900	6.89848400	22.76726500
H	9.94806700	6.91343600	23.11120300
C	10.98774100	7.26619900	21.27940500
H	10.41725500	6.54006600	20.68912500
H	12.00396000	7.30839400	20.87062000
H	10.53440100	8.25171400	21.13055300
C	11.77775200	7.90227600	23.60777500
H	12.83746600	7.92045900	23.32640100
H	11.71099600	7.67008700	24.67477600
H	11.38338000	8.91355600	23.46236000
C	8.45409000	6.60537600	25.22172100
H	8.75684600	7.42898800	25.86308800
H	8.28409400	6.90442900	24.19064500
C	7.55601700	5.59695800	25.74808300
H	6.93101500	5.05637300	25.04379800
C	7.16511900	5.45967000	27.10720300
C	6.44441400	4.22608600	27.56913100
H	7.14551200	3.38776900	27.59394300
H	5.63822000	3.96039800	26.87959500
H	6.03752200	4.35099200	28.57557400

H	7.76501000	5.96154400	27.85580800
C	5.91917000	9.43462000	24.83585800
C	5.57091200	8.23536200	25.45666800
C	5.88696300	8.03716700	26.80539400
C	6.54816900	9.03513800	27.52988500
C	6.89055800	10.23070700	26.90021900
C	6.58329600	10.43376400	25.55168500
H	5.67047500	9.58631900	23.78986000
H	5.05847200	7.45280800	24.90535400
H	6.79105100	8.86921800	28.57544600
H	7.40031900	11.00491200	27.46492400
H	6.85314900	11.36593000	25.06533000
N	5.63191100	6.78061600	27.40550500
O	8.81124400	4.25922400	23.53208000
C	7.89231100	3.38132700	23.34922700
O	7.24802700	2.73567700	24.18185000
O	7.66894400	3.20087600	22.00234700
C	6.67667400	2.22610700	21.67215300
H	5.69679900	2.50039600	22.07526400
H	6.63122600	2.20260000	20.58130400
H	6.94875700	1.23578400	22.05055100
H	5.52405000	6.82603700	28.41685500
H	4.83725000	6.29453300	26.99480800

E-IM3a

Rh	9.91327700	5.01105400	25.61622300
C	11.01255300	6.56229300	28.55198100
O	9.17273900	0.84037400	26.72922500
N	9.85300200	2.80286500	25.88084200
P	10.73528900	4.97706000	27.67038800
N	11.99777800	5.01520400	24.86682400
O	14.21296300	4.74593500	24.60675400
C	12.28792700	7.14689000	28.49453700
H	13.11616700	6.60933100	28.04724100
C	12.50435400	8.42522600	29.01060200
H	13.49715200	8.86182700	28.95828400
C	8.73814800	3.42450700	30.94222200
H	8.56129800	3.72983500	31.96871400
C	9.49742100	4.23940000	30.10114300
H	9.90992200	5.15884000	30.49618800
C	9.74134700	3.88673800	28.76961700
C	9.95855100	7.28912200	29.13150800
H	8.96090000	6.87008400	29.17416400
C	10.18315000	8.56006800	29.65946300
H	9.35940600	9.10367500	30.10890500

C	11.45413300	9.13422700	29.59595500
H	11.62363800	10.12776700	29.99979100
C	8.22094800	2.22404100	30.46197600
H	7.62760600	1.58215600	31.10502800
C	8.47643800	1.84087700	29.14820800
H	8.08751100	0.90222200	28.77388700
C	9.44678900	2.15348800	26.91691900
C	9.22868400	2.65496800	28.28633400
C	9.24656000	0.60558900	25.29148900
H	8.22270800	0.52037600	24.91684500
H	9.77352600	-0.33557500	25.13591800
C	11.45449600	1.62894000	24.37151800
H	11.85177100	2.62490900	24.15983500
C	9.97685300	1.84848600	24.75347800
H	9.46172600	2.28080500	23.89540800
C	12.28184700	1.01161500	25.50375000
H	11.98270700	-0.02418200	25.70157700
H	12.18415600	1.57925600	26.43263800
H	13.34288300	0.99992300	25.23445700
C	12.39931000	4.17675500	27.79076900
C	11.54825400	0.79841000	23.08762700
H	10.99301500	1.27014200	22.26910800
H	11.14467000	-0.21105600	23.23067400
H	12.59184500	0.69414500	22.77250200
C	12.74309400	3.61564900	29.02891700
H	12.02939400	3.63578800	29.84333100
C	13.98763000	3.02769900	29.24617200
H	14.21676200	2.59794400	30.21621500
C	14.92662600	2.99750000	28.21705100
H	15.89883700	2.54000200	28.36944700
C	14.61085900	3.55639600	26.98424700
H	15.33255000	3.52879300	26.17804400
C	13.35594600	4.14738400	26.75047300
C	13.11582500	4.67173900	25.39888700
C	13.74518100	5.08243600	23.27043700
H	13.89834000	4.20668500	22.63487600
H	14.35528800	5.90886300	22.90376300
C	12.25599400	5.42842600	23.46594600
H	11.61801100	4.81804600	22.82660800
C	11.88291300	6.90153400	23.22811300
H	10.81959200	6.96622000	23.46345200
C	12.05389700	7.25508800	21.74775000
H	11.46824800	6.57713200	21.11723400
H	13.10230000	7.19304400	21.43283600

