

Supporting Information

Mechanism and Origins of Stereo- and Enantioselectivities of Palladium-Catalyzed Hydroamination of Racemic Internal Allenes via Dynamic Kinetic Resolution: A Computational Study

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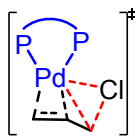
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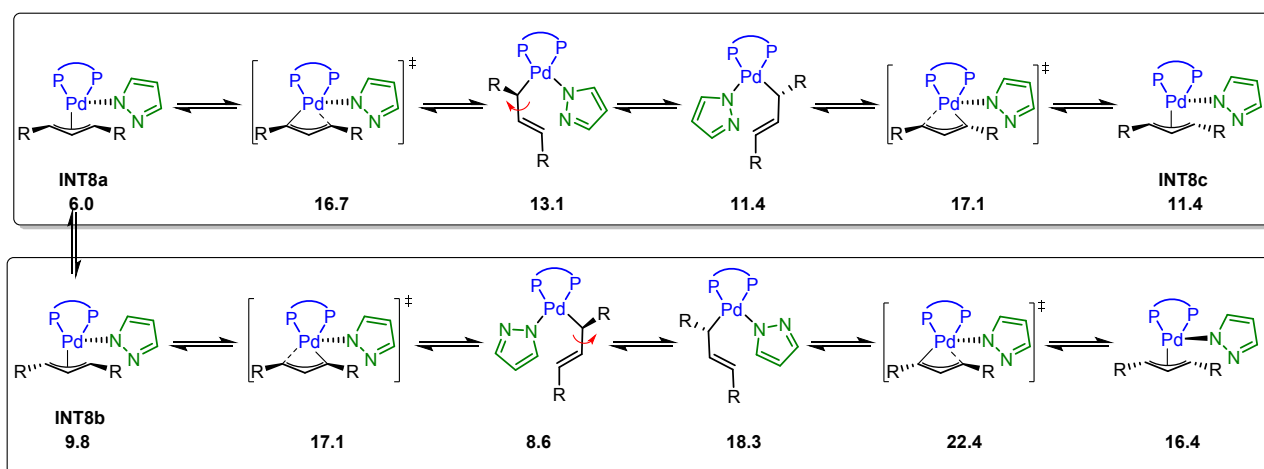
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1. C-Cl reductive elimination.

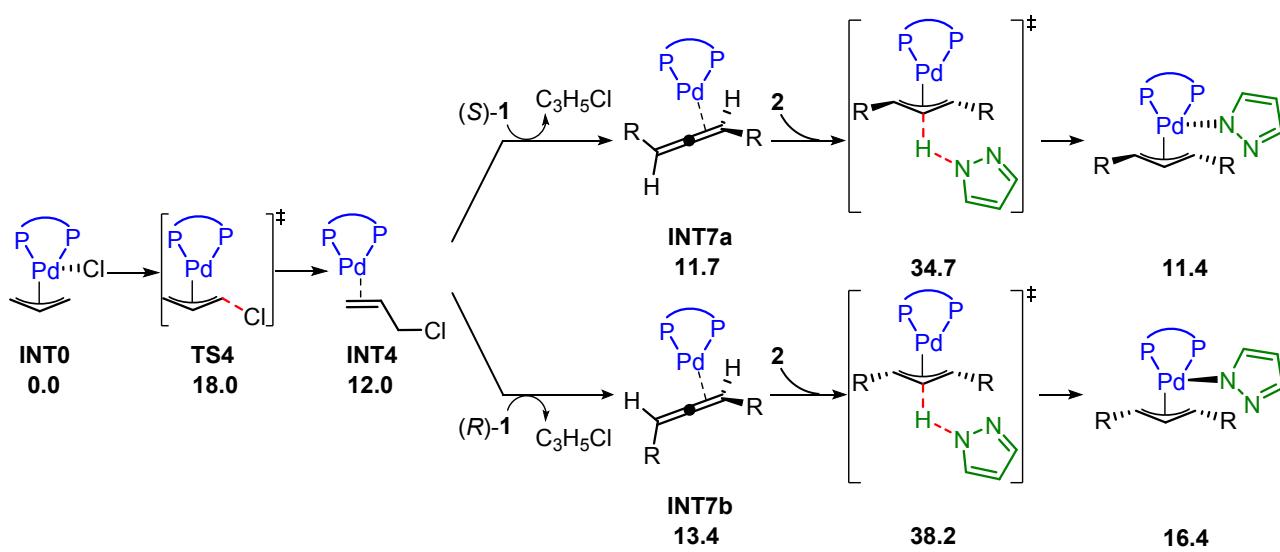


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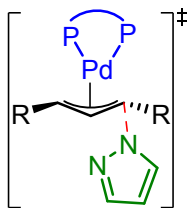
2. Other possibilities of η^3 - η^1 - η^3 allylic isomerization.



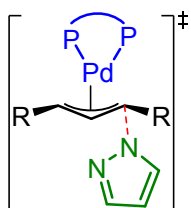
3. Other possibilities of protonation.



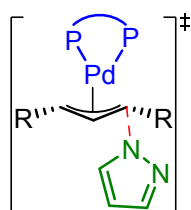
4. Other possibilities of nucleophilic attack.



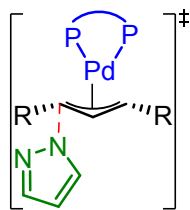
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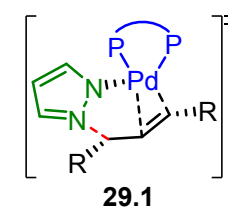
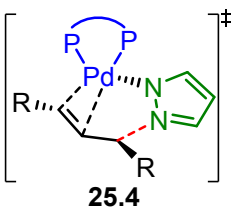
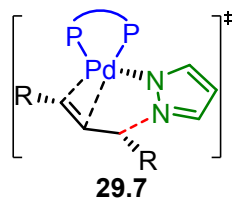
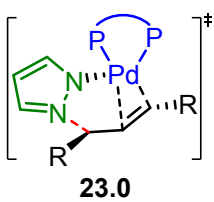
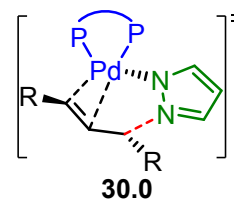
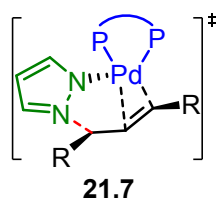
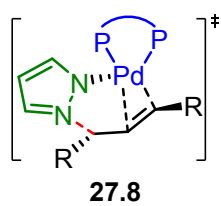
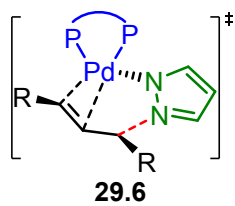


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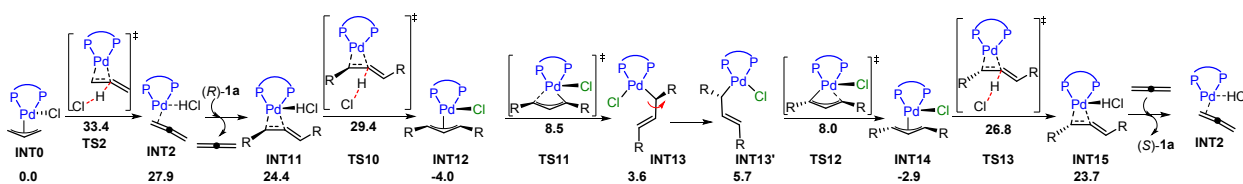
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5. C-N reductive elimination.



6. Racemization in the absence of the pyrazole substrate

As shown in below, **INT2** undergoes the ligand exchange step with (*R*)-**1a** to afford intermediate **INT11**, from which the protonation of the central carbon of allene using HCl as the proton source takes place through transition state **TS10**, leading to η^3 -allyl Pd(II) complex **INT12**. The subsequent η^3 - η^1 - η^3 allylic isomerization to give intermediate **INT14** is quite feasible. Finally, the deprotonation of the central carbon of the allyl ligand via **TS13** delivers intermediate **INT15**, from which the ligand exchange with propadiene could release (*S*)-**1a**.



The computations show that the formation of **INT2** via **TS2** is the rate-determining step of this process, with an energy barrier of 33.4 kcal/mol relative to **INT0**, which can take place under the reaction conditions. However, since that the energy barrier is 3.2 kcal/mol higher than the process with the pyrazole substrate, this process is less likely to occur in the presence of the pyrazole substrate.

7. Table of calculated energies and energy corrections

Stationary point	Single-point energy M06/6-311++G(<i>d,p</i>), SDD (a.u.)	Thermal correction to Gibbs free energy B3LYP-(D3)BJ/6-31G(<i>d</i>), LANL2DZ (a.u.)
(R)-1	-735.604813	0.283884
(S)-1	-735.6048196	0.283472
2	-226.104244	0.045253
propadiene	-116.590101	0.032005
INT0	-3153.081546	0.558205
TS1	-3153.010319	0.550265
INT1	-3036.425417	0.498367
TS2	-3153.016510	0.546464
INT2	-3153.027383	0.548458
INT3	-3036.397263	0.492791
TS3	-3036.393742	0.491475
TS4	-3153.050077	0.555380
INT4	-3153.060877	0.556722
INT5	-2801.712204	0.554215
C ₃ H ₅ Cl	-577.427825	0.043936
TS5	-2801.669382	0.548257
INT6	-2801.696768	0.553852
INT7a	-3311.242880	0.801130
TS6a	-3537.331104	0.864504
INT8a	-3537.371843	0.871869
INT7b	-3311.237875	0.798796
TS6b	-3537.327721	0.866398
INT8b	-3537.366055	0.872250
TS7	-3537.356435	0.870771
INT9	-3537.357501	0.868157
TS8	-3537.354977	0.867698
INT9'	-3537.360046	0.866220
(E)-(S)-TS9	-3537.347548	0.866279
(E)-(S)-INT10	-3537.402010	0.873117
(E)-(S)-3	-961.759074	0.352641
(E)-(R)-TS9	-3537.343752	0.866332
(E)-(R)-INT10	-3537.402635	0.874479

(E)-(R)-3	-961.760065	0.354108
INT8c	-3537.364646	0.873261
(Z)-(S)-TS9	-3537.348641	0.870934
(Z)-(S)-INT10	-3537.404930	0.876883
(Z)-(S)-3	-961.758112	0.353795
(Z)-(R)-TS9	-3537.346446	0.871193
(Z)-(R)-INT10	-3537.398861	0.873374
(Z)-(R)-3	-961.760253	0.356676

8. Cartesian coordinates

(R)-1

C	1.04229300	0.63474900	0.78085200
C	-0.20945300	0.33396100	0.54187700
H	-0.50221100	0.04418900	-0.46969300
C	2.28505000	0.95709900	1.03816700
H	2.98390200	0.17907800	1.35305000
C	-1.31733900	0.39780600	1.56819100
H	-0.89560700	0.56696200	2.56467700
H	-1.84724600	-0.56398300	1.60102800
C	-2.33942900	1.51279600	1.24755800
H	-1.81403300	2.47512800	1.24007900
H	-2.73303100	1.35629400	0.23545400
C	-3.47349200	1.54289700	2.24435300
C	-3.35454400	2.26329400	3.44036500
C	-4.64633500	0.81041700	2.02007300
C	-4.37986700	2.25457500	4.38685500
H	-2.45037600	2.83835400	3.62696400
C	-5.67532200	0.79836700	2.96310100
H	-4.75341600	0.24805800	1.09524100
C	-5.54490000	1.52102600	4.15089300
H	-4.27127900	2.82339800	5.30631500
H	-6.57958100	0.22794500	2.76888300
H	-6.34566900	1.51574000	4.88495500
C	2.85225000	2.35050000	0.88870000
H	3.31407500	2.66547800	1.83460500
H	2.04598000	3.05993300	0.67360600
C	3.91724400	2.42875600	-0.22888600
H	4.71597300	1.70835700	-0.01213100
H	3.45580900	2.11888600	-1.17380800
C	4.49431700	3.81810200	-0.36087300
C	3.88744100	4.76727700	-1.19387900
C	5.61496700	4.20463000	0.38583500
C	4.38685400	6.06742000	-1.28186300
H	3.01736200	4.48087800	-1.78033800
C	6.11858000	5.50367800	0.30204300
H	6.09814800	3.47816400	1.03535700
C	5.50533900	6.44013000	-0.53301900
H	3.90539000	6.78798500	-1.93740800
H	6.99169700	5.78332200	0.88536600
H	5.89771800	7.45074800	-0.60227100

(S)-1

C	1.09741200	0.69792700	1.16526000
C	-0.12676400	0.34973700	0.85751900
H	-0.33462500	-0.02984800	-0.14541100

C	2.31891200	1.02733900	1.50300800
H	2.66210700	2.04919800	1.32681400
C	-1.31246100	0.46737700	1.78773800
H	-0.97685500	0.76788100	2.78597200
H	-1.79629700	-0.51356900	1.89276700
C	-2.36091200	1.47829400	1.27003000
H	-1.88767100	2.46369400	1.18790000
H	-2.66727500	1.18596800	0.25773200
C	-3.56759600	1.55119500	2.17533600
C	-3.60838800	2.45730800	3.24307400
C	-4.64812700	0.67654600	2.00030600
C	-4.69959100	2.49136900	4.11264400
H	-2.77711300	3.14302700	3.39040000
C	-5.74160300	0.70587400	2.86692800
H	-4.63144000	-0.03106700	1.17440000
C	-5.77061300	1.61448000	3.92725800
H	-4.71497800	3.20439300	4.93247700
H	-6.57222500	0.02255200	2.71227300
H	-6.62215900	1.64124500	4.60125400
C	3.33062700	0.07284500	2.09509200
H	4.17156883	-0.05598892	1.40544099
H	2.87031227	-0.91573986	2.22950857
C	3.85836093	0.55942239	3.46422240
H	4.33438355	1.53755481	3.32817952
H	3.00791498	0.70951414	4.14110405
C	4.83629531	-0.41846303	4.07074049
C	4.38889450	-1.47048395	4.88086470
C	6.20630536	-0.32643432	3.79230763
C	5.28504626	-2.40553276	5.40080593
H	3.32840505	-1.55337184	5.10804295
C	7.10704118	-1.25854533	4.30973299
H	6.56807368	0.48613280	3.16636595
C	6.64848944	-2.30238925	5.11633532
H	4.91965756	-3.21183096	6.03101964
H	8.16653743	-1.16788251	4.08614479
H	7.34806732	-3.02739108	5.52264755
2			
C	0.73738200	-1.55851900	0.00000900
C	2.12062200	-1.56172500	0.00003700
C	2.47852300	-0.19374900	-0.00003000
N	0.36218300	-0.25345700	-0.00007000
H	-0.57606600	0.11845800	-0.00011000
H	0.01159600	-2.35859400	0.00003600
H	2.77209400	-2.42303400	0.00009600
H	3.46862200	0.24308500	-0.00003500
N	1.40743300	0.60294500	-0.00009100
propadiene			
C	-0.66427800	0.95206400	0.00000000
C	0.64281600	0.95206400	0.00000000
C	1.94991100	0.95206400	0.00000000
H	2.51943300	1.00590900	-0.92585500
H	2.51943300	0.89821900	0.92585500
H	-1.23380000	1.87791600	0.05389700
H	-1.23380000	0.02621200	-0.05389700
INTO			
P	-1.27042400	1.63722300	-0.13917400
C	-2.27148200	0.39854500	-1.06119000
C	-1.46263400	3.18035100	-1.11162000