H	11.71259300	8.27775100	21.55501500
C	12.63198900	7.86588100	24.15030400
H	13.71320700	7.84704200	23.96906600
H	12.45883700	7.62201600	25.20333500
H	12.29249600	8.89389700	23.98419800
C	8.82334900	7.82274300	24.77922300
H	9.68849800	8.48556200	24.74607100
H	8.64009800	7.35891800	23.81219100
C	8.88804100	6.83628300	25.89770500
H	9.15744400	7.31384000	26.83573200
C	7.97488000	5.71377800	25.98799800
C	7.19095500	5.37844800	27.23728600
H	6.22797800	5.90978400	27.25051900
H	7.72319000	5.64756100	28.15122300
H	6.96767100	4.30693500	27.29437000
O	7.75488000	5.85702700	22.64799800
C	8.74621700	5.11514300	22.60691800
O	9.42295900	4.60194800	23.55645200
O	9.25820700	4.72277700	21.38295800
C	8.58243600	5.24366100	20.23647300
H	8.61952400	6.33730000	20.21408800
H	9.10961000	4.84141000	19.36866900
H	7.53526400	4.92651100	20.20992900
H	7.41636400	5.50799400	25.07350200
C	8.49655300	11.33291400	27.53296800
C	8.46535100	10.63073200	26.32796000
C	7.61255300	9.53658700	26.21467000
C	6.80374800	9.11934100	27.26616800
C	6.84180400	9.83162000	28.46606900
C	7.68502000	10.93654900	28.59920400
H	9.15304600	12.19078500	27.63532900
H	9.08861700	10.92947600	25.49086100
H	6.15704800	8.25606200	27.14844800
H	6.21298100	9.51949700	29.29352700
H	7.71221800	11.48775900	29.53377000
N	7.61040500	8.77103300	24.96513100
H	6.76261900	8.19639400	24.91414700
H	7.57488700	9.41055000	24.16368200
(R)-IM4			
Rh	9.90567800	5.40585000	25.27230600
C	11.69703700	7.26307600	27.62676700
O	8.83530400	1.69800700	27.29039700
N	9.70960800	3.30275600	25.98884300
P	11.09025400	5.61385300	27.11898500

N	11.75540000	5.06086300	24.17293400
O	13.89518800	4.65525400	23.62984100
C	13.04643600	7.60287600	27.45045100
H	13.75863600	6.85807600	27.11384900
C	13.48403200	8.90361500	27.70722200
H	14.53178500	9.15281600	27.56904300
C	9.29976300	5.17661200	30.82123000
H	9.28338600	5.73490900	31.75178400
C	10.09372400	5.62391100	29.76276500
H	10.68976100	6.51727400	29.89742000
C	10.12682100	4.94639100	28.54012100
C	10.79296100	8.24974200	28.05973400
H	9.74575700	8.00932800	28.20259100
C	11.23725100	9.54414800	28.32303500
H	10.53031600	10.29351200	28.66625200
C	12.58306600	9.87545600	28.14468700
H	12.92650000	10.88543400	28.34703400
C	8.53798800	4.02054600	30.67655600
H	7.91345400	3.66590300	31.49001600
C	8.58471500	3.30994800	29.47903100
H	8.00473600	2.40230100	29.36499400
C	9.33531700	2.95005700	27.16862900
C	9.36383200	3.75663600	28.40126500
C	8.71104200	1.17148200	25.93383400
H	7.64960700	1.17822000	25.67260400
H	9.07999800	0.14582200	25.94168200
C	10.91167600	1.61421400	24.61009200
H	11.42217400	2.47088000	24.15810000
C	9.54316300	2.14808200	25.08029500
H	8.98626200	2.49346500	24.20783600
C	11.77753400	1.09008400	25.76046300
H	11.34699200	0.18692500	26.20812200
H	11.90103800	1.83657600	26.54929600
H	12.77498600	0.82839300	25.39373600
C	12.60370800	4.57122400	27.09831200
C	10.71621300	0.55019400	23.52495200
H	10.13696600	0.94398100	22.68225100
H	10.18855400	-0.32824500	23.91519900
H	11.68360400	0.20954300	23.14126500
C	13.07139200	4.07836700	28.32309100
H	12.52483100	4.30246400	29.23213700
C	14.22896900	3.30501000	28.40031300
H	14.56394100	2.93152300	29.36278000
C	14.94867500	3.02074300	27.24102500

H	15.85047900	2.41881000	27.28622400
C	14.50443700	3.50781900	26.01587500
H	15.05549600	3.28174200	25.11155200
C	13.33157200	4.27641700	25.92151300
C	12.92392600	4.70081700	24.57277300
C	13.24222300	4.89425300	22.34926900
H	13.22207800	3.94619700	21.80528800
H	13.84543700	5.61766900	21.80043400
C	11.83439300	5.39246700	22.73153600
H	11.06040900	4.82557600	22.21215500
C	11.57467800	6.89312200	22.48668900
H	10.56601000	7.08387600	22.86435000
C	11.58116500	7.18748300	20.98342200
H	10.87601500	6.53854800	20.45317900
H	12.57444100	7.03716900	20.54442800
H	11.29210700	8.22665000	20.79447200
C	12.54287300	7.79460200	23.25754600
H	13.58050600	7.64682700	22.93569700
H	12.48878900	7.60598600	24.33432400
H	12.29545600	8.84829200	23.09027500
C	9.14511000	7.35720500	25.24163100
H	9.76932300	8.11469100	25.71039900
H	8.76004200	7.62727300	24.26156200
C	8.32629400	6.49562500	26.07041600
H	8.40788300	6.59316700	27.15028000
C	6.93786800	6.10369200	25.66072500
C	6.48840500	4.73139600	26.13486100
H	5.42075500	4.56804600	25.95250200
H	6.69566900	4.57974700	27.19708000
H	7.05328900	3.98816100	25.57074300
O	7.79219900	6.53093000	22.51662500
C	8.38848200	5.44645100	22.51456000
O	8.85863800	4.77205100	23.49333200
O	8.59922600	4.78369500	21.31918700
C	8.05879100	5.41984700	20.15845200
H	8.47954500	6.41957500	20.01774000
H	8.33070500	4.78373300	19.31326100
H	6.96884500	5.50195900	20.22020000
H	6.81335700	6.20577000	24.58141400
C	7.04628400	8.63312300	29.48754200
C	6.86695400	8.45893600	28.11510000
C	6.03599900	7.43373600	27.66872700
C	5.36735000	6.59444200	28.55532100
C	5.55733300	6.77613900	29.92626700

C	6.40108500	7.78658500	30.39235800
H	7.69443300	9.42632900	29.84562600
H	7.37640500	9.09748100	27.40091000
H	4.71499800	5.81212800	28.18327700
H	5.04476700	6.12524100	30.62705500
H	6.54965200	7.91934900	31.45929700
N	5.93963600	7.18213700	26.22860500
H	4.98503900	6.89777100	25.98312000
H	6.12386700	8.05213700	25.71955200

E-IM3b

Rh	9.62328900	4.96037500	25.75371300
C	11.18858300	6.89835900	28.29229900
O	9.51132000	0.93104700	27.38597300
N	9.94495300	2.82659800	26.26597600
P	10.85462600	5.24503400	27.57631800
N	11.45316000	5.12342900	24.52237200
O	13.60103000	5.17996300	23.86904400
C	12.38389300	7.55911600	27.97313100
H	13.15095100	7.05281000	27.39801900
C	12.59682000	8.87356400	28.39251700
H	13.52680900	9.37272300	28.13769900
C	9.71869000	3.92257300	31.34050700
H	9.74037000	4.32506400	32.34834300
C	10.21273900	4.68935300	30.28313900
H	10.62404400	5.66578900	30.50087200
C	10.20047100	4.21631200	28.96609900
C	10.20844800	7.58041100	29.03459700
H	9.26779000	7.09550100	29.27170300
C	10.43145600	8.88811100	29.46367600
H	9.66913400	9.39904900	30.04390500
C	11.62475600	9.53936900	29.14060400
H	11.79496800	10.55944500	29.47119500
C	9.21088800	2.64920200	31.09849300
H	8.82135900	2.04544400	31.91169100
C	9.22015900	2.14321500	29.80167600
H	8.84881800	1.14464200	29.60677600
C	9.72994600	2.26662800	27.40561700
C	9.70902200	2.90523000	28.72931800
C	9.39066000	0.56117500	25.97845500
H	8.32734800	0.42163400	25.76320900
H	9.92195600	-0.37953700	25.83595600
C	11.43375400	1.55843300	24.71836700
H	11.76546600	2.54186100	24.37227800
C	9.99426700	1.76294600	25.23372300

H	9.36313700	2.08157700	24.40458500
C	12.40275100	1.07600700	25.80299800
H	12.15063200	0.06551900	26.14434100
H	12.40690400	1.73926500	26.67185100
H	13.42347700	1.04286200	25.40950700
C	12.55182300	4.54278600	27.36142600
C	11.42726800	0.61105200	23.51366300
H	10.76598600	0.98032200	22.72173400
H	11.08809500	-0.39310100	23.79461900
H	12.43465200	0.51291100	23.09565200
C	13.19794100	4.06200000	28.50859000
H	12.68919200	4.09908500	29.46435600
C	14.48578500	3.53166200	28.45527300
H	14.95298400	3.16228700	29.36270800
C	15.16279200	3.48165100	27.23840800
H	16.16443500	3.06823700	27.18009700
C	14.54561300	3.96418000	26.08984900
H	15.06371000	3.92360200	25.14015800
C	13.24273800	4.49248200	26.12746500
C	12.68639500	4.95000400	24.84402500
C	12.84496900	5.38717100	22.64154300
H	12.92458400	4.47448500	22.04370900
H	13.30376400	6.21831500	22.10618700
C	11.41211600	5.65136900	23.13600000
H	10.68292200	5.07487700	22.56590000
C	10.97286700	7.12910400	23.11759800
H	9.98091400	7.13146900	23.57152800
C	10.81240200	7.61305700	21.67396200
H	10.10855700	6.97400200	21.13255300
H	11.76633200	7.61816700	21.13343200
H	10.41993900	8.63570600	21.65720500
C	11.90126700	8.03884700	23.92704700
H	12.91374300	8.06707700	23.50762700
H	11.97485400	7.71664500	24.97035000
H	11.52130700	9.06630000	23.92441100
C	8.80906300	7.98428500	26.02061100
C	8.34512200	6.61060100	25.67927900
H	7.90276500	6.56433500	24.68790300
C	7.84809600	5.66633000	26.65720100
C	6.58723500	4.86008500	26.42533800
H	6.59426400	3.93265200	27.01163000
H	6.48341300	4.58646800	25.37276100
H	5.68902100	5.42208400	26.72367600
H	7.97986900	5.95123300	27.70411900

C	5.10811600	8.40568700	23.31238100
C	5.71548600	8.39594600	24.56951700
C	6.92765400	9.05814500	24.72916800
C	7.55293200	9.72236600	23.67790400
C	6.93645600	9.72427400	22.42694600
C	5.71771800	9.06537900	22.24331600
H	4.16181200	7.89356500	23.17171300
H	5.26090000	7.87598700	25.40679600
H	8.50422500	10.22184600	23.83331800
H	7.41042000	10.23921700	21.59767300
H	5.24380300	9.06677500	21.26688400
N	7.62127400	8.98057300	26.01850800
O	8.54373600	4.14534300	24.07941900
C	8.08348400	4.66474200	23.00540200
O	8.11339000	5.83737200	22.61437500
O	7.47684700	3.69722600	22.22691500
C	6.93436100	4.16323600	20.99038900
H	7.70961000	4.59824200	20.35141600
H	6.50500100	3.28630500	20.50063100
H	6.15296800	4.91280500	21.15203400
H	7.97299400	9.90636900	26.28707600
H	6.96374800	8.69356500	26.75087700
H	9.50145300	8.39724000	25.28750100
H	9.23516900	8.07650700	27.01425900
(S)-IM4			
Rh	9.57354600	4.84924700	25.31506600
C	10.94790200	7.21260700	27.55222900
O	9.64630800	1.10073100	27.66811600
N	9.90080400	2.79279200	26.21181300
P	10.64386500	5.44654000	27.16577300
N	11.51073200	4.94707900	24.30546000
O	13.70203700	4.98702300	23.81621200
C	12.24544400	7.74223300	27.46887300
H	13.08923200	7.09550500	27.26233500
C	12.46485900	9.10921200	27.64704800
H	13.47501000	9.50133500	27.57771100
C	9.06163900	4.81875800	30.93068200
H	8.87011800	5.41708300	31.81590800
C	9.63326600	5.41412500	29.80430100
H	9.89186900	6.46557800	29.83544300
C	9.88428900	4.67384000	28.64556900
C	9.87593700	8.08292000	27.81425500
H	8.86417100	7.70436600	27.87604900
C	10.10144700	9.44528500	28.00246800