C	-2.25115100	1.87606300	1.38244400
C	-2.54765700	-0.85696300	-0.44039200
C	-2.69904700	0.64741800	-2.36812300
C	-2.26918500	4.24650700	-0.69797600
C	-0.72638100	3.30316300	-2.30292500
C	-1.59777200	1.90851000	2.61987900
C	-3.65046100	1.97640800	1.32345700
C	-3.26406200	-1.76170700	-1.20073100
C	-2.15982700	-1.22789000	0.95027800
C	-3.40027400	-0.30742600	-3.12622000
H	-2.49288100	1.60780800	-2.82265700
C	-2.34509800	5.41089300	-1.46707400
H	-2.83223600	4.17606600	0.22544800
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H	-0.07610800	2.49040000	-2.61553300
C	-2.34570900	2.03528400	3.79221900
H	-0.51502800	1.81391800	2.66927800
C	-4.38774100	2.12323300	2.49644000
H	-4.16000100	1.92262200	0.36609200
C	-3.66360500	-1.51162400	-2.51173000
O	-3.64784700	-3.02528400	-0.83477300
C	-3.14624400	-1.32728800	1.91383800
C	-0.83235200	-1.52834900	1.38449400
H	-3.71656600	-0.10430000	-4.14284600
C	-1.62713100	5.51764700	-2.65773200
H	-2.96846800	6.23432500	-1.13085700
H	-0.24802800	4.53566600	-3.99860300
C	-3.73583000	2.14400300	3.73409700
H	-1.83543800	2.04362200	4.75078800
H	-5.46973100	2.20853100	2.44640400
O	-4.30645100	-2.60856900	-3.01888600
C	-4.34505700	-3.57730000	-1.95923600
C	-2.88241800	-1.63753700	3.24627400
O	-4.49213800	-1.13259600	1.74302600
C	-0.58177800	-1.85421900	2.71982100
P	0.56811300	-1.28450600	0.22687700
H	-1.69003800	6.42332800	-3.25371600
H	-4.31344900	2.24316000	4.64896100
H	-3.84033600	-4.49018200	-2.28654900
H	-5.38618000	-3.77295500	-1.68173400
C	-1.60418000	-1.90864700	3.68345300
O	-4.04881100	-1.63553500	3.96264000
C	-5.08343700	-1.25085200	3.04415400
H	0.43224700	-2.06573300	3.03525000

C	1.96504200	-2.26656700	0.89242500
C	0.05430400	-2.15332900	-1.29655300
H	-1.39414100	-2.15207100	4.71837400
H	-5.85561700	-2.02501300	3.02166000
H	-5.49170800	-0.28135500	3.34521700
C	2.34641700	-3.50500000	0.35624600
C	2.70437400	-1.71706800	1.95375200
C	0.21336100	-1.51346700	-2.53141200
C	-0.51207000	-3.43609100	-1.24951900
C	3.43892300	-4.19259500	0.88786400
H	1.80610200	-3.93303600	-0.47956700
C	3.78644300	-2.41698300	2.48664000
C	-0.19350300	-2.14521700	-3.70682800
H	0.62863800	-0.50988300	-2.55636800
C	-0.90202600	-4.07191800	-2.42671100
H	-0.66754900	-3.92443600	-0.29272200
C	4.15701100	-3.65512300	1.95707400
H	3.72769800	-5.14922000	0.46162000
H	4.34575200	-1.98394200	3.31099400
C	-0.74929300	-3.42493900	-3.65617600
H	-0.08496000	-1.63560000	-4.65959400
H	-1.33279100	-5.06818700	-2.38403000
H	5.00582600	-4.19382600	2.36875600
H	-1.06891300	-3.91545800	-4.57087900
H	2.44012900	-0.73849100	2.35118600
Pd	0.98958100	0.99812400	0.00553800
Cl	1.88324600	1.55361400	2.85689500
C	2.71035300	2.00321900	-1.00441700
C	1.99926300	2.99245500	-0.30215800
C	3.18548600	0.86267000	-0.32078400
H	2.65087100	1.98049900	-2.09135800
H	2.18968600	3.16014200	0.75418400
H	1.47502300	3.76827000	-0.84960400
H	3.57393200	0.02046600	-0.88478500
H	3.46843600	0.93059400	0.72546100
TS1			
P	-3.37665300	0.28360700	0.03714400
C	-4.41286800	-0.92012500	-0.88781400
C	-3.55107200	1.84303400	-0.91415100
C	-4.31626700	0.51627900	1.58435300
C	-4.74248200	-2.16775100	-0.27731600
C	-4.81129900	-0.64898100	-2.19981000
C	-4.43583000	2.86542600	-0.55393400
C	-2.74112400	2.00657700	-2.05016800
C	-3.63438800	0.52722300	2.80703000

C	-5.71535100	0.63381300	1.55886400
C	-5.48625900	-3.03902600	-1.05056400
C	-4.36773000	-2.56735600	1.10880100
C	-5.53964500	-1.57175200	-2.97109800
H	-4.55803200	0.30377800	-2.64715800
C	-4.51047000	4.03147100	-1.32058700
H	-5.05648700	2.76405200	0.32878000
C	-2.83092700	3.16177100	-2.82354300
H	-2.03686700	1.22444200	-2.31846000
C	-4.35428700	0.65060100	3.99701000
H	-2.55217800	0.42044300	2.82796700
C	-6.42370900	0.77886600	2.74970500
H	-6.24855100	0.59083300	0.61407000
C	-5.86044600	-2.76633600	-2.36465700
O	-5.91950800	-4.29040000	-0.69802400
C	-5.35396700	-2.65197500	2.07404800
C	-3.04786500	-2.90746100	1.53571800
H	-5.83237900	-1.35317500	-3.99152900
C	-3.71540800	4.18050700	-2.45667000
H	-5.19160300	4.82387400	-1.02434200
H	-2.20423600	3.27175000	-3.70388300
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H	-3.82323700	0.64229500	4.94420300
H	-7.50526900	0.87865000	2.72469300
O	-6.53777100	-3.83516300	-2.88604200
C	-6.63118600	-4.80525100	-1.83112100
C	-5.09363700	-2.98030300	3.40276400
O	-6.69419600	-2.41778800	1.90998000
C	-2.80078400	-3.25099800	2.86705700
P	-1.64541100	-2.69910200	0.37294500
H	-3.77733100	5.08784600	-3.05028000
H	-6.29909300	0.87466500	4.90077900
H	-6.16619400	-5.73912900	-2.15767400
H	-7.68290000	-4.95330000	-1.56395700
C	-3.82126100	-3.28673700	3.83381600
O	-6.25688800	-2.95222100	4.12384600
C	-7.28822200	-2.55214800	3.20852200
H	-1.79157100	-3.49442800	3.17565900
C	-0.27787600	-3.72839000	1.02889500
C	-2.18781500	-3.54698900	-1.15259900
H	-3.61479600	-3.54417800	4.86608800
H	-8.06319400	-3.32350400	3.17379300
H	-7.69469900	-1.58614800	3.52223000
C	0.04247400	-4.99113000	0.50964300

C	0.50235000	-3.19164600	2.06739400
C	-1.99333200	-2.91445700	-2.38640000
C	-2.80499400	-4.80638700	-1.11096500
C	1.11452100	-5.71417600	1.03526000
H	-0.53025400	-5.41088100	-0.30857900
C	1.56491300	-3.92589200	2.59398700
C	-2.41236300	-3.53189000	-3.56541000
H	-1.54036900	-1.92730300	-2.41134700
C	-3.20796900	-5.42798800	-2.29127700
H	-2.98992100	-5.28662300	-0.15527300
C	1.87386500	-5.18765400	2.08138500
H	1.35563300	-6.68970000	0.62249200
H	2.15737900	-3.50156000	3.39945200
C	-3.01721400	-4.78923800	-3.51980400
H	-2.27413200	-3.02762900	-4.51717100
H	-3.67804500	-6.40650400	-2.25190300
H	2.70705600	-5.75377100	2.48813900
H	-3.34568600	-5.26834200	-4.43741300
H	0.28774500	-2.19487000	2.44843300
Pd	-1.14160800	-0.38863600	0.15617900
C	0.99998500	-0.72478400	-0.35290800
C	0.68480500	0.46822200	-0.95213200
H	-0.72829300	1.14372000	-0.03306400
C	0.89780000	1.48520900	-1.76522200
H	1.86697700	1.58432400	-2.25080100
H	0.15536300	2.24857300	-1.96581400
Cl	-0.12688300	0.16403000	2.76724100
H	1.45675800	-0.74194500	0.63285900
H	1.04581800	-1.63231500	-0.94899900
INT1			
P	-1.23793900	1.77804300	-0.27802400
C	-2.26874400	0.53262000	-1.14849600
C	-1.61700900	3.34553500	-1.15292500
C	-1.97483000	1.90718100	1.38537100
C	-2.54900200	-0.72679000	-0.53746200
C	-2.67337900	0.78521300	-2.46380700
C	-2.68182000	4.18015100	-0.79126200
C	-0.82144300	3.68757400	-2.25749000
C	-1.12290000	1.92350000	2.49684300
C	-3.36436900	1.94914100	1.57510600
C	-3.25994600	-1.62613200	-1.31061400
C	-2.15536500	-1.12325100	0.84358200
C	-3.36474200	-0.16509900	-3.23431300
H	-2.44899900	1.74386400	-2.91447300
C	-2.94954500	5.33543000	-1.52762200

H	-3.29349500	3.94674300	0.07178000
C	-1.10256300	4.83231800	-3.00163500
H	0.02377300	3.05857800	-2.51973200
C	-1.65420400	1.98727800	3.78495300
H	-0.04959400	1.86305700	2.34092800
C	-3.89063400	2.03381400	2.86268100
H	-4.03258300	1.88034600	0.72292100
C	-3.64301400	-1.36958000	-2.62541600
O	-3.66539400	-2.88421100	-0.94981700
C	-3.13109100	-1.25219400	1.81395900
C	-0.82279500	-1.42946200	1.25038600
H	-3.66407400	0.04102700	-4.25531400
C	-2.16714300	5.65984300	-2.63666700
H	-3.76953000	5.98247700	-1.23004400
H	-0.48169900	5.08389600	-3.85629300
C	-3.03693100	2.04762700	3.96894600
H	-0.98928700	1.98404100	4.64329000
H	-4.96686300	2.07652100	3.00284000
O	-4.29728300	-2.45474800	-3.13920400
C	-4.28926200	-3.45510000	-2.10800800
C	-2.85256600	-1.60393700	3.13251100
O	-4.47504400	-1.02407800	1.67016600
C	-0.55857000	-1.80307100	2.57102600
P	0.55430100	-1.16809400	0.05970400
H	-2.37880800	6.55869100	-3.20837200
H	-3.44993800	2.09663300	4.97212300
H	-3.70553000	-4.31570200	-2.44657900
H	-5.31827000	-3.73567600	-1.86550000
C	-1.56970600	-1.89053800	3.54481100
O	-4.00864000	-1.60447900	3.86702700
C	-5.06504400	-1.27033800	2.95441900
H	0.45793300	-2.03390100	2.86470600
C	1.96814600	-2.03950500	0.82426300
C	0.05964200	-2.15880700	-1.39312000
H	-1.34880600	-2.17142500	4.56813200
H	-5.76224500	-2.11134400	2.87864700
H	-5.56826800	-0.36391800	3.30154200
C	2.33154900	-3.35205400	0.49953600
C	2.71130900	-1.33871000	1.78771000
C	0.22248500	-1.59815100	-2.66675300
C	-0.51164700	-3.43353500	-1.26530100
C	3.40984300	-3.96157600	1.14354500
H	1.78399100	-3.89833600	-0.25977700
C	3.77605000	-1.95588600	2.44121300