H	9.26195300	10.09980700	28.20911500
C	11.39549600	9.96361100	27.91600700
H	11.56732900	11.02642100	28.05718800
C	8.75404300	3.46004400	30.91678200
H	8.31605900	2.98597500	31.78913600
C	9.00729600	2.70465200	29.77419000
H	8.76034200	1.65037200	29.75642800
C	9.72930700	2.43378600	27.43817100
C	9.55781200	3.29306500	28.62547000
C	9.56577900	0.46660000	26.35708200
H	8.52261600	0.18332300	26.19058600
H	10.19036300	-0.42602600	26.37876700
C	11.47893000	1.40304900	24.86496400
H	11.72369600	2.34850500	24.37024400
C	10.03921100	1.56632900	25.39071000
H	9.35351200	1.65408200	24.54904200
C	12.50077100	1.16187300	25.98127000
H	12.36417000	0.17696700	26.44201500
H	12.43215500	1.91913300	26.76597200
H	13.51748700	1.19520900	25.57802700
C	12.34813200	4.73844300	27.24031300
C	11.52571900	0.28837800	23.81448800
H	10.83355500	0.49092500	22.98938100
H	11.25561300	-0.68115400	24.25012600
H	12.53344700	0.19284100	23.39663500
C	12.87400100	4.42394900	28.49988900
H	12.26583300	4.56537900	29.38530300
C	14.17414700	3.94056800	28.64484700
H	14.55048700	3.70040900	29.63423600
C	14.98264400	3.77707200	27.52143800
H	15.99609600	3.40218400	27.62122200
C	14.48323000	4.09543700	26.26298300
H	15.10217000	3.96401100	25.38426200
C	13.16988700	4.56831100	26.10431200
C	12.71931300	4.84856100	24.73547200
C	13.04613000	5.06563100	22.51765000
H	13.22799300	4.12245600	21.99557400
H	13.50758400	5.88434200	21.96574100
C	11.56025600	5.28293000	22.86066100
H	10.91910300	4.57788000	22.33129700
C	11.02678700	6.70599800	22.59878000
H	9.98102300	6.68521100	22.91400900
C	11.06265000	7.01973100	21.09938500
H	10.53996600	6.25032400	20.51963200

H	12.08896700	7.08732200	20.72010500
H	10.57658000	7.98036700	20.89914600
C	11.75138500	7.77240500	23.42480200
H	12.81681500	7.82906000	23.17102100
H	11.66514700	7.57028300	24.49646200
H	11.31722400	8.76000800	23.23553500
C	8.40165400	6.55185300	25.06188300
H	8.68962100	7.42424400	25.64116200
H	8.22028300	6.77502200	24.01178200
C	7.60386500	5.51069200	25.67352700
H	6.97053200	4.93428600	24.99902300
C	6.98750700	5.57328500	27.03670700
C	6.44814000	4.23180600	27.51536800
H	7.24643900	3.49330200	27.49985000
H	5.65366400	3.88037700	26.84821700
H	6.05190600	4.29742600	28.53352000
H	7.63399800	6.02847900	27.78480800
C	6.25368900	9.95940300	25.64004100
C	5.97468700	8.59309100	25.69866600
C	6.00200900	7.95802900	26.93574600
C	6.29012400	8.64524600	28.11237000
C	6.55772700	10.01252500	28.04197500
C	6.54556900	10.66750000	26.80750400
H	6.23675800	10.46789300	24.68161400
H	5.73924000	8.03060100	24.80157400
H	6.29991600	8.12119500	29.06318000
H	6.77400000	10.56324400	28.95152500
H	6.75755900	11.73077700	26.75733900
N	5.73688000	6.52188300	27.01214000
O	8.82922600	4.18692200	23.42522300
C	7.93243600	3.29556500	23.21973600
O	7.28537500	2.62340000	24.03069500
O	7.73134200	3.12466300	21.86467400
C	6.76979500	2.12957100	21.50957700
H	5.77614500	2.37443400	21.89826300
H	6.74225100	2.11451400	20.41774300
H	7.05913700	1.14216400	21.88326300
H	5.18429600	6.32842200	27.85471400
H	5.15457500	6.23278200	26.21825000
E-3a			
C	-1.80515900	0.96769300	-0.69129600
H	-2.13338900	1.49850200	0.20362200
C	-1.19025700	1.63643300	-1.66886700
H	-0.87377100	1.08466300	-2.55338300

C	-0.89600400	3.10724600	-1.65117000
H	-1.24137600	3.57900000	-0.72555400
H	0.18067900	3.29785700	-1.75074400
H	-1.37914100	3.61710900	-2.49510800
C	-2.11211900	-0.51033900	-0.69221200
H	-1.57127300	-0.98743500	0.13376800
H	-3.18219100	-0.65001600	-0.46802000
N	-1.74968400	-1.21050000	-1.91369100
H	-1.16270200	-2.02193000	-1.78133600
C	-2.60138300	-1.28819600	-3.00296800
C	-2.38114800	-2.27303100	-3.99019100
C	-3.67571700	-0.39252200	-3.17984000
C	-3.20499600	-2.35518300	-5.10806400
H	-1.55749700	-2.97145300	-3.86287800
C	-4.49441500	-0.48992300	-4.30579400
H	-3.85666500	0.38717500	-2.44923800
C	-4.27241400	-1.46591800	-5.27925000
H	-3.01414600	-3.12536200	-5.85084300
H	-5.31590600	0.21273600	-4.41957900
H	-4.91373300	-1.53334300	-6.15249400
(R)-2a			
C	-0.77974900	-2.86386900	-1.30541900
H	0.12478600	-3.43279200	-1.05953400
H	-0.50348900	-2.07716700	-2.01270300
H	-1.49145200	-3.54070500	-1.78848500
C	-1.39305300	-2.25420500	-0.04256200
H	-2.28530200	-1.68565500	-0.32727800
C	-0.41847600	-1.32344000	0.64189500
H	0.49831500	-1.79678600	0.99713400
C	-0.61969000	-0.02029800	0.83692300
H	-1.52865400	0.47067300	0.49461000
H	0.11507300	0.60535400	1.33724700
N	-1.81170900	-3.35087600	0.83753900
H	-1.12251400	-4.09179600	0.90362700
C	-2.51128900	-3.14025200	2.01948800
C	-2.50163400	-4.14378300	3.01180900
C	-3.27906800	-1.98132400	2.25191300
C	-3.23783700	-3.99664800	4.18296800
H	-1.90784600	-5.03968300	2.84617200
C	-4.01239300	-1.84767500	3.43175300
H	-3.30397100	-1.18748900	1.51548100
C	-4.00221200	-2.84622100	4.40755000
H	-3.21012700	-4.78661800	4.92894800
H	-4.59632400	-0.94408600	3.58666100

H	-4.57339700	-2.73143100	5.32351400
(S)-2a			
C	-0.77974900	-2.86386900	1.30541900
H	0.12478600	-3.43279200	1.05953400
H	-0.50348900	-2.07716700	2.01270300
H	-1.49145200	-3.54070500	1.78848500
C	-1.39305300	-2.25420500	0.04256200
H	-2.28530200	-1.68565500	0.32727800
C	-0.41847600	-1.32344000	-0.64189500
H	0.49831500	-1.79678600	-0.99713400
C	-0.61969000	-0.02029800	-0.83692300
H	-1.52865400	0.47067300	-0.49461000
H	0.11507300	0.60535400	-1.33724700
N	-1.81170900	-3.35087600	-0.83753900
H	-1.12251400	-4.09179600	-0.90362700
C	-2.51128900	-3.14025200	-2.01948800
C	-2.50163400	-4.14378300	-3.01180900
C	-3.27906800	-1.98132400	-2.25191300
C	-3.23783700	-3.99664800	-4.18296800
H	-1.90784600	-5.03968300	-2.84617200
C	-4.01239300	-1.84767500	-3.43175300
H	-3.30397100	-1.18748900	-1.51548100
C	-4.00221200	-2.84622100	-4.40755000
H	-3.21012700	-4.78661800	-4.92894800
H	-4.59632400	-0.94408600	-3.58666100
H	-4.57339700	-2.73143100	-5.32351400

IM2a'-endo

Rh	9.63551800	5.02370700	25.46724400
C	11.40954500	6.94159200	27.82059400
O	9.18078900	1.15030700	27.38891600
N	9.76894600	2.89204500	26.10750000
P	10.84636200	5.28327800	27.32110900
N	11.46534300	5.36937900	24.48694500
O	13.55161200	5.05707300	23.76123500
C	12.78457600	7.22080400	27.87639200
H	13.51301000	6.45003300	27.65832300
C	13.22641500	8.50052200	28.21203700
H	14.29188200	8.70409500	28.24817600
C	9.22671500	4.54292700	31.02090100
H	9.14280700	5.06821500	31.96663500
C	9.87072000	5.15857200	29.94497300
H	10.29170600	6.14864700	30.07056600
C	9.98448500	4.50354900	28.71748700
C	10.48807400	7.96054600	28.11692300

H	9.42360300	7.76647600	28.10534000
C	10.93763800	9.23540700	28.45377900
H	10.21595700	10.01271600	28.68361300
C	12.30671300	9.50999600	28.49607100
H	12.65328500	10.50589900	28.75399700
C	8.70567900	3.25940700	30.87763800
H	8.20800900	2.77331500	31.71009500
C	8.81938900	2.59290700	29.65870800
H	8.40543000	1.59905500	29.54428000
C	9.49302800	2.45570100	27.29548600
C	9.44621600	3.20275300	28.56408700
C	9.02553400	0.66315500	26.02120100
H	7.95443000	0.62020400	25.80770100
H	9.45572400	-0.33578900	25.97140000
C	11.18482000	1.33271000	24.75336200
H	11.65746600	2.25331100	24.39522600
C	9.75599000	1.72288100	25.18613100
H	9.16841100	1.98471400	24.30865200
C	12.03789500	0.78727900	25.90235200
H	11.66371900	-0.17847000	26.25886000
H	12.07482400	1.47557100	26.74923900
H	13.06509200	0.63203800	25.56059200
C	12.38401000	4.30232900	27.15909200
C	11.11905700	0.33900300	23.58892900
H	10.56738300	0.75489900	22.73989100
H	10.62381000	-0.59124600	23.89117100
H	12.12684300	0.08155100	23.24778200
C	12.90150800	3.68687700	28.30238300
H	12.37443200	3.76724100	29.24577700
C	14.10263600	2.97658300	28.24674400
H	14.48810400	2.50676100	29.14564400
C	14.79877000	2.87419400	27.04412500
H	15.72926900	2.31886200	26.99405500
C	14.29738400	3.48718000	25.89836600
H	14.83302400	3.41227500	24.95987300
C	13.09407100	4.20352200	25.94335000
C	12.64037900	4.88225900	24.72700700
C	12.83458200	5.62619600	22.61471300
H	12.64021900	4.81044700	21.91453600
H	13.48627700	6.36824800	22.15717100
C	11.55505200	6.18986400	23.24232700
H	10.68382700	5.99640100	22.62063200
C	11.59786300	7.70020300	23.55350600
H	10.71472600	7.90550800	24.16177200

C	11.45991900	8.48575400	22.24385900
H	10.54290700	8.20796400	21.71377000
H	12.30791300	8.30018300	21.57418900
H	11.42730900	9.56130300	22.44503200
C	12.83192100	8.13349600	24.34816100
H	13.75133200	8.02675300	23.76196900
H	12.94250100	7.55874500	25.27029200
H	12.74347400	9.18717200	24.63188100
C	8.72368400	6.95351700	25.35207400
H	9.27814500	7.82014300	25.69689800
H	8.31821200	7.03542400	24.34890800
C	7.98830600	6.21131600	26.33329200
H	8.07508400	6.46340000	27.38804100
C	7.37963000	4.99845900	26.00876200
C	6.71479800	4.13282700	27.03228100
H	5.62939800	4.28677000	26.96701300
H	7.03178000	4.36791900	28.05003600
H	6.88804100	3.07037300	26.83778400
O	8.60406900	5.87413000	21.52630800
C	8.04711100	5.43772100	22.53496500
O	6.95239200	5.64019700	23.06866000
O	8.87100400	4.44879600	23.33175500
C	9.73978900	3.64686100	22.51143100
H	10.02654900	4.20529300	21.62085700
H	10.62931200	3.38492700	23.07785000
H	9.21046300	2.73708600	22.20912300
H	7.09182500	4.84333700	24.97081700