C	-0.18597000	-2.30211300	-3.79977900
H	0.65111100	-0.60474200	-2.76052400
C	-0.89967800	-4.14295500	-2.40071300
H	-0.67286900	-3.85772400	-0.27917300
C	4.12784100	-3.26907200	2.11948300
H	3.68728600	-4.97822200	0.88019100
H	4.34195300	-1.40512600	3.18667300
C	-0.74502600	-3.57489000	-3.66851900
H	-0.07142700	-1.85552500	-4.78288100
H	-1.32942300	-5.13522400	-2.29593900
H	4.96550700	-3.74600400	2.62021600
H	-1.06227400	-4.12277800	-4.55102800
H	2.46244700	-0.30633100	2.00958300
Pd	0.96052500	1.20071700	-0.32491400
H	1.20734500	2.75427300	-0.45330500
Cl	3.33524800	0.94815800	-0.65240300
TS2			
P	-1.30497500	1.73975900	-0.23034800
C	-2.33450000	0.50565300	-1.11749800
C	-1.57452700	3.30397600	-1.14487200
C	-2.15681200	1.92528700	1.37621100
C	-2.55827100	-0.76942800	-0.51446400
C	-2.79091700	0.76513400	-2.41310700
C	-2.50117200	4.28107400	-0.76087100
C	-0.77290300	3.52768700	-2.27746800
C	-1.38500100	1.92303000	2.54563100
C	-3.55359800	2.01095700	1.47026400
C	-3.27252900	-1.67724300	-1.27392400
C	-2.13081600	-1.15787900	0.86126600
C	-3.48180500	-0.19529800	-3.17324300
H	-2.60847500	1.73668900	-2.85558300
C	-2.63021900	5.45742400	-1.50267800
H	-3.11500900	4.13437400	0.12056000
C	-0.91673300	4.69411300	-3.02623600
H	-0.03188900	2.78600000	-2.56395100
C	-2.00112000	2.00370600	3.79433000
H	-0.30554000	1.82999800	2.46583200
C	-4.16589500	2.11287100	2.71858200
H	-4.16028200	1.97436800	0.57080900
C	-3.70615300	-1.41425900	-2.57165800
O	-3.64102300	-2.94738200	-0.91336200
C	-3.09497000	-1.27583100	1.84566700
C	-0.79305600	-1.46799500	1.25654900
H	-3.82321100	0.01531200	-4.18017700
C	-1.84520000	5.66387500	-2.63762000

H	-3.34635300	6.21229000	-1.19073000
H	-0.29526700	4.85161400	-3.90284200
C	-3.39150800	2.10143500	3.88201400
H	-1.39778400	1.98324900	4.69697900
H	-5.24762400	2.18907700	2.78375700
O	-4.35289300	-2.51022100	-3.07675300
C	-4.29435300	-3.51760300	-2.05514500
C	-2.80474800	-1.61892200	3.16386100
O	-4.44270500	-1.06217800	1.71072000
C	-0.51818600	-1.83185600	2.57784800
P	0.58341700	-1.18994900	0.06460600
H	-1.94906000	6.57933800	-3.21276200
H	-3.87179500	2.16369200	4.85419500
H	-3.70980600	-4.36677300	-2.42032900
H	-5.31014700	-3.81696200	-1.78005300
C	-1.51872700	-1.90829900	3.56397100
O	-3.95505900	-1.62216400	3.90822200
C	-5.01358300	-1.24962600	3.01249600
H	0.50075800	-2.06460300	2.86289600
C	2.00331300	-2.11045300	0.77470500
C	0.06229600	-2.14384200	-1.40468300
H	-1.28806700	-2.18586300	4.58615200
H	-5.75544500	-2.05308800	2.97078600
H	-5.45868800	-0.30954600	3.35139900
C	2.37693200	-3.39881500	0.37220600
C	2.76666300	-1.45361400	1.75334400
C	0.20005800	-1.55779000	-2.66942600
C	-0.50360800	-3.42243200	-1.29053100
C	3.48584700	-4.02205700	0.94827300
H	1.81601000	-3.91353100	-0.39911900
C	3.86300300	-2.08380000	2.33934400
C	-0.23250100	-2.24059100	-3.80666700
H	0.64618000	-0.57258600	-2.75418100
C	-0.91376700	-4.11063800	-2.43112000
H	-0.64350100	-3.86698700	-0.31001300
C	4.22641600	-3.37119900	1.93579200
H	3.77108600	-5.01766200	0.62061000
H	4.44116100	-1.56415500	3.09805300
C	-0.78752300	-3.51652500	-3.68999600
H	-0.13513500	-1.77579500	-4.78325700
H	-1.33861700	-5.10614300	-2.33695500
H	5.08874800	-3.85895600	2.38099600
H	-1.12194800	-4.04742500	-4.57666100
H	2.50697900	-0.43852700	2.03811300

Pd	0.94336900	1.15623900	-0.09586200
C	1.94295800	3.02280700	0.01331700
C	2.88865400	1.98041100	0.20578800
H	2.95094600	1.03695600	-1.01788100
C	4.01625900	1.75367800	0.88903300
H	4.60230900	2.56399800	1.32424200
H	4.43527400	0.75368900	0.96900400
Cl	3.35184800	0.41229100	-2.36837600
H	1.88569600	3.52383200	-0.95194100
H	1.60142700	3.61900400	0.85876400
INT2			
P	-1.37456600	1.77107900	-0.21248800
C	-2.36701700	0.51105200	-1.10996800
C	-1.69959600	3.33627400	-1.11381600
C	-2.27367000	1.93424600	1.37611200
C	-2.54803900	-0.77158000	-0.50767400
C	-2.84076800	0.75793100	-2.40135600
C	-2.65193000	4.28267900	-0.71248100
C	-0.90714200	3.60408300	-2.24303900
C	-1.52666400	1.98730900	2.56053500
C	-3.67421900	1.96102700	1.44527900
C	-3.25140700	-1.69555500	-1.25823100
C	-2.10734200	-1.14428500	0.86896600
C	-3.51341100	-0.22071800	-3.15586200
H	-2.69006000	1.73553900	-2.84327100
C	-2.81608500	5.46750500	-1.43282300
H	-3.25994100	4.10466700	0.16697000
C	-1.08469200	4.78045700	-2.96978900
H	-0.14750300	2.89353400	-2.55289200
C	-2.16857200	2.06215200	3.79679100
H	-0.44230000	1.94600500	2.50493600
C	-4.31445800	2.05811500	2.68007000
H	-4.26132400	1.88631000	0.53521600
C	-3.70475300	-1.44357000	-2.55101800
O	-3.59272300	-2.97191600	-0.89055500
C	-3.07591300	-1.28825700	1.84626800
C	-0.76385400	-1.41673700	1.27705100
H	-3.86938000	-0.01899500	-4.15968400
C	-2.03887300	5.71716800	-2.56473900
H	-3.55350600	6.19551600	-1.10646200
H	-0.46804300	4.96944100	-3.84375900
C	-3.56320700	2.09992300	3.85791800
H	-1.58171500	2.08536900	4.71030800
H	-5.39959200	2.09000800	2.72365200
O	-4.33362200	-2.55518200	-3.04840100

C	-4.25065100	-3.55561300	-2.02224900
C	-2.78998600	-1.61514000	3.16900400
O	-4.42888800	-1.11999700	1.69603000
C	-0.49366600	-1.76350500	2.60430000
P	0.62125200	-1.15586200	0.08074500
H	-2.16948600	6.63941800	-3.12356000
H	-4.06415000	2.15856000	4.81991500
H	-3.65935900	-4.39949000	-2.38929500
H	-5.25944100	-3.86713900	-1.73417400
C	-1.49962000	-1.86160100	3.58271200
O	-3.94739800	-1.65231200	3.90144900
C	-5.00687500	-1.31424900	2.99304100
H	0.52631600	-1.97375400	2.90121200
C	2.01948900	-2.11164500	0.79914100
C	0.06780300	-2.14870400	-1.35704400
H	-1.26936400	-2.12673800	4.60830200
H	-5.72635200	-2.13773800	2.94975600
H	-5.47978200	-0.38424300	3.32166200
C	2.42622900	-3.37332000	0.34462300
C	2.74163100	-1.50147700	1.83871800
C	0.12311400	-1.59170800	-2.63994300
C	-0.44907100	-3.44318500	-1.19044700
C	3.51672500	-4.01816900	0.93245500
H	1.90287100	-3.85362200	-0.47353100
C	3.81726100	-2.15502500	2.43761600
C	-0.33410200	-2.31645700	-3.74135300
H	0.50649500	-0.58751700	-2.77613800
C	-0.88257400	-4.17422500	-2.29470200
H	-0.52982000	-3.86911000	-0.19522700
C	4.20830300	-3.41754200	1.98499100
H	3.82389900	-4.99303400	0.56439300
H	4.35990500	-1.67012300	3.24399200
C	-0.83324800	-3.60888800	-3.57215700
H	-0.30241600	-1.86825000	-4.72992400
H	-1.26920600	-5.18016500	-2.15680900
H	5.05440000	-3.92304200	2.44148000
H	-1.18680100	-4.17309600	-4.43036100
H	2.46891500	-0.50066900	2.15937400
Pd	0.94424500	1.20418700	0.05395800
C	2.05927400	3.01455800	0.42464600
C	2.88942400	1.89766900	0.45672200
H	1.72595200	1.30994100	-1.76388100
C	4.09380600	1.36531700	0.58971700
H	4.96874900	1.98627400	0.78933600

H	4.26534100	0.29595900	0.50968800
Cl	2.14390800	1.50360600	-3.05923900
H	2.01930300	3.65232700	-0.45728700
H	1.71235200	3.47649600	1.34841000
INT3			
P	-1.30406900	2.04842000	-0.18774300
C	-2.33515200	0.83598800	-1.12787500
C	-1.73939300	3.68906700	-0.89907000
C	-2.06050000	2.03924400	1.48150300
C	-2.44727600	-0.51745300	-0.66593200
C	-2.85500900	1.19626400	-2.37405900
C	-2.66270300	4.57684200	-0.32922000
C	-1.04853600	4.08040500	-2.05923100
C	-1.22146100	1.93231100	2.59830400
C	-3.44930900	2.09468800	1.67028200
C	-3.11802400	-1.38334600	-1.51010500
C	-2.05290100	-1.02378300	0.68719600
C	-3.50511000	0.27949800	-3.22054400
H	-2.74848400	2.21811300	-2.71650300
C	-2.90348500	5.81995000	-0.91768800
H	-3.18782800	4.30960900	0.58007100
C	-1.30484900	5.31446000	-2.65486000
H	-0.31342300	3.41305300	-2.49884700
C	-1.75979500	1.88144400	3.88426600
H	-0.14695800	1.86540700	2.44962800
C	-3.98513700	2.07183600	2.95734100
H	-4.10961400	2.13250600	0.80966900
C	-3.61697300	-1.01250100	-2.75905100
O	-3.43995900	-2.69623200	-1.26405200
C	-3.05465800	-1.14398400	1.63340600
C	-0.75515500	-1.46289300	1.10042600
H	-3.90187000	0.57928500	-4.18368800
C	-2.23294200	6.18918000	-2.08449700
H	-3.61780000	6.49940400	-0.46102400
H	-0.77041100	5.59613100	-3.55759400
C	-3.14222400	1.95570900	4.06564400
H	-1.10194300	1.77967300	4.74235700
H	-5.06114700	2.13275900	3.09465700
O	-4.23980100	-2.08300600	-3.34720400
C	-3.96714200	-3.20570200	-2.49515600
C	-2.83536400	-1.57879800	2.93877300
O	-4.38197600	-0.83512400	1.47042800
C	-0.55113300	-1.90915300	2.41092400
P	0.67595300	-1.34423400	-0.06320300
H	-2.42476300	7.15573800	-2.54157100

H	-3.56268600	1.91722900	5.06628800
H	-3.21832600	-3.85007800	-2.96977600
H	-4.89631200	-3.74323800	-2.29472600
C	-1.58414600	-1.96415400	3.36432300
O	-4.00855800	-1.54343500	3.64562400
C	-5.02592600	-1.16221200	2.70756900
H	0.43829800	-2.23048500	2.71198700
C	2.03672000	-2.18021700	0.85010200
C	0.23795700	-2.54188100	-1.37817600
H	-1.40452200	-2.30385100	4.37797400
H	-5.71100400	-2.00311700	2.54958500
H	-5.55195100	-0.28300700	3.08614200
C	2.24314600	-3.56668000	0.85026300
C	2.90840800	-1.36125200	1.58427700
C	0.72043700	-2.32393700	-2.67556400
C	-0.52769300	-3.68644400	-1.11143400
C	3.29694100	-4.12134300	1.57801200
H	1.58632500	-4.21285200	0.27802600
C	3.95252200	-1.91697600	2.32300600
C	0.44563500	-3.23952300	-3.69191800
H	1.29587700	-1.43063100	-2.89258200
C	-0.78911900	-4.60760800	-2.12572100
H	-0.92658000	-3.84910400	-0.11578400
C	4.14973700	-3.29989900	2.31868800
H	3.45172000	-5.19658300	1.56610800
H	4.61731800	-1.27181600	2.89023400
C	-0.30570600	-4.38433500	-3.41794600
H	0.81544200	-3.05567700	-4.69631700
H	-1.37552500	-5.49615300	-1.90830600
H	4.96916600	-3.73474900	2.88379100
H	-0.51735400	-5.09896600	-4.20834000
H	2.76200700	-0.28337200	1.56724800
Pd	0.73156800	0.95235500	-0.34047600
H	0.69206700	0.97560300	-2.14601300
Cl	0.89351100	1.20757300	-3.55271300
TS3			
P	-1.30032200	1.92619100	-0.22107800
C	-2.26982500	0.62123000	-1.10397800
C	-1.72339600	3.48369500	-1.10067700
C	-2.15558700	2.03858500	1.39562300
C	-2.40970900	-0.68105000	-0.52509800
C	-2.77567300	0.87423200	-2.38323600
C	-2.61913800	4.44180800	-0.60691700
C	-1.05201700	3.74124400	-2.30848700
C	-1.38480900	2.03249500	2.56537200