TS4a-endo

Rh	9.65814000	5.01648900	25.45021700
C	11.39313700	6.93859700	27.89119600
O	9.24454000	1.12372000	27.37412000
N	9.79498000	2.88243900	26.09748000
P	10.85043100	5.28351600	27.34818600
N	11.49983600	5.31294000	24.48210500
O	13.59881400	4.99371600	23.79602700
C	12.75814400	7.26495200	27.89114400
H	13.50018600	6.52228000	27.62523800
C	13.17252900	8.55285900	28.23241000
H	14.23127300	8.79213900	28.22478400
C	9.20199900	4.47690100	31.03231600
H	9.10788600	4.98712100	31.98546800
C	9.86282100	5.10672300	29.97508300
H	10.28548000	6.09270400	30.12440400
C	9.99137700	4.47539100	28.73630300

C	10.45329700	7.92049200	28.24887000
H	9.39602100	7.68748600	28.27977800
C	10.87442600	9.20295900	28.59500800
H	10.13851200	9.94972500	28.87595300
C	12.23401800	9.52407300	28.58151600
H	12.55859400	10.52561800	28.84637200
C	8.67712100	3.19848700	30.86092400
H	8.16475600	2.70080000	31.67755400
C	8.80944100	2.55182200	29.63361400
H	8.39721400	1.55998200	29.49769500
C	9.52593400	2.43857300	27.28339300
C	9.45471800	3.17683000	28.55752200
C	9.10548200	0.63466900	26.00666800
H	8.03630300	0.55638800	25.79256000
H	9.56756400	-0.34999400	25.95489100
C	11.23162600	1.37200400	24.71513900
H	11.67086900	2.30943300	24.35747300
C	9.79959900	1.71889300	25.17158200
H	9.19653900	1.97235200	24.30333700
C	12.11347200	0.83701400	25.84727100
H	11.76972100	-0.14337500	26.19462300
H	12.13923600	1.51497900	26.70327500
H	13.14113900	0.71507100	25.49345300
C	12.40851200	4.32381800	27.20944600
C	11.17547100	0.38936900	23.54092700
H	10.59949500	0.80085300	22.70566400
H	10.70948700	-0.55730100	23.83914800
H	12.18410900	0.16249200	23.18077600
C	12.93060900	3.73360200	28.36428000
H	12.39844900	3.82453500	29.30390500
C	14.13745800	3.03253600	28.32811900
H	14.52252700	2.58193500	29.23709900
C	14.84072300	2.91641800	27.13090700
H	15.77707800	2.36980500	27.09413000
C	14.33678600	3.50290200	25.97312400
H	14.87649600	3.41439900	25.03830900
C	13.12427100	4.20668700	25.99785900
C	12.67371100	4.84427100	24.75687700
C	12.89351200	5.51211200	22.62096500
H	12.71408200	4.67014500	21.94766400
H	13.54574200	6.24192000	22.14473300
C	11.60193300	6.08752300	23.21132200
H	10.73726000	5.86309800	22.59392800
C	11.63146700	7.60840700	23.46830600

H	10.72499200	7.83283400	24.03352900
C	11.54617500	8.35149600	22.12971600
H	10.65419500	8.05351400	21.56902500
H	12.42349600	8.15359600	21.50310700
H	11.49840100	9.43232700	22.29704700
C	12.83257200	8.06999700	24.29686600
H	13.77747100	7.91996100	23.76294300
H	12.88944900	7.54467600	25.25304700
H	12.74636900	9.13875300	24.51843400
C	8.78577700	6.95370400	25.29807500
H	9.34244900	7.81302000	25.66075800
H	8.42460500	7.05701700	24.28175600
C	8.01297000	6.23299400	26.26732600
H	8.09604800	6.50302900	27.31714300
C	7.39288800	5.02032000	25.97022800
C	6.72282500	4.18713400	27.01862300
H	5.63751800	4.34184700	26.95387000
H	7.04584200	4.44872600	28.02824800
H	6.89472400	3.11932500	26.85392000
O	8.43889700	6.24445800	21.61059100
C	7.65927700	5.81752200	22.39996000
O	6.58713500	5.71155800	22.90161100
O	8.79576800	4.52742700	23.52664000
C	9.52245800	3.73018800	22.61966900
H	9.71613800	4.26917700	21.68091100
H	10.49545300	3.41982900	23.01409200
H	8.96119800	2.81886800	22.35644800
H	7.12100600	4.80795800	24.94259800

IM5a-endo

Rh	9.72437300	5.07097400	25.54828600
C	11.32821300	6.94379400	28.10677800
O	9.23596800	1.11858800	27.18752700
N	9.83695100	2.96022900	26.07218300
P	10.87905400	5.28228100	27.49588800
N	11.60531200	5.15095500	24.56453900
O	13.73018900	4.78737200	23.97321100
C	12.62556100	7.42454500	27.86484900
H	13.37591100	6.78006000	27.42250500
C	12.96243000	8.73839300	28.19088800
H	13.96937800	9.09500800	27.99746800
C	9.24661500	4.16530400	31.11626600
H	9.16235000	4.59499200	32.10929200
C	9.89749600	4.88036500	30.10800200
H	10.32514200	5.84786700	30.33913200

C	10.01504300	4.35966800	28.81725300
C	10.37816300	7.80365900	28.68365200
H	9.37433700	7.45661300	28.89628800
C	10.72379100	9.11327800	29.01474300
H	9.98182700	9.76239500	29.46926500
C	12.01396900	9.58574200	28.76501100
H	12.27856400	10.60721900	29.02035800
C	8.71992300	2.90574400	30.84446300
H	8.21432100	2.34129300	31.62097500
C	8.84537300	2.36348200	29.56701000
H	8.43698900	1.38361000	29.35378700
C	9.54664900	2.43009500	27.21397700
C	9.48173200	3.07406200	28.53969500
C	9.10090800	0.75675800	25.77607800
H	8.03171400	0.72047900	25.55005300
H	9.54169900	-0.23038900	25.64489400
C	11.25967500	1.54844700	24.57709700
H	11.70340800	2.49308200	24.24969300
C	9.82939300	1.89149800	25.04264000
H	9.25911800	2.26840400	24.19286700
C	12.13605900	0.96298300	25.68948200
H	11.78290800	-0.02753800	25.99747300
H	12.16339600	1.60684100	26.57227200
H	13.16501800	0.84736200	25.33555400
C	12.48482800	4.39324800	27.41746700
C	11.19991900	0.61345900	23.36407200
H	10.61430800	1.05511200	22.55028800
H	10.74488100	-0.34982100	23.62305800
H	12.20735300	0.41079900	22.98612700
C	13.00323400	3.87081200	28.60826000
H	12.45111600	3.98960400	29.53297800
C	14.22412500	3.19726400	28.62991000
H	14.59995700	2.79750800	29.56621200
C	14.95193900	3.04224800	27.45163900
H	15.90029000	2.51524400	27.45528000
C	14.45665200	3.56429500	26.26137300
H	15.01470500	3.44076500	25.34222300
C	13.22514700	4.23943000	26.22686900
C	12.77929800	4.75181300	24.92529100
C	13.05732300	5.10440700	22.71857600
H	12.97897000	4.17752800	22.14426200
H	13.67994100	5.82018000	22.18397500
C	11.69317200	5.64868600	23.16502400
H	10.88073300	5.18971700	22.60499500

C	11.55681700	7.18289400	23.09798000
H	10.56094600	7.41145800	23.48198400
C	11.61073700	7.65215700	21.63965300
H	10.88183200	7.11574500	21.02202100
H	12.60274300	7.50118200	21.19893600
H	11.38463600	8.72154500	21.57708400
C	12.58087600	7.91461200	23.97002200
H	13.60805200	7.72065500	23.63991700
H	12.49785900	7.61953200	25.01996000
H	12.41848000	8.99614400	23.91615300
C	8.97429700	7.06572700	25.33996600
H	9.59989900	7.89340800	25.66431700
H	8.57896500	7.16079200	24.33527200
C	8.19238400	6.40916200	26.34218600
H	8.30534800	6.69475600	27.38320700
C	7.51384500	5.21364700	26.08084000
C	6.83099500	4.42774300	27.15976100
H	5.75514300	4.64682800	27.14170200
H	7.21366800	4.67135700	28.15293100
H	6.93497500	3.35106100	26.99450800
O	8.94757700	4.44255900	23.70720600
C	8.28741800	5.25882000	22.79294400
H	7.35679100	5.71993700	23.17911500
H	8.90428700	6.08819600	22.39791300
H	7.98458100	4.65458300	21.92053100
H	7.18512000	5.00326600	25.06982400

E-TS5a

Rh	9.93503500	5.08849700	25.59575800
C	11.16267700	6.61882400	28.53156400
O	9.09210500	1.00109800	26.70052700
N	9.83129200	2.94246300	25.86332200
P	10.83153900	5.04281200	27.65583700
N	12.01430900	5.10588200	24.83249600
O	14.17233000	4.61149700	24.46578100
C	12.45716300	7.16132300	28.49365800
H	13.27687100	6.59000700	28.07263900
C	12.70266800	8.44014400	28.99615200
H	13.70979500	8.84445300	28.96029400
C	8.86785900	3.53109000	30.96490600
H	8.72741400	3.82871000	31.99927500
C	9.64047800	4.32578700	30.11616400
H	10.09695700	5.22630600	30.50803500
C	9.83554700	3.98061800	28.77577100
C	10.12050500	7.38529200	29.08212700

H	9.11075200	6.99493500	29.11786500
C	10.37237700	8.65931200	29.58996300
H	9.55564300	9.23658000	30.01114200
C	11.66253800	9.19224400	29.54469800
H	11.85502000	10.18708800	29.93479500
C	8.28815300	2.36073300	30.48121100
H	7.68421700	1.73540100	31.13063300
C	8.49137800	1.98681800	29.15524800
H	8.05031600	1.07256500	28.77802400
C	9.41838000	2.29793200	26.90362000
C	9.25534100	2.78216200	28.28671400
C	9.12073700	0.79191400	25.25570600
H	8.08654200	0.80024400	24.89986100
H	9.56738100	-0.18454800	25.07131400
C	11.41197400	1.66962700	24.40744800
H	11.88239600	2.63778700	24.22000700
C	9.93780200	1.98293500	24.73604800
H	9.48048300	2.44214600	23.86164500
C	12.15849400	0.98497000	25.55730100
H	11.77878500	-0.02742500	25.73628600
H	12.07936200	1.55067400	26.48903600
H	13.22255100	0.89763100	25.31605800
C	12.46927300	4.18701100	27.73332000
C	11.49543000	0.84753700	23.11703500
H	11.00444400	1.36403500	22.28472700
H	11.01874200	-0.13294500	23.23360200
H	12.54044100	0.67486800	22.83924700
C	12.83855800	3.62459900	28.96314500
H	12.16376700	3.69426100	29.80766200
C	14.05702600	2.96988200	29.13239800
H	14.30784500	2.54171100	30.09778300
C	14.94181000	2.86954800	28.06051800
H	15.89202000	2.35800300	28.17487800
C	14.60084400	3.42928500	26.83481800
H	15.28217200	3.35056600	25.99765300
C	13.37305500	4.09088300	26.65067200
C	13.11248200	4.63698600	25.31109500
C	13.65560600	4.96459000	23.15067500
H	13.58688500	4.04455100	22.56281000
H	14.37009000	5.64333500	22.68539700
C	12.28297800	5.58458700	23.45387500
H	11.49535500	5.18615200	22.81385500
C	12.23888200	7.12346100	23.38094500
H	11.22912900	7.39770200	23.69098100