C	-3.55366800	2.08580700	1.49401600
C	-3.10195800	-1.60486100	-1.28749500
C	-1.98959700	-1.10191700	0.84813600
C	-3.43221300	-0.10557800	-3.14991000
H	-2.66596300	1.86317400	-2.80985800
C	-2.85063500	5.62296600	-1.31501300
H	-3.13151100	4.27529100	0.33334800
C	-1.29756300	4.91252900	-3.02206600
H	-0.32996200	3.02426500	-2.68631600
C	-2.00033200	2.06990700	3.81651300
H	-0.30276500	1.97419800	2.48216200
C	-4.16738700	2.15012100	2.74442100
H	-4.15993700	2.05694400	0.59402900
C	-3.58034700	-1.34513600	-2.56921600
O	-3.41772100	-2.89262400	-0.93244200
C	-2.97690900	-1.20335100	1.81217700
C	-0.68012800	-1.51067900	1.25697500
H	-3.81188200	0.11045500	-4.14203100
C	-2.19829200	5.85851400	-2.52574000
H	-3.54387500	6.35877700	-0.91712000
H	-0.77377700	5.09250100	-3.95630100
C	-3.39259400	2.13218800	3.90719900
H	-1.39542900	2.04776100	4.71817300
H	-5.25058700	2.20136800	2.81122700
O	-4.19103100	-2.46259500	-3.07587400
C	-4.12829600	-3.45573900	-2.04172500
C	-2.73547200	-1.59765000	3.12576700
O	-4.31247300	-0.93191900	1.65250200
C	-0.45492000	-1.92254100	2.57513300
P	0.75314600	-1.33366900	0.10322800
H	-2.38127700	6.77772400	-3.07468200
H	-3.87336300	2.16378800	4.88069400
H	-3.58618000	-4.32871200	-2.41437400
H	-5.14353900	-3.71919400	-1.72605700
C	-1.47540300	-1.96526900	3.54247100
O	-3.90196200	-1.56608400	3.84497000
C	-4.93084700	-1.18269000	2.92033800
H	0.54265600	-2.22385400	2.87144200
C	2.07669500	-2.34647400	0.88005000
C	0.21693200	-2.26423500	-1.37965100
H	-1.28014600	-2.28344500	4.56025100
H	-5.65173800	-2.00090900	2.81644500
H	-5.41165800	-0.26780600	3.27625700
C	2.28942800	-3.71123400	0.64205400

C	2.93726900	-1.66838600	1.75925100
C	0.40982000	-1.67046400	-2.63457900
C	-0.40999500	-3.51628300	-1.30137700
C	3.33051400	-4.38474500	1.28299200
H	1.65386100	-4.24927000	-0.05150800
C	3.96523800	-2.34593900	2.41378500
C	-0.01424200	-2.31866200	-3.79453200
H	0.87111400	-0.68818000	-2.68947100
C	-0.80894700	-4.17541600	-2.46372500
H	-0.61241100	-3.96081000	-0.33217400
C	4.16454000	-3.70772700	2.17497200
H	3.48898500	-5.44107100	1.08465900
H	4.61766600	-1.80906300	3.09635800
C	-0.61969100	-3.57441200	-3.71082700
H	0.12450200	-1.84316600	-4.76099900
H	-1.27859500	-5.15272000	-2.39503400
H	4.97240600	-4.23585000	2.67323000
H	-0.94803700	-4.08147500	-4.61350900
H	2.79514200	-0.60244200	1.92284800
Pd	0.77176700	1.01086100	-0.10023700
H	1.46504200	2.24857300	-1.25481900
Cl	2.51007500	2.83006400	-2.01232200
TS4			
P	-1.30253700	1.69380400	-0.27001100
C	-2.35413000	0.46574000	-1.14377100
C	-1.59402500	3.27070400	-1.15797900
C	-2.11090000	1.87057700	1.35895800
C	-2.59276900	-0.80271900	-0.53160100
C	-2.79990600	0.71441100	-2.44545500
C	-2.43509000	4.28475700	-0.68352800
C	-0.89006700	3.47462000	-2.35762900
C	-1.31276500	1.81720500	2.50894200
C	-3.50175000	2.00007300	1.48698200
C	-3.29800700	-1.71651700	-1.29286900
C	-2.20587300	-1.18286000	0.85852200
C	-3.48804900	-0.24949500	-3.20407200
H	-2.61408300	1.68178800	-2.89509800
C	-2.57837900	5.47413600	-1.40200600
H	-2.97153500	4.15681700	0.24944200
C	-1.04898200	4.65385800	-3.08225700
H	-0.21029800	2.70585800	-2.71498700
C	-1.89675300	1.89035500	3.77339100
H	-0.23907600	1.68989600	2.40175800
C	-4.08113400	2.09413500	2.75134600
H	-4.12924100	2.00393900	0.60116800

C	-3.71831100	-1.46456600	-2.59707100
O	-3.67485500	-2.98160200	-0.92385900
C	-3.19990900	-1.27430800	1.81531500
C	-0.88811300	-1.52265400	1.29217200
H	-3.82311300	-0.04348400	-4.21411200
C	-1.89377900	5.65921500	-2.60326100
H	-3.22772300	6.25604200	-1.01890800
H	-0.50330900	4.79417100	-4.01069200
C	-3.28066200	2.03184300	3.89552200
H	-1.27403900	1.83046300	4.66084000
H	-5.15771500	2.20582000	2.84423800
O	-4.36341900	-2.56291500	-3.09827100
C	-4.30211600	-3.56682300	-2.07282400
C	-2.95647300	-1.62424000	3.14130500
O	-4.53593600	-1.02202300	1.64251300
C	-0.66135200	-1.89899400	2.61903000
P	0.51826800	-1.29332100	0.12553400
H	-2.00847600	6.58483500	-3.15952400
H	-3.73618400	2.08811700	4.87978400
H	-3.69675900	-4.40643200	-2.42679300
H	-5.31607800	-3.88266500	-1.81150900
C	-1.69106500	-1.95105400	3.57607600
O	-4.12553600	-1.59235600	3.85310000
C	-5.15264800	-1.21605100	2.92276300
H	0.33974100	-2.16570300	2.93367000
C	1.91334100	-2.20971800	0.88599200
C	0.01291700	-2.27446600	-1.33189800
H	-1.49646000	-2.23767900	4.60314100
H	-5.89221500	-2.01984600	2.85122800
H	-5.61001700	-0.27829900	3.25029200
C	2.39750200	-3.42689600	0.39063800
C	2.57395300	-1.60509700	1.96956600
C	0.11079800	-1.68918200	-2.60063500
C	-0.51224400	-3.56895500	-1.20584400
C	3.51428700	-4.03013100	0.97446100
H	1.91551200	-3.90161300	-0.45606300
C	3.67825900	-2.21483200	2.55925100
C	-0.31652200	-2.38592700	-3.73089200
H	0.49749500	-0.67787900	-2.68866600
C	-0.91793500	-4.27219800	-2.33897900
H	-0.61748100	-4.01649600	-0.22234500
C	4.15332500	-3.43071600	2.05962300
H	3.88470900	-4.96981500	0.57494600
H	4.17884700	-1.73226700	3.39308100

C	-0.82834500	-3.67872800	-3.60153600
H	-0.25510100	-1.91915900	-4.70934600
H	-1.31156700	-5.27951200	-2.23654800
H	5.02390200	-3.90000300	2.50790100
H	-1.16003700	-4.22230900	-4.48134700
H	2.22676800	-0.64601400	2.34280500
Pd	0.93252500	1.00782700	-0.25443300
Cl	5.78649300	1.84280600	0.68090400
C	2.94103400	1.84117400	-0.77792300
C	2.01015600	2.86805200	-0.48412700
C	3.52984000	1.04306200	0.22278500
H	3.19239700	1.62643100	-1.81379800
H	1.99720900	3.30684800	0.51260500
H	1.65450000	3.51590400	-1.27903000
H	3.96446000	0.08627800	-0.02481300
H	3.29687200	1.21551500	1.26449000
INT4			
P	-1.31312900	1.72389900	-0.25501800
C	-2.36920100	0.49757700	-1.13800800
C	-1.65050900	3.30795700	-1.12543700
C	-2.14916200	1.87856300	1.36806200
C	-2.59039400	-0.78182500	-0.54122200
C	-2.82799700	0.75525500	-2.43345800
C	-2.52344200	4.29724900	-0.65497900
C	-0.93392200	3.54550500	-2.31153500
C	-1.35991600	1.82540400	2.52420900
C	-3.54192500	1.99013500	1.49051500
C	-3.29666400	-1.69181500	-1.30673200
C	-2.19376200	-1.17627200	0.84301400
C	-3.51281100	-0.20629200	-3.19894600
H	-2.65444200	1.72979100	-2.87298400
C	-2.68515400	5.49131700	-1.36178700
H	-3.07162800	4.14592100	0.26769600
C	-1.11159600	4.72799200	-3.02686400
H	-0.23027800	2.79686600	-2.66489300
C	-1.95208500	1.88319200	3.78590100
H	-0.28439500	1.70899700	2.42138900
C	-4.13126400	2.06958400	2.75153200
H	-4.16380100	1.99203400	0.60065400
C	-3.72973300	-1.42946800	-2.60387600
O	-3.66635000	-2.96310100	-0.94626900
C	-3.18591700	-1.28401600	1.80058900
C	-0.87298400	-1.51607000	1.26950900
H	-3.85757900	0.00856400	-4.20405000
C	-1.98780700	5.70734400	-2.55070300

H	-3.35982500	6.25257100	-0.98015200
H	-0.55604400	4.89150900	-3.94588100
C	-3.33808700	2.00910400	3.90086800
H	-1.33433400	1.82305500	4.67707900
H	-5.20987800	2.16792300	2.83791000
O	-4.37449100	-2.52777700	-3.11133100
C	-4.29986200	-3.53941600	-2.09528700
C	-2.94009100	-1.64475300	3.12250400
O	-4.52543400	-1.04135600	1.63066800
C	-0.64460700	-1.90204400	2.59373600
P	0.53251300	-1.27415500	0.09654800
H	-2.11735600	6.63612300	-3.09873800
H	-3.80060100	2.05386600	4.88263200
H	-3.69425000	-4.37381900	-2.46165000
H	-5.31038700	-3.86276500	-1.82840500
C	-1.67213000	-1.96687300	3.55266100
O	-4.11028300	-1.62880000	3.83600200
C	-5.13839800	-1.24533700	2.91007700
H	0.35799400	-2.16701000	2.90531900
C	1.91343700	-2.21217700	0.86737900
C	0.01510600	-2.28514100	-1.34193800
H	-1.47428400	-2.26105300	4.57713700
H	-5.87846600	-2.04854100	2.83392400
H	-5.59573500	-0.31028200	3.24605900
C	2.36774900	-3.45675700	0.41305400
C	2.59301800	-1.59132300	1.93023500
C	0.11528200	-1.72053700	-2.61999700
C	-0.52217500	-3.57272800	-1.19858800
C	3.46816000	-4.07115600	1.01632900
H	1.87230600	-3.94643100	-0.41730800
C	3.67828900	-2.21319800	2.54391600
C	-0.31915300	-2.42944000	-3.74012800
H	0.51037600	-0.71338600	-2.72049600
C	-0.93458000	-4.28977700	-2.32085800
H	-0.63356000	-4.00394200	-0.20839900
C	4.12117000	-3.45714800	2.08518400
H	3.81296800	-5.03311600	0.64754100
H	4.18748300	-1.72090600	3.36738600
C	-0.84141900	-3.71611600	-3.59220600
H	-0.25553300	-1.97689100	-4.72529900
H	-1.33819900	-5.29160500	-2.20290200
H	4.97563900	-3.93773800	2.55256100
H	-1.17893200	-4.26960600	-4.46376800
H	2.26998700	-0.61037400	2.26839900

Pd	0.93371200	1.02030900	-0.30351400
Cl	5.63642700	1.95471200	0.33147200
C	3.05047400	1.60929900	-0.71417900
C	2.22747100	2.74986500	-0.67666700
C	3.89387200	1.20023300	0.42983400
H	3.33365700	1.19204800	-1.67869900
H	2.21457400	3.38178000	0.21005200
H	1.91791500	3.23914400	-1.59595600
H	4.09384500	0.13250000	0.47226200
H	3.51722200	1.55564300	1.38825400
INT5			
P	-1.07997400	1.99635900	0.00178300
C	-2.06959600	0.80171300	-1.00661200
C	-1.46417000	3.62940700	-0.76262000
C	-1.98562200	1.99981700	1.59784700
C	-2.31240400	-0.51842600	-0.51040700
C	-2.44001500	1.13176800	-2.31479500
C	-2.40930000	4.54459600	-0.28062200
C	-0.68787300	3.98637300	-1.87944900
C	-1.24192300	1.86016500	2.77700000
C	-3.38387500	2.07867000	1.67595300
C	-2.94268300	-1.38597600	-1.38505300
C	-2.01495400	-1.01664900	0.86697900
C	-3.04973600	0.21327000	-3.18881000
H	-2.25214100	2.13372500	-2.68113100
C	-2.58532100	5.77883500	-0.91097300
H	-3.00263600	4.30506000	0.59405900
C	-0.88027900	5.20772200	-2.52216400
H	0.07532800	3.29844900	-2.23301000
C	-1.88264300	1.80135100	4.01481700
H	-0.16140700	1.76644300	2.70816000
C	-4.02264000	2.04508800	2.91492800
H	-3.97291300	2.13989400	0.76617900
C	-3.28573700	-1.04913300	-2.69117700
O	-3.31748700	-2.68268400	-1.13130700
C	-3.06598800	-1.18971600	1.74864700
C	-0.72907300	-1.41640600	1.34455200
H	-3.32468900	0.48925500	-4.20056300
C	-1.83044800	6.11068100	-2.03667200
H	-3.31697500	6.48066200	-0.51998200
H	-0.27913000	5.46122200	-3.39103700
C	-3.27385500	1.89868000	4.08575100
H	-1.29836700	1.67264200	4.92134200
H	-5.10544300	2.12018100	2.96617500
O	-3.87550100	-2.12158600	-3.31135100