C	12.42892000	7.59026300	21.93388400
H	11.70746400	7.10965200	21.26330600
H	13.43514500	7.36239200	21.56378900
H	12.28981800	8.67388300	21.85888900
C	13.22701000	7.80471700	24.33253400
H	14.26594800	7.55578500	24.08706000
H	13.04470700	7.51887200	25.37334300
H	13.12730500	8.89339700	24.26608300
C	8.96261000	7.63095500	24.74995600
H	9.74896400	8.37815900	24.73694000
H	8.75384900	7.14885200	23.80167800
C	8.78283800	6.89492500	25.94902900
H	9.07567200	7.40443200	26.86020700
C	7.97347900	5.70239600	26.05689900
C	7.24160600	5.36958700	27.33704700
H	6.27440600	5.89019500	27.37171900
H	7.80032800	5.65948700	28.22817500
H	7.03386400	4.29713800	27.41302900
O	9.40811400	4.85839800	23.57599600
C	8.13807700	4.51543800	23.13405700
H	7.66044600	3.69477300	23.70713500
H	7.41136400	5.35483800	23.13538900
H	8.18670000	4.16717700	22.08578300
H	7.37244800	5.46897900	25.18158900
C	8.09687200	11.11115700	27.62181800
C	8.17693300	10.63387600	26.31449500
C	7.35815800	9.57121800	25.91721300
C	6.47510400	8.97987900	26.82564600
C	6.40414700	9.46371700	28.13255300
C	7.21296700	10.52859500	28.53566000
H	8.72896400	11.93918000	27.92776500
H	8.86933000	11.07552000	25.60357200
H	5.85432300	8.14830600	26.50748700
H	5.71554100	9.00422900	28.83506300
H	7.15547100	10.90328800	29.55278400
N	7.53417400	8.98911500	24.63376100
H	6.71919200	8.47096100	24.31231900
H	7.83005400	9.65187000	23.91921700
(R)-TS6			
Rh	9.80888400	5.16862500	25.33673800
C	11.50962400	7.06141500	27.79086600
O	9.13208600	1.29180000	27.20763900
N	9.80397300	3.04150500	25.97661100
P	11.01185500	5.39962100	27.21147700

N	11.65167500	5.08688800	24.25183500
O	13.79393000	4.79824800	23.65954000
C	12.84446400	7.47955300	27.68446300
H	13.61039800	6.78425400	27.36017900
C	13.19781200	8.79469200	27.99252500
H	14.23504700	9.10413900	27.90657200
C	9.36858200	4.60346300	30.92051500
H	9.32324200	5.10623500	31.88143900
C	10.06049500	5.19770100	29.86263100
H	10.55185900	6.14932100	30.02328900
C	10.13306800	4.58617400	28.60780600
C	10.53496100	7.98594700	28.20707900
H	9.49686500	7.68888600	28.29693900
C	10.89461700	9.29483300	28.52275700
H	10.13115300	9.99276500	28.85218400
C	12.22631700	9.70391300	28.41336400
H	12.50389500	10.72523400	28.65587400
C	8.74802600	3.37038800	30.73800700
H	8.20753900	2.89918300	31.55250000
C	8.82537200	2.73539300	29.50038300
H	8.34642200	1.77503700	29.35406300
C	9.51208200	2.59041100	27.14709000
C	9.50500600	3.32559900	28.42452600
C	8.96941400	0.85120300	25.82374800
H	7.89674900	0.81839700	25.61290900
H	9.39043100	-0.15064900	25.74338900
C	11.09977200	1.51878200	24.48946500
H	11.54964600	2.43491700	24.09330600
C	9.70535600	1.92833500	25.00774000
H	9.10908700	2.28824600	24.16724600
C	12.01488300	0.97060400	25.58954000
H	11.65153900	0.00970200	25.97138900
H	12.10122100	1.66296700	26.43085800
H	13.02216800	0.80489100	25.19495000
C	12.58881600	4.45821600	27.13156900
C	10.95623400	0.52197200	23.33439200
H	10.34383000	0.93596100	22.52555800
H	10.48685500	-0.41130000	23.66778600
H	11.93755900	0.26750400	22.92037600
C	13.11804800	3.94413200	28.32166200
H	12.59150900	4.10809000	29.25497700
C	14.31249000	3.22454300	28.33286400
H	14.69619300	2.83252300	29.26942000
C	15.00573200	3.01568200	27.14159600

H	15.93395600	2.45363200	27.13604700
C	14.50171100	3.52845100	25.95066700
H	15.03362600	3.36328200	25.02209500
C	13.29345500	4.24569800	25.92456300
C	12.83763600	4.73396300	24.61452400
C	13.10716800	5.09453800	22.40820600
H	13.05256200	4.16656400	21.83192600
H	13.70477800	5.82893500	21.86917500
C	11.72606800	5.59443300	22.86055000
H	10.92524700	5.12707600	22.28742000
C	11.53937600	7.12614700	22.82316600
H	10.54871200	7.31061300	23.24806500
C	11.53549300	7.62396500	21.37423800
H	10.79408600	7.08739800	20.77172500
H	12.51399800	7.49531400	20.89679100
H	11.29166100	8.69085600	21.33816600
C	12.56453200	7.87615600	23.67946700
H	13.58724300	7.72732600	23.31389500
H	12.52484400	7.55832700	24.72560800
H	12.36148100	8.95202000	23.65313700
C	8.96098700	7.06490000	25.28274700
H	9.54235200	7.88507600	25.70026500
H	8.51622800	7.31014300	24.32040200
C	8.18186300	6.26103200	26.20882500
H	8.31271400	6.40881300	27.27702900
C	6.97656500	5.57733800	25.87166200
C	6.44392200	4.51560700	26.78983800
H	5.38860400	4.30389400	26.60015900
H	6.57995100	4.78714000	27.84011600
H	7.00060400	3.59112900	26.60589500
O	8.80113900	4.52453100	23.61051200
C	8.24418900	5.36096300	22.65446300
H	8.94022600	6.11885800	22.24657200
H	7.89995500	4.76501900	21.78871300
H	7.35252400	5.92714400	22.99836200
H	6.77280800	5.42934600	24.81732200
C	7.08471400	9.68953400	28.07768300
C	6.65931000	8.93855900	26.98165800
C	5.85203200	7.81438600	27.18372800
C	5.47203900	7.44115600	28.47818800
C	5.90339600	8.19789100	29.56710100
C	6.71425800	9.32024000	29.37301000
H	7.70861900	10.56318500	27.91633900
H	6.95304200	9.21333800	25.97370400

H	4.84701000	6.56541000	28.62434600
H	5.60497700	7.90822900	30.57006200
H	7.04940800	9.90485500	30.22402200
N	5.53923900	6.97281000	26.08451300
H	4.65866500	6.47244900	26.18858400
H	5.55673300	7.46130600	25.19175800