C	-3.85294500	-3.19423500	-2.35791400
C	-2.90492300	-1.65781500	3.05020100
O	-4.39140000	-0.91802900	1.51766500
C	-0.58348700	-1.90615600	2.64642300
P	0.73784000	-1.09789800	0.28386500
H	-1.97268200	7.06977300	-2.52650400
H	-3.77441200	1.85322400	5.04871900
H	-3.20506900	-3.99401400	-2.73003800
H	-4.87308500	-3.55111600	-2.18703400
C	-1.66915300	-2.02820500	3.53296000
O	-4.11771600	-1.68167700	3.69089400
C	-5.08578200	-1.23491100	2.73010700
H	0.39902100	-2.20309500	2.99353900
C	2.09554100	-2.01420800	1.11882300
C	0.37293100	-2.07834800	-1.22337500
H	-1.53992000	-2.40155800	4.54260400
H	-5.80558900	-2.03761800	2.53687000
H	-5.58199700	-0.33715800	3.10934500
C	2.52149400	-3.30116700	0.76403300
C	2.78705000	-1.32930800	2.13407500
C	0.66742700	-1.50191400	-2.46736000
C	-0.21693100	-3.34973100	-1.17838800
C	3.60587400	-3.89298100	1.41609900
H	2.01319100	-3.84192900	-0.02647100
C	3.85636900	-1.92782600	2.79804500
C	0.37797600	-2.18610400	-3.64827900
H	1.10079600	-0.50542200	-2.50025100
C	-0.48861400	-4.04071500	-2.35908300
H	-0.48103800	-3.78752400	-0.22059200
C	4.27157100	-3.21297100	2.43700200
H	3.92801100	-4.88925500	1.12576600
H	4.37371700	-1.38807600	3.58628200
C	-0.19830300	-3.45724000	-3.59576400
H	0.59672300	-1.72516900	-4.60715000
H	-0.93450200	-5.03072100	-2.31485900
H	5.11349500	-3.67638300	2.94323800
H	-0.42445200	-3.99096300	-4.51451200
H	2.47987700	-0.31900800	2.39403500
Pd	1.11070700	1.17208800	-0.09103200
C	2.84991200	2.64353600	-2.17943100
N	3.67860800	0.71839400	-1.77885400
H	3.79758000	-0.25923600	-2.00038300
H	2.53384900	3.49598400	-2.76701000
C	2.87642900	2.52878900	-0.74906800

H	2.83028300	3.34090700	-0.03774400
C	3.36375000	1.21634200	-0.52372200
H	3.81937800	0.78319900	0.35692100
N	3.28105700	1.55035300	-2.78472600
C₃H₅Cl			
Cl	5.67704500	1.75734800	0.31480400
C	3.10328100	1.84698400	-0.65633300
C	2.14323100	2.76406100	-0.52767800
C	3.89492400	1.32949800	0.49548700
H	3.34036300	1.42512300	-1.63105400
H	1.89877600	3.20250600	0.43731600
H	1.56390900	3.10454400	-1.38098000
H	3.87680100	0.23998900	0.55973900
H	3.57415900	1.76046900	1.44439700
TS5			
P	-1.04872600	1.75580900	-0.02364900
C	-2.08322900	0.61151500	-1.02726200
C	-1.29426600	3.40625300	-0.78824800
C	-1.93117000	1.82360100	1.57972500
C	-2.35567100	-0.70067700	-0.52986300
C	-2.46427100	0.96605200	-2.32481700
C	-2.26539500	4.33153700	-0.38011400
C	-0.40612300	3.75656900	-1.81932800
C	-1.17415800	1.72355400	2.75444600
C	-3.32752000	1.92574200	1.66897400
C	-3.04366800	-1.53969500	-1.38746400
C	-2.02907800	-1.18147800	0.84528200
C	-3.12985900	0.07387600	-3.18530200
H	-2.23998100	1.96206000	-2.68848400
C	-2.35515700	5.57775400	-1.00179600
H	-2.94237000	4.09085900	0.43137100
C	-0.50564800	4.99924000	-2.44440700
H	0.37648000	3.06832700	-2.12359300
C	-1.80155600	1.72847700	4.00069200
H	-0.09548900	1.61383200	2.68229400
C	-3.95157900	1.95160200	2.91535200
H	-3.92594300	1.95644800	0.76385800
C	-3.40668600	-1.17899500	-2.68314000
O	-3.46625700	-2.81951200	-1.13031200
C	-3.06003000	-1.32008700	1.75675800
C	-0.73066600	-1.54553800	1.31636500
H	-3.41758200	0.36202000	-4.18995200
C	-1.48015900	5.91283600	-2.03752000
H	-3.10839500	6.28853200	-0.67322100
H	0.19368100	5.25514000	-3.23495100

C	-3.19039600	1.84621400	4.08272200
H	-1.20818600	1.63245200	4.90520200
H	-5.03256400	2.04326400	2.97569200
O	-4.05958300	-2.22070400	-3.29048100
C	-4.03902800	-3.30582700	-2.35150700
C	-2.86765900	-1.72245100	3.07622200
O	-4.38896500	-1.05656800	1.54472600
C	-0.55246400	-1.96368100	2.63919300
P	0.73094100	-1.33380400	0.22073600
H	-1.55121700	6.88532700	-2.51656900
H	-3.67988100	1.84885900	5.05230700
H	-3.41519200	-4.11351200	-2.74711300
H	-5.06184600	-3.64343200	-2.16214300
C	-1.61784400	-2.05226600	3.55263100
O	-4.06360200	-1.71858100	3.74349400
C	-5.05740400	-1.32905900	2.78300500
H	0.44009700	-2.23055300	2.98144800
C	2.04687400	-2.28070200	1.08398700
C	0.29267000	-2.32527600	-1.25552700
H	-1.46295500	-2.36749700	4.57811300
H	-5.76765500	-2.15029300	2.63959200
H	-5.55884500	-0.42236500	3.13162500
C	2.17477800	-3.67470300	1.01396100
C	2.95048400	-1.55106100	1.87062400
C	0.64161300	-1.82948800	-2.51935800
C	-0.39772700	-3.54254000	-1.16056100
C	3.18590900	-4.32474500	1.72242600
H	1.49653500	-4.25447800	0.39840400
C	3.95088200	-2.20315300	2.59143100
C	0.31000100	-2.54255300	-3.67154000
H	1.15824600	-0.87604400	-2.58958100
C	-0.70854200	-4.26432100	-2.31227500
H	-0.71665000	-3.91164100	-0.19119300
C	4.07119400	-3.59243500	2.51653300
H	3.28221400	-5.40452000	1.65284500
H	4.64182000	-1.62641600	3.19949600
C	-0.36121300	-3.76300500	-3.56958700
H	0.57320000	-2.14384500	-4.64676200
H	-1.23118700	-5.21303600	-2.22808700
H	4.85657600	-4.10171600	3.06758300
H	-0.61737000	-4.31990200	-4.46632300
H	2.86603900	-0.46786000	1.90328900
Pd	1.21271000	0.85904200	-0.25503800
C	3.23813700	3.73323000	-2.57707600

N	2.66820500	2.30802400	-1.07634300
H	2.78698000	0.88488300	-0.71747400
H	3.35708200	4.14252500	-3.57310400
C	3.62442700	4.29221600	-1.34182800
H	4.11113000	5.23977500	-1.15805500
C	3.24947100	3.33729700	-0.40627700
H	3.34462200	3.31474300	0.67038900
N	2.67159300	2.52887700	-2.41816300
INT6			
P	-0.88129600	1.60294300	-0.22525200
C	-1.98200100	0.44423700	-1.13059200
C	-1.04867900	3.19390400	-1.10890100
C	-1.70705100	1.82188100	1.38935500
C	-2.32187700	-0.80351200	-0.52814400
C	-2.37254500	0.72357500	-2.44315000
C	-1.87931200	4.23348100	-0.67127800
C	-0.26826200	3.37505900	-2.26206000
C	-0.92565400	1.75618900	2.55035100
C	-3.09330800	2.00704300	1.49854900
C	-3.07356800	-1.66572000	-1.30415400
C	-1.95969900	-1.20012800	0.86166700
C	-3.10310600	-0.19241400	-3.22093100
H	-2.10578700	1.67591200	-2.88459200
C	-1.93681700	5.43194200	-1.38411500
H	-2.46870500	4.12037500	0.23116000
C	-0.33365600	4.57069600	-2.97341800
H	0.42423500	2.60228100	-2.57521300
C	-1.52179300	1.87441900	3.80604200
H	0.14318400	1.58297400	2.46293800
C	-3.68424500	2.14221200	2.75369500
H	-3.70926800	2.02068000	0.60486200
C	-3.43791800	-1.38576400	-2.61920800
O	-3.53174100	-2.90903200	-0.95242800
C	-2.95462300	-1.25633500	1.82009500
C	-0.64813100	-1.54762200	1.30509500
H	-3.38985900	0.03171700	-4.24188200
C	-1.16877000	5.60145800	-2.53701200
H	-2.57906000	6.23465400	-1.03294500
H	0.28655600	4.70335400	-3.85448900
C	-2.90045200	2.06974400	3.90888200
H	-0.91206800	1.80611300	4.70191300
H	-4.75689900	2.29602200	2.83115000
O	-4.13079000	-2.44408300	-3.14412300
C	-4.24355000	-3.41290300	-2.09127400
C	-2.71421900	-1.57771400	3.15427100

O	-4.28478600	-0.97932600	1.64470600
C	-0.42206200	-1.88664900	2.64299400
P	0.78378300	-1.40391200	0.16217400
H	-1.21045000	6.53797500	-3.08580800
H	-3.36519300	2.16017300	4.88631300
H	-3.78941800	-4.35298100	-2.41549100
H	-5.29855900	-3.54726300	-1.82977700
C	-1.45160000	-1.90307500	3.59988900
O	-3.88000400	-1.50934900	3.86606700
C	-4.90262300	-1.13321200	2.92978000
H	0.57919200	-2.14624700	2.96384200
C	2.07963000	-2.41988900	0.96845000
C	0.26196900	-2.30286800	-1.33726700
H	-1.25992700	-2.15788700	4.63572400
H	-5.65729400	-1.92425700	2.87793400
H	-5.34069200	-0.17998600	3.23807900
C	2.18685900	-3.80455100	0.78554000
C	2.96794900	-1.77197100	1.84034300
C	0.53922400	-1.73558400	-2.58809400
C	-0.44213000	-3.51412900	-1.26586300
C	3.16488300	-4.52890000	1.46866200
H	1.52396000	-4.31993100	0.10062900
C	3.93246600	-2.50079900	2.53487000
C	0.11707800	-2.37356300	-3.75459600
H	1.06624300	-0.78674800	-2.63633800
C	-0.84416100	-4.15849700	-2.43427500
H	-0.70925200	-3.93146900	-0.30043500
C	4.03374400	-3.88130400	2.34853600
H	3.24787500	-5.60012100	1.30978600
H	4.61219100	-1.98825700	3.20911500
C	-0.57090200	-3.58626800	-3.67948800
H	0.32106600	-1.92078500	-4.72015300
H	-1.38178300	-5.10025000	-2.37191900
H	4.79302400	-4.44811000	2.87943800
H	-0.90044600	-4.08139500	-4.58813900
H	2.90587400	-0.69448600	1.95819200
Pd	1.39562700	0.77679500	-0.20091100
C	3.05802600	4.35472100	-1.49919000
N	2.16600500	2.68051200	-0.47236300
H	2.88060400	0.23006200	-0.29818900
H	3.59683600	4.87051700	-2.28576200
C	2.51118600	4.87868300	-0.31417700
H	2.52265900	5.90054400	0.03959000
C	1.94782900	3.76703900	0.30749400

H	1.39815900	3.68260600	1.23596900
N	2.85105600	3.02910200	-1.59034500
INT7a			
P	-1.09732200	0.24835600	1.13761600
C	-2.39995500	0.34164600	-0.16334500
C	-1.52999500	1.49861000	2.41522800
C	-1.43244100	-1.35364700	1.96041900
C	-2.43576600	-0.69356600	-1.15150400
C	-3.19022300	1.48411900	-0.31716900
C	-1.83782600	1.15683500	3.73984900
C	-1.36917500	2.85889900	2.09339400
C	-0.36222100	-2.23388700	2.16154100
C	-2.72109700	-1.72988500	2.36701600
C	-3.26938600	-0.47034600	-2.23092400
C	-1.75085700	-2.01665700	-1.03802000
C	-4.02234200	1.68416100	-1.43504400
H	-3.16562900	2.25389500	0.44433700
C	-1.98976900	2.14813700	4.71272600
H	-1.94874800	0.11577000	4.01981100
C	-1.53950600	3.84750500	3.05958200
H	-1.08883600	3.13824500	1.08330400
C	-0.57658100	-3.47944700	2.75300000
H	0.62986200	-1.94648300	1.82491000
C	-2.93116500	-2.96714700	2.97389200
H	-3.55723200	-1.05807500	2.19742000
C	-4.02707100	0.69004500	-2.38860600
O	-3.51689800	-1.32299900	-3.27856600
C	-2.50571700	-3.10644100	-0.64511100
C	-0.38004900	-2.27988400	-1.33377500
H	-4.63069900	2.57571500	-1.53705300
C	-1.84666300	3.49459000	4.37728100
H	-2.22006800	1.86287100	5.73538800
H	-1.41627100	4.89205300	2.78813700
C	-1.86027100	-3.84674100	3.16044100
H	0.25541000	-4.16409500	2.88848200
H	-3.92965700	-3.24823000	3.29754200
O	-4.75721700	0.61180600	-3.54754200
C	-4.27674100	-0.56014300	-4.22429100
C	-1.98032500	-4.38740100	-0.49358600
O	-3.83914300	-3.11389600	-0.32125000
C	0.13184600	-3.57393700	-1.19404100
P	0.72478200	-0.86506400	-1.73697100
H	-1.96544300	4.26336600	5.13529600
H	-2.02842900	-4.81655300	3.61972400
H	-3.62415100	-0.26037300	-5.05278900

H	-5.12580800	-1.15319600	-4.56913900
C	-0.65735000	-4.65700300	-0.76507900
O	-2.95915500	-5.24437200	-0.06213800
C	-4.14836200	-4.45323900	0.08421900
H	1.17534600	-3.75663600	-1.41813200
C	2.30307000	-1.70472600	-2.16081700
C	0.05572800	-0.28141800	-3.34422400
H	-0.24325800	-5.65248800	-0.65194200
H	-4.93513900	-4.85577600	-0.56136300
H	-4.45320600	-4.45211800	1.13481100
C	2.57820500	-2.28604000	-3.40544500
C	3.26808200	-1.78055100	-1.14498800
C	0.08931800	1.09457500	-3.61351800
C	-0.48500400	-1.15301400	-4.30017300
C	3.79183700	-2.93494700	-3.62772100
H	1.85649900	-2.21449000	-4.21101200
C	4.47691700	-2.44066500	-1.36359700
C	-0.38055900	1.58806300	-4.83112600
H	0.47740600	1.76957300	-2.85592100
C	-0.94780700	-0.66005900	-5.52063800
H	-0.55775600	-2.21386500	-4.08257700
C	4.74186500	-3.01462700	-2.60903700
H	4.00807100	-3.34888500	-4.60712000
H	5.21671500	-2.49054400	-0.56950700
C	-0.89319500	0.71039700	-5.78968600
H	-0.35154200	2.65568800	-5.02894200
H	-1.35646600	-1.34471800	-6.25879200
H	5.69149300	-3.50943800	-2.79007300
H	-1.25682300	1.09301600	-6.73920500
H	3.06570300	-1.30297200	-0.18959900
C	3.38665600	2.46372500	-1.12871200
C	2.48138300	2.13836900	-0.21355900
C	1.81952200	2.42249000	0.97802300
Pd	0.90153500	0.75576700	-0.03429900
C	3.52234100	1.80666300	-2.47510600
H	3.38579700	2.56450900	-3.26214400
H	2.71039900	1.08593400	-2.58501500
C	4.85962200	1.09382500	-2.69906900
H	5.68505700	1.81396800	-2.60417700
H	5.00168700	0.36357600	-1.89276900
C	4.97967400	0.36595000	-4.02553100
C	3.94700700	0.33548600	-4.96988300
C	6.15766400	-0.33882300	-4.31435500
C	4.08234600	-0.38395300	-6.16015700

H	3.01652400	0.85771100	-4.77700600
C	6.29911700	-1.05763200	-5.49952900
H	6.96906800	-0.32985100	-3.58969100
C	5.25637200	-1.08582600	-6.43026900
H	3.26134700	-0.39766700	-6.87242500
H	7.22089900	-1.59883900	-5.69692400
H	5.36163400	-1.64673000	-7.35499300
H	1.12941800	3.26940400	0.96408500
C	2.26715600	2.03873700	2.37505900
H	3.00021300	1.22444400	2.33783200
H	1.40630200	1.66794900	2.94439900
C	2.85913500	3.23962400	3.14949800
H	3.80707800	3.54406000	2.69039800
H	2.16644400	4.08567800	3.04745200
C	3.05193700	2.92002800	4.61188800
C	1.94378000	2.88544400	5.47224800
C	4.31102100	2.59900000	5.13218900
C	2.09224000	2.54221300	6.81556800
H	0.95843200	3.12955700	5.08151700
C	4.46487200	2.25633700	6.47772600
H	5.17836900	2.62032400	4.47632700
C	3.35536000	2.22664800	7.32429400
H	1.22231700	2.52355400	7.46698300
H	5.45145400	2.01421300	6.86396200
H	3.47295600	1.96149700	8.37135200
H	4.07793800	3.28844600	-0.92512600
TS6a			
P	-1.15816800	0.57493900	0.79634500
C	-2.52080700	0.35211800	-0.41678600
C	-1.59907200	2.07686500	1.74777400
C	-1.35939900	-0.82503800	1.95152100
C	-2.60988500	-0.88050200	-1.13285800
C	-3.35913300	1.42003100	-0.75147100
C	-2.04272500	2.04423200	3.07577100
C	-1.37320900	3.32240600	1.13575900
C	-0.22688900	-1.57504500	2.29620500
C	-2.61516400	-1.17952400	2.46717300
C	-3.56108200	-0.93077600	-2.13513300
C	-1.81715100	-2.11163800	-0.84575300
C	-4.30130500	1.34313600	-1.79329200
H	-3.28824100	2.34538700	-0.19367400
C	-2.27223100	3.23352600	3.77158300
H	-2.19759600	1.09407000	3.57344600
C	-1.62127100	4.50722100	1.82520700
H	-0.99073000	3.35734600	0.11943800

C	-0.35508900	-2.67272200	3.14842400
H	0.74864300	-1.32357100	1.88856700
C	-2.73318200	-2.26545500	3.33308000
H	-3.49828200	-0.61720800	2.17900300
C	-4.37196600	0.14898800	-2.47673400
O	-3.85359700	-2.00016000	-2.94253100
C	-2.44556200	-3.16712300	-0.21198500
C	-0.45942800	-2.33081800	-1.23031700
H	-4.94126400	2.18188900	-2.04245400
C	-2.06939000	4.46516300	3.14846200
H	-2.60905800	3.19371400	4.80350300
H	-1.44870500	5.46178700	1.33652700
C	-1.60349800	-3.01842900	3.66888100
H	0.52488000	-3.25654600	3.40217300
H	-3.70548600	-2.52788400	3.74094700
O	-5.19482700	-0.19725300	-3.51586500
C	-4.82901000	-1.53652000	-3.88494800
C	-1.80867800	-4.36995500	0.08430700
O	-3.74378000	-3.21232700	0.22915100
C	0.15921900	-3.55291300	-0.95290100
P	0.50044800	-0.91601400	-1.90674400
H	-2.24886200	5.38801400	3.69232400
H	-1.69959300	-3.87259600	4.33318900
H	-4.38752700	-1.52697000	-4.88638100
H	-5.71206000	-2.17987900	-3.83983100
C	-0.50140600	-4.59907400	-0.28380600
O	-2.67757500	-5.20989400	0.72935900
C	-3.89228100	-4.46540600	0.90963700
H	1.18612500	-3.71044900	-1.25605600
C	2.04505500	-1.63476700	-2.57074200
C	-0.47452200	-0.38719400	-3.35955200
H	-0.00411000	-5.53809100	-0.06969200
H	-4.72695400	-5.01958300	0.47148600
H	-4.04659700	-4.28102100	1.97719000
C	2.38316100	-1.60065800	-3.92936000
C	2.99553800	-2.08737100	-1.63773300
C	-0.78341800	0.97275900	-3.49376600
C	-0.96131900	-1.30344500	-4.30274500
C	3.64811800	-2.02038300	-4.34882500
H	1.67229400	-1.22929400	-4.65929600
C	4.24666500	-2.52612300	-2.06386400
C	-1.57656500	1.41221200	-4.55360700
H	-0.42202300	1.67241600	-2.74516500
C	-1.73712200	-0.85981600	-5.37293600

H	-0.74417000	-2.36132200	-4.18958300
C	4.57802400	-2.48877400	-3.42135300
H	3.91369300	-1.96142200	-5.39952600
H	4.96916900	-2.86728800	-1.32803600
C	-2.05296000	0.49681900	-5.49452400
H	-1.82849200	2.46496300	-4.64086400
H	-2.10263500	-1.57253800	-6.10700200
H	5.56396000	-2.79699000	-3.75238600
H	-2.67130700	0.83791200	-6.31982700
H	2.76889900	-2.06746800	-0.57662500
C	2.93358300	2.15901200	-1.13599700
C	2.82907400	1.63450700	0.13022600
C	1.86412400	2.15724200	1.04779800
Pd	0.91012700	0.71252800	-0.24265000
C	3.60643200	1.44755200	-2.27473900
H	2.96795900	1.46516800	-3.16889000
H	3.75297000	0.40063200	-2.00449900
C	4.97575400	2.06407400	-2.65125100
H	4.83136600	3.09700600	-2.99416900
H	5.60278900	2.10836500	-1.75299900
C	5.65989200	1.24229600	-3.71779100
C	5.23080800	1.30085000	-5.05092200
C	6.68882400	0.35237100	-3.38891400
C	5.81087300	0.49114600	-6.02737100
H	4.43198200	1.98704600	-5.32322800
C	7.27742000	-0.45655900	-4.36256300
H	7.02623800	0.28964500	-2.35716600
C	6.83805900	-0.39262200	-5.68583600
H	5.46492400	0.55254400	-7.05584200
H	8.07756300	-1.13826000	-4.08643000
H	7.29410400	-1.02140500	-6.44549300
H	1.32757300	3.08991400	0.82470900
C	1.93040400	1.78779400	2.51394700
H	1.96906600	0.69896700	2.61414700
H	1.02733400	2.12385600	3.03695000
C	3.18134700	2.36220400	3.22036900
H	4.05737000	2.11111000	2.61047100
H	3.11662700	3.45678500	3.26094700
C	3.34017200	1.78646500	4.60601500
C	2.89091100	2.47567700	5.73875600
C	3.88751600	0.50512500	4.77473700
C	2.98646900	1.90568000	7.01043000
H	2.46188200	3.46833400	5.62086200
C	3.98345600	-0.06762900	6.04259700

H	4.23756300	-0.04457200	3.90542700
C	3.53330600	0.63065700	7.16664500
H	2.63546000	2.45817700	7.87823700
H	4.41215500	-1.06041800	6.15236800
H	3.60971600	0.18549800	8.15496900
H	3.61444400	0.18150400	0.74809200
H	2.65209900	3.20642900	-1.34543400
C	5.29732400	-1.03195100	1.49979900
C	5.28062700	-2.24739800	2.17635300
C	3.90996900	-2.56081300	2.28647400
N	4.01385800	-0.69344300	1.25237100
H	6.11430700	-0.39679300	1.18647700
H	6.12776600	-2.81426400	2.53541900
H	3.44604200	-3.42482300	2.74572100
N	3.14661600	-1.61336300	1.72410000
INT8a			
P	-1.57355300	1.28949300	-0.84135700
C	-2.64334400	-0.06948600	-1.46312900
C	-1.55473900	2.49412200	-2.22314900
C	-2.60489000	2.07532000	0.44639500
C	-2.96025300	-1.14197800	-0.58002200
C	-3.08061000	-0.10382700	-2.79118600
C	-2.10930900	3.77415400	-2.11062100
C	-0.83666000	2.16161900	-3.38498400
C	-1.96135000	2.61308200	1.56829500
C	-4.00150100	2.14453300	0.34085600
C	-3.69884700	-2.17723700	-1.12203900
C	-2.59469900	-1.22703500	0.86300500
C	-3.81228600	-1.18251200	-3.31892200
H	-2.85186200	0.72400000	-3.44899100
C	-1.93316800	4.71181000	-3.13157900
H	-2.65560600	4.04997100	-1.21524900
C	-0.69340800	3.08566900	-4.41714500
H	-0.37317500	1.18217700	-3.46605800
C	-2.71241300	3.20996400	2.58220600
H	-0.88202300	2.52658800	1.65658900
C	-4.74651800	2.75046700	1.35170200
H	-4.50100900	1.71534800	-0.52204800
C	-4.09806700	-2.21665900	-2.45540600
O	-4.11651300	-3.31508400	-0.48148200
C	-3.58228000	-1.04265900	1.81118700
C	-1.31339700	-1.61614300	1.36230800
H	-4.13185000	-1.19841000	-4.35457100
C	-1.22861400	4.37100600	-4.28488900
H	-2.32863400	5.71561500	-3.01501700

H	-0.13859600	2.81436800	-5.31087200
C	-4.10316200	3.27968800	2.47557000
H	-2.20897900	3.60796800	3.45848300
H	-5.82840700	2.80411400	1.26683900
O	-4.77310900	-3.38123300	-2.70522000
C	-4.79968300	-4.10431300	-1.46438500
C	-3.37008500	-1.21731500	3.17966700
O	-4.89663000	-0.71307100	1.59111400
C	-1.12098700	-1.81639800	2.73088600
P	0.12124100	-1.59667500	0.21976700
H	-1.08013600	5.10823700	-5.06721800
H	-4.68723900	3.74265000	3.26616300
H	-4.27774400	-5.05705500	-1.59078600
H	-5.83806400	-4.25522900	-1.15273300
C	-2.15078600	-1.62878200	3.67117500
O	-4.53616300	-0.98130300	3.85987400
C	-5.44310900	-0.43841900	2.88738600
H	-0.14080700	-2.09694900	3.09417700
C	1.45719500	-2.50062300	1.09897800
C	-0.37803000	-2.70059200	-1.14968800
H	-1.98449700	-1.78462300	4.73078000
H	-6.41322300	-0.92880100	2.98300700
H	-5.51685300	0.64700700	3.02488600
C	1.81499300	-3.82135700	0.79323700
C	2.18818500	-1.79890300	2.07328300
C	-0.16349400	-2.27783200	-2.46632700
C	-0.99238100	-3.93926600	-0.91175300
C	2.87164900	-4.43775300	1.46642700
H	1.28521500	-4.36919400	0.02328800
C	3.23830800	-2.42208400	2.74517700
C	-0.55718600	-3.08271200	-3.53584700
H	0.28869200	-1.30472700	-2.63665800
C	-1.37139200	-4.74861900	-1.98128500
H	-1.19152400	-4.25700500	0.10693900
C	3.58198700	-3.74329000	2.44716000
H	3.14266700	-5.45935300	1.21562400
H	3.78815000	-1.86382400	3.49689300
C	-1.15888400	-4.31906300	-3.29448900
H	-0.40213200	-2.74160500	-4.55515200
H	-1.83787300	-5.71123700	-1.79157700
H	4.40487200	-4.22492900	2.96783000
H	-1.46796600	-4.94493400	-4.12653200
H	1.94731000	-0.76641900	2.28971700
C	1.81148600	2.59007900	-0.59000900

C	2.44129600	1.53089400	-1.26525600
C	2.83909500	0.38621700	-0.53489600
Pd	0.63177800	0.63698200	-0.26715700
C	1.23353100	3.78515100	-1.27974000
H	0.28588900	4.05471000	-0.80349300
H	1.00443500	3.55656200	-2.32259100
C	2.14129500	5.03806500	-1.24532200
H	2.35293700	5.31115100	-0.20447500
H	3.10069900	4.81137200	-1.72512100
C	1.44158800	6.16682700	-1.96520700
C	0.47116300	6.93501200	-1.30863000
C	1.66116700	6.39317800	-3.32914600
C	-0.26451500	7.90007900	-1.99709900
H	0.28693200	6.76747900	-0.24984600
C	0.92970200	7.35848200	-4.02321100
H	2.40707900	5.79953800	-3.85254300
C	-0.03943400	8.11345400	-3.35947800
H	-1.01187200	8.48735900	-1.47023200
H	1.11686100	7.52107900	-5.08135000
H	-0.61008400	8.86580900	-3.89676300
C	3.41353800	-0.82514200	-1.21344200
H	3.04115800	-1.73562600	-0.73689100
H	3.10026300	-0.86332400	-2.26454400
C	4.95852700	-0.85864100	-1.13186000
H	5.25052500	-0.75159700	-0.07964900
H	5.37377400	0.00135100	-1.67041000
C	5.50544900	-2.15010400	-1.68995000
C	5.45984400	-3.32054400	-0.91924900
C	6.00609100	-2.22708500	-2.99479200
C	5.90249600	-4.53621700	-1.43939500
H	5.06955500	-3.27544600	0.09380100
C	6.45328400	-3.44211700	-3.51916800
H	6.04714800	-1.32667300	-3.60358400
C	6.40179400	-4.60146100	-2.74304800
H	5.86003300	-5.43249600	-0.82601300
H	6.84277500	-3.48215300	-4.53294700
H	6.74978300	-5.54715500	-3.14923700
H	3.08607800	0.53733800	0.51732300
H	2.02181100	2.68353100	0.47436600
H	2.41596700	1.49549600	-2.35492600
C	2.56587800	1.40782200	3.74950000
C	1.37454500	1.06085800	4.40808000
C	0.43535000	1.01571200	3.37153300
N	2.35430700	1.55467300	2.42573700

H	3.55622400	1.56314300	4.16523700
H	1.21545900	0.88365300	5.46410100
H	-0.62227500	0.79408300	3.41340600
N	1.02916400	1.30896400	2.19102300
INT7b			
P	-2.19441800	1.03655700	0.23666800
C	-2.95895500	0.11054700	-1.16009800
C	-2.35530100	2.79656700	-0.27551200
C	-3.41138100	0.81778600	1.59088600
C	-3.31139800	-1.26588100	-0.99933100
C	-3.03427500	0.71037900	-2.42159200
C	-3.52593500	3.55656700	-0.14392100
C	-1.21325700	3.39593700	-0.82885200
C	-2.91718500	0.57700700	2.88030200
C	-4.79770200	0.83429500	1.38042900
C	-3.74488800	-1.91373000	-2.14268200
C	-3.29742400	-2.03817700	0.28043000
C	-3.45029100	0.01269300	-3.56969200
H	-2.75778900	1.75284500	-2.52741800
C	-3.55368500	4.88709100	-0.56333200
H	-4.41397700	3.11828900	0.29699500
C	-1.24583000	4.72262200	-1.26059500
H	-0.29649900	2.81707100	-0.89865900
C	-3.79379800	0.35722400	3.94318000
H	-1.84132900	0.54164500	3.03248000
C	-5.67328800	0.63368700	2.44689300
H	-5.19139700	0.96623000	0.37778100
C	-3.79878300	-1.30848800	-3.39558500
O	-4.15915600	-3.21843200	-2.24407700
C	-4.50391200	-2.36141500	0.87398300
C	-2.13097200	-2.56013600	0.92081800
H	-3.49596300	0.49196400	-4.54100100
C	-2.41670400	5.47132100	-1.12688500
H	-4.46456100	5.46816500	-0.44910500
H	-0.35423700	5.17281500	-1.68779600
C	-5.17333400	0.38783500	3.72828700
H	-3.40089500	0.15690300	4.93581100
H	-6.74594800	0.65817700	2.27566800
O	-4.24128700	-2.20860100	-4.33024200
C	-4.42940800	-3.44888700	-3.63239900
C	-4.60520400	-3.09572700	2.05321300
O	-5.75783800	-2.01176700	0.44004100
C	-2.24649600	-3.31763300	2.08972200
P	-0.48686600	-2.04011700	0.28899600
H	-2.44163600	6.50760200	-1.45184600

H	-5.85709600	0.21517400	4.55444900
H	-3.72474800	-4.19097700	-4.01974500
H	-5.46572800	-3.77955500	-3.75047900
C	-3.48923200	-3.59592400	2.68771100
O	-5.92249900	-3.22146300	2.41234100
C	-6.68091500	-2.55340500	1.39339000
H	-1.35106200	-3.70792900	2.55866400
C	0.73542100	-3.15470400	1.08785800
C	-0.52648800	-2.57493300	-1.46161700
H	-3.56444000	-4.17937000	3.59829400
H	-7.33659600	-3.27468200	0.89422500
H	-7.25487400	-1.73960000	1.84571600
C	1.41530500	-4.17386000	0.40792700
C	1.10606200	-2.86112700	2.41239500
C	-0.07590500	-1.67620600	-2.43724900
C	-1.02685500	-3.82486700	-1.85378700
C	2.43610700	-4.88811200	1.04080100
H	1.16221200	-4.40334800	-0.62076200
C	2.11071700	-3.58624200	3.04869600
C	-0.13171700	-2.01815500	-3.78860800
H	0.29218200	-0.70210400	-2.12651000
C	-1.06353500	-4.17321300	-3.20330900
H	-1.40280800	-4.51496300	-1.10449700
C	2.78391200	-4.60101400	2.36103900
H	2.96106000	-5.66809300	0.49642400
H	2.38081400	-3.34887200	4.07367100
C	-0.62401800	-3.26708100	-4.17292100
H	0.20314800	-1.30921200	-4.54007100
H	-1.44138400	-5.14796800	-3.49946400
H	3.57915500	-5.15645000	2.84970300
H	-0.66816300	-3.53396000	-5.22491700
H	0.61547600	-2.04402900	2.93388100
C	1.66705200	2.91469500	1.32927700
C	1.47796300	1.60469400	1.22781600
C	2.02169000	0.32208800	1.32773200
Pd	-0.02871400	0.24294600	0.70415900
C	2.99635300	-0.29033600	0.33954900
H	2.70498200	-1.32486000	0.12270800
H	2.96725200	0.25492400	-0.61101700
C	4.44432700	-0.31353300	0.88019300
H	4.80922600	0.71330500	1.00072800
H	4.42974700	-0.76887000	1.87942300
C	5.36149300	-1.10005300	-0.02401500
C	5.32165600	-2.50249600	-0.01597300

C	6.22023900	-0.46185800	-0.92658200
C	6.11971100	-3.24549300	-0.88531700
H	4.65609000	-3.01186000	0.67687900
C	7.02282600	-1.20189100	-1.79803800
H	6.26009400	0.62486700	-0.94449100
C	6.97485500	-2.59693500	-1.78065100
H	6.07626200	-4.33137300	-0.86293500
H	7.68612700	-0.68829300	-2.48898300
H	7.59900200	-3.17425900	-2.45713900
H	2.05604300	-0.13633400	2.32034200
C	2.95758700	3.54843900	1.79243500
H	3.75095400	2.79337100	1.82931800
H	3.28214700	4.32193700	1.08100100
C	2.81771700	4.20056500	3.18827200
H	2.01777900	4.95071100	3.15380800
H	2.50023300	3.42780200	3.89900500
C	4.10610900	4.83624500	3.65154500
C	5.08648200	4.07072900	4.29773700
C	4.37638400	6.18737700	3.39853900
C	6.30168700	4.63802900	4.68283700
H	4.89072800	3.02021800	4.50114900
C	5.59028100	6.76063600	3.78152600
H	3.62492600	6.79480800	2.89910300
C	6.55800600	5.98699000	4.42569900
H	7.04715100	4.02852400	5.18664900
H	5.77874800	7.81182500	3.58017100
H	7.50231500	6.43153400	4.72728700
H	0.84872800	3.60151800	1.11046900
TS6b			
P	-2.09663700	1.29063600	0.38695800
C	-2.65220900	0.20522700	-0.99059600
C	-2.42620800	3.00849200	-0.17379800
C	-3.32802700	0.97953500	1.70492200
C	-2.87812900	-1.18433000	-0.74093500
C	-2.66144200	0.69521000	-2.29932800
C	-3.52748400	3.77179300	0.23725200
C	-1.47166700	3.59131600	-1.02404100
C	-2.87535000	0.73466500	3.00719800
C	-4.70517100	0.94991700	1.43816600
C	-3.13075400	-1.96385000	-1.85493000
C	-2.89435400	-1.83932500	0.60069700
C	-2.89109400	-0.13241800	-3.41286400
H	-2.46841800	1.74585900	-2.47519100
C	-3.67898900	5.08573800	-0.21105500
H	-4.26299700	3.35269100	0.91361200

C	-1.63659200	4.89611700	-1.48584300
H	-0.60219100	3.01976500	-1.32275400
C	-3.78407600	0.46463600	4.03060000
H	-1.80923800	0.73083200	3.20568800
C	-5.61333900	0.69885700	2.46552400
H	-5.06276200	1.10085200	0.42434300
C	-3.12153000	-1.46619300	-3.15581700
O	-3.40927900	-3.30690200	-1.87716100
C	-4.10329700	-2.23828200	1.13852200
C	-1.73587000	-2.15066600	1.37583600
H	-2.88529400	0.26224500	-4.42241300
C	-2.74108300	5.64826700	-1.07851600
H	-4.53412900	5.66869500	0.11963100
H	-0.89392800	5.31836000	-2.15572400
C	-5.15402000	0.44963600	3.76199300
H	-3.42151600	0.25975200	5.03363500
H	-6.67875100	0.68900100	2.25307700
O	-3.38253800	-2.47809500	-4.04234900
C	-3.47617300	-3.67881100	-3.26005200
C	-4.22042200	-2.86164900	2.37897200
O	-5.34803700	-2.06819000	0.58895400
C	-1.86332100	-2.79774700	2.60834400
P	-0.10721300	-1.55462400	0.77624900
H	-2.86558500	6.66936100	-1.42778200
H	-5.86242200	0.23865300	4.55779500
H	-2.63164900	-4.33279900	-3.49905000
H	-4.43435800	-4.16702700	-3.45791100
C	-3.11286100	-3.16283900	3.14068700
O	-5.54030700	-3.09878600	2.65787200
C	-6.28439500	-2.59390300	1.53838200
H	-0.97467800	-3.03210400	3.18119100
C	1.12887900	-2.36192000	1.86145000
C	0.05365500	-2.36262000	-0.85456100
H	-3.19856900	-3.65742600	4.10145600
H	-6.84932500	-3.41058400	1.07797500
H	-6.94553100	-1.79134700	1.87771600
C	1.99694400	-3.36747700	1.41819200
C	1.28658100	-1.85379100	3.16326400
C	0.44213300	-1.58427000	-1.95208700
C	-0.25390300	-3.71969500	-1.03378500
C	2.99143500	-3.86508700	2.26502100
H	1.90760200	-3.75665200	0.41048400
C	2.26335500	-2.36653500	4.01363000
C	0.52557400	-2.16339400	-3.21900400

H	0.64477000	-0.52376100	-1.83516100
C	-0.15292700	-4.29674100	-2.29882500
H	-0.58332600	-4.31664700	-0.18844100
C	3.12405300	-3.37235000	3.56331500
H	3.66084000	-4.64123900	1.90505600
H	2.35854500	-1.97181300	5.02068500
C	0.23286600	-3.51704900	-3.39449800
H	0.81384700	-1.54807300	-4.06627400
H	-0.38351100	-5.35014600	-2.43227100
H	3.89599500	-3.76326400	4.21962500
H	0.29981100	-3.96587300	-4.38170300
H	0.64210500	-1.05006900	3.50763700
C	1.35622500	2.92136400	1.67191500
C	1.86476000	2.08953800	0.69943500
C	2.32514900	0.77412100	1.00518800
Pd	0.16890900	0.75107100	0.73752300
C	3.20107100	-0.01526300	0.06486000
H	2.92570100	-1.07598200	0.08865700
H	3.06080600	0.32856600	-0.96554600
C	4.69564800	0.08681200	0.44858100
H	5.03024600	1.12369200	0.32379600
H	4.79937600	-0.15863400	1.51376000
C	5.54547400	-0.84891500	-0.37489200
C	5.65533200	-2.20051000	-0.01734000
C	6.18572500	-0.41337100	-1.54142600
C	6.38723600	-3.09185600	-0.80183300
H	5.15716100	-2.55152700	0.88338300
C	6.92050200	-1.30138500	-2.32982500
H	6.10585000	0.63147100	-1.83247400
C	7.02423400	-2.64445400	-1.96232900
H	6.46357100	-4.13522300	-0.50661900
H	7.41326400	-0.94359500	-3.22998900
H	7.59708700	-3.33625300	-2.57365500
H	2.39047000	0.41418900	2.04120000
C	1.69325300	2.88449600	3.14423100
H	2.63064600	2.34140900	3.29735000
H	1.82953400	3.89547900	3.54937100
C	0.56294800	2.17683600	3.93645500
H	-0.34882700	2.78298200	3.88793700
H	0.33633300	1.24061400	3.40940900
C	0.92115500	1.87782600	5.37128500
C	1.94367400	0.96176400	5.66275500
C	0.25103300	2.48931800	6.43651200
C	2.28275300	0.66196400	6.98131100

H	2.47588200	0.48086300	4.84616000
C	0.58704800	2.19270900	7.76005500
H	-0.54296000	3.20183500	6.22595500
C	1.60311300	1.27719200	8.03691400
H	3.07748000	-0.05043600	7.18668700
H	0.05369200	2.67702000	8.57355700
H	1.86502200	1.04463600	9.06521000
H	0.66045600	3.70948500	1.37215400
C	1.66362000	3.72794400	-2.83674000
C	1.04532400	3.48283000	-4.05696100
C	0.58374200	2.15347400	-3.94929900
N	1.56238500	2.59664500	-2.10137700
H	1.74630500	2.44604700	-1.04593900
H	2.15868400	4.60703300	-2.44801500
H	0.94987500	4.15855100	-4.89505600
H	0.04347100	1.56036300	-4.67662200
N	0.89327900	1.62527200	-2.75924100
INT8b			
P	-1.71813200	1.40235700	-0.32216400
C	-2.71960700	0.15369300	-1.22101300
C	-1.77517500	2.86869600	-1.42406400
C	-2.76832600	1.85145900	1.10228400
C	-3.04981500	-1.06582900	-0.56133800
C	-3.08453600	0.35174900	-2.55666000
C	-2.54287400	4.00182700	-1.13385800
C	-0.97659200	2.86233000	-2.58104500
C	-2.14362700	2.16152100	2.31630100
C	-4.16670700	1.89714600	1.00248700
C	-3.73860700	-1.99491500	-1.31920500
C	-2.74884600	-1.41219300	0.85821800
C	-3.76256100	-0.62425700	-3.30736400
H	-2.84077000	1.28682700	-3.04301100
C	-2.51865500	5.10689300	-1.98927900
H	-3.15748100	4.02620100	-0.24113500
C	-0.96785000	3.95710600	-3.44178100
H	-0.35779800	1.99545900	-2.79784000
C	-2.91469700	2.50662400	3.42740700
H	-1.06264000	2.09380100	2.39529800
C	-4.93120600	2.25671500	2.11147900
H	-4.65264000	1.64160800	0.06633100
C	-4.06997200	-1.79901000	-2.65762900
O	-4.15091500	-3.24006700	-0.92051900
C	-3.79229600	-1.44858300	1.76397200
C	-1.47927100	-1.84811700	1.34973900
H	-4.02579900	-0.45997500	-4.34588800

C	-1.73810300	5.08612400	-3.14460600
H	-3.11405400	5.98305100	-1.74929100
H	-0.35189500	3.93586000	-4.33614300
C	-4.30644400	2.55661700	3.32655000
H	-2.42406800	2.72541200	4.37123700
H	-6.01387200	2.29714500	2.02984100
O	-4.69613500	-2.91188500	-3.15000400
C	-4.81498700	-3.82537800	-2.04803100
C	-3.64513300	-1.87266600	3.08478800
O	-5.10716400	-1.12878600	1.53045500
C	-1.35176000	-2.29784100	2.66588400
P	0.01510500	-1.59443100	0.31278400
H	-1.72280500	5.94533600	-3.80864600
H	-4.90580000	2.82559200	4.19181600
H	-4.32735800	-4.76879000	-2.30673000
H	-5.87394000	-3.97439200	-1.81060200
C	-2.43532700	-2.32579800	3.56253500
O	-4.85516200	-1.81341900	3.72594300
C	-5.73858500	-1.13869000	2.81736500
H	-0.38207500	-2.61301500	3.02758900
C	1.30847300	-2.66631600	1.05580400
C	-0.40269000	-2.42019300	-1.26734700
H	-2.31692800	-2.67432100	4.58194900
H	-6.68124700	-1.68509100	2.75426800
H	-5.88557900	-0.10598100	3.15461600
C	1.70906700	-3.88619500	0.49064400
C	1.95934300	-2.20180900	2.21119300
C	-0.11344000	-1.76454800	-2.46942700
C	-1.01743100	-3.68115100	-1.29970700
C	2.71703900	-4.64257700	1.09147300
H	1.24713900	-4.24766600	-0.42006400
C	2.95596200	-2.96790900	2.81383400
C	-0.43653700	-2.35815600	-3.69038500
H	0.34106600	-0.77798700	-2.43377700
C	-1.32801400	-4.27811600	-2.52002300
H	-1.27118700	-4.18240100	-0.37094900
C	3.33360800	-4.19374400	2.26071600
H	3.02119800	-5.58264400	0.64027300
H	3.43860200	-2.59234200	3.71105700
C	-1.04206900	-3.61548900	-3.71710200
H	-0.22286700	-1.83617100	-4.61854300
H	-1.79735900	-5.25773100	-2.53805600
H	4.11513600	-4.78725200	2.72688500
H	-1.29733100	-4.07640200	-4.66682000

H	1.70130300	-1.23598200	2.62109400
C	1.40980800	2.72610700	-0.23003900
C	2.27133100	1.71455500	-0.73572400
C	2.77825600	0.69135400	0.07842000
Pd	0.47565600	0.73313100	0.14983000
C	3.53699700	-0.46489100	-0.50490200
H	3.21357000	-1.39526300	-0.03231900
H	3.32945600	-0.56086200	-1.57851800
C	5.06248800	-0.33071000	-0.28486500
H	5.42706600	0.57686600	-0.78008900
H	5.24810700	-0.20756600	0.78963200
C	5.79360000	-1.54555900	-0.80448500
C	5.72887300	-2.75576100	-0.09971900
C	6.49067300	-1.51459900	-2.01762100
C	6.34207100	-3.90534100	-0.59537100
H	5.18492500	-2.79632300	0.83954600
C	7.11107600	-2.66282600	-2.51625100
H	6.54824700	-0.58273400	-2.57556900
C	7.03728200	-3.86298000	-1.80714700
H	6.27762200	-4.83424300	-0.03475800
H	7.65131000	-2.61876200	-3.45818700
H	7.51817200	-4.75714300	-2.19398300
H	2.87371800	0.85351000	1.15606100
C	1.57126600	3.42489200	1.09371100
H	0.62263600	3.90741000	1.35762000
H	1.80042400	2.71367800	1.88422800
C	2.68896400	4.49276000	1.04829000
H	3.62965300	3.98786400	0.78932500
H	2.49231700	5.22137700	0.25170800
C	2.83316600	5.20577900	2.37426900
C	2.71085700	6.59707000	2.46412300
C	3.07536800	4.47550800	3.54911000
C	2.83453200	7.25172200	3.69230000
H	2.51735100	7.17355900	1.56223800
C	3.19673400	5.12672700	4.77614300
H	3.14799900	3.39156000	3.50294000
C	3.07909900	6.51761400	4.85341100
H	2.73763700	8.33326700	3.74016900
H	3.38029800	4.54521700	5.67581700
H	3.17389500	7.02294400	5.81071300
H	0.90571700	3.31500400	-0.99222100
H	2.32475900	1.58162400	-1.81651600
C	0.17272600	0.32505400	3.88001700
C	1.04524500	0.11378700	4.95452200

C	2.28474300	0.54122400	4.45226600
N	0.84569500	0.83052100	2.82008300
H	-0.88973700	0.13533300	3.81434200
H	0.81457200	-0.27210600	5.93918000
H	3.25170900	0.56604300	4.94408700
N	2.15993400	0.96520600	3.17783900
TS7			
P	-1.37350000	1.41381000	-0.41926900
C	-2.42233700	0.23116500	-1.38418000
C	-1.47687100	2.97357300	-1.37619700
C	-2.40565200	1.70497600	1.06349600
C	-2.82041200	-0.98833900	-0.75744100
C	-2.74631800	0.45430100	-2.72584000
C	-2.07998600	4.12910900	-0.86143600
C	-0.87705600	3.03293600	-2.64433400
C	-1.82512700	1.63358800	2.33464700
C	-3.77917300	1.96251200	0.93821000
C	-3.51983400	-1.88452400	-1.54412600
C	-2.59035800	-1.32299600	0.67388800
C	-3.43573400	-0.48918600	-3.50959900
H	-2.47421000	1.39078400	-3.19268300
C	-2.10973200	5.30432400	-1.61393800
H	-2.51851200	4.11415000	0.12890700
C	-0.92999400	4.20041800	-3.40505900
H	-0.34331300	2.16794800	-3.02784000
C	-2.61653800	1.80774300	3.47030400
H	-0.76562600	1.43305700	2.43107300
C	-4.56210300	2.15439500	2.07518900
H	-4.23458200	2.00418200	-0.04666300
C	-3.80353600	-1.66171000	-2.88822800
O	-4.01382800	-3.10664800	-1.16447300
C	-3.67308800	-1.33848400	1.53381600
C	-1.33007100	-1.66455000	1.24655100
H	-3.67030500	-0.29637900	-4.55027500
C	-1.54823000	5.34124000	-2.89134100
H	-2.57429100	6.19352400	-1.19727500
H	-0.45325500	4.23003700	-4.38014900
C	-3.98196300	2.06915000	3.34488200
H	-2.15872400	1.74346700	4.45279700
H	-5.62319000	2.36431700	1.97119100
O	-4.47600800	-2.73677600	-3.40767300
C	-4.59929100	-3.68638600	-2.33758500
C	-3.56480400	-1.61829400	2.89349000
O	-4.98088200	-1.07469800	1.22002500
C	-1.23727600	-1.96067600	2.61083200

P	0.18698900	-1.58924500	0.20774500
H	-1.56650300	6.25738900	-3.47322100
H	-4.59414600	2.20811000	4.23168600
H	-4.05547500	-4.59863000	-2.60062100
H	-5.65824400	-3.89046600	-2.15189700
C	-2.35289100	-1.93869300	3.46547600
O	-4.79541300	-1.53235900	3.48551900
C	-5.70511400	-1.10933600	2.45663900
H	-0.27796200	-2.22357000	3.03649000
C	1.39452400	-2.58598800	1.16619800
C	-0.24783400	-2.60186700	-1.25336800
H	-2.26173100	-2.16409800	4.52167900
H	-6.52353300	-1.83019900	2.37745500
H	-6.07104800	-0.10502800	2.69024100
C	1.74218900	-3.90491300	0.85179300
C	2.05593100	-1.93761100	2.22222400
C	0.02319300	-2.08569300	-2.52646500
C	-0.88856500	-3.84380300	-1.13309500
C	2.72842600	-4.56641900	1.58712100
H	1.26980500	-4.41133600	0.01868800
C	3.02887100	-2.60357700	2.96357100
C	-0.33750600	-2.80230300	-3.66709600
H	0.48497500	-1.10564100	-2.60724900
C	-1.23038900	-4.56779100	-2.27434500
H	-1.14153800	-4.23066700	-0.15093000
C	3.36953900	-3.92196400	2.64544000
H	3.00253000	-5.58303900	1.32136900
H	3.53060000	-2.09011200	3.77858500
C	-0.96081400	-4.04573300	-3.54253200
H	-0.14049900	-2.38732600	-4.65109800
H	-1.71741600	-5.53364000	-2.17401300
H	4.13872500	-4.43800400	3.21263600
H	-1.24259300	-4.60410500	-4.43045500
H	1.81429200	-0.90290800	2.44149200
C	2.56429200	2.49841300	-1.21360700
C	2.77996800	1.17768400	-1.49536600
C	2.95744700	0.16932800	-0.47143400
Pd	0.86942700	0.57834300	-0.14573700
C	2.25133700	3.55225500	-2.21746500
H	1.28136900	3.98976700	-1.96136100
H	2.15184400	3.12591100	-3.22350300
C	3.28117200	4.70538500	-2.24094200
H	3.39295200	5.09595200	-1.22177600
H	4.26078400	4.32376900	-2.55067800

C	2.82270400	5.80264500	-3.17329900
C	1.79369900	6.67263700	-2.78575800
C	3.35513100	5.92965900	-4.46140200
C	1.31200600	7.64488700	-3.66167500
H	1.36157400	6.57848300	-1.79255700
C	2.87622300	6.90188800	-5.34283900
H	4.15177600	5.25945300	-4.77604300
C	1.85172900	7.76261800	-4.94550200
H	0.51619900	8.31218900	-3.34175800
H	3.30426600	6.98660200	-6.33808500
H	1.47814400	8.52050300	-5.62841100
C	3.46181600	-1.18221500	-0.91239300
H	3.26532500	-1.93195500	-0.14821300
H	2.93543200	-1.50814100	-1.81841400
C	4.98470400	-1.19037900	-1.18427900
H	5.50040500	-0.81241600	-0.29177000
H	5.22089000	-0.50340300	-2.00528500
C	5.46117400	-2.58629100	-1.50744000
C	5.56534500	-3.54580200	-0.48983000
C	5.73826400	-2.97601700	-2.82281000
C	5.93513900	-4.85854300	-0.77891600
H	5.34212300	-3.26096600	0.53500500
C	6.11289200	-4.28923100	-3.11750600
H	5.65968800	-2.24321900	-3.62266400
C	6.21144300	-5.23551600	-2.09615900
H	6.00938800	-5.58743100	0.02388200
H	6.32747100	-4.57189800	-4.14465300
H	6.50207700	-6.25739400	-2.32340900
H	3.38235100	0.52294300	0.46847100
H	2.65936700	2.82867900	-0.18373800
H	2.69544500	0.83723300	-2.52920100
C	0.70371100	3.87622000	2.70103100
C	1.27063000	3.01139100	3.65239100
C	1.66043700	1.90690300	2.88861500
N	0.74746100	3.33643000	1.46875100
H	0.27012700	4.85962700	2.84956700
H	1.39658200	3.16755800	4.71594800
H	2.16845600	1.00117200	3.19879000
N	1.34543900	2.11331600	1.58739500
INT9			
P	-1.59065400	1.43565100	0.03529100
C	-2.59516400	0.40982300	-1.12427500
C	-1.72809800	3.11338900	-0.68825400
C	-2.57865100	1.47779400	1.57080700
C	-2.93944600	-0.91829000	-0.73652300

C	-2.90241900	0.85767100	-2.41338100
C	-2.56928600	4.09816400	-0.15813200
C	-0.96388900	3.40909900	-1.82653400
C	-1.90560300	1.37042800	2.79556700
C	-3.97626900	1.58766400	1.55188500
C	-3.58731000	-1.68864800	-1.68315700
C	-2.69550900	-1.48004700	0.61749500
C	-3.53572800	0.04018500	-3.36731000
H	-2.65112500	1.87017000	-2.70014800
C	-2.65028000	5.35390300	-0.76173700
H	-3.15126400	3.89353700	0.73273200
C	-1.06298700	4.65692800	-2.44205200
H	-0.28540100	2.66069100	-2.22437100
C	-2.62990000	1.35595400	3.98772500
H	-0.82320100	1.29591400	2.80764700
C	-4.69385400	1.59105800	2.74726200
H	-4.50081100	1.65297300	0.60372700
C	-3.86163800	-1.23854100	-2.97162500
O	-4.02744400	-2.97965000	-1.54061500
C	-3.77682600	-1.66132800	1.46004200
C	-1.42292300	-1.87012400	1.12851300
H	-3.75850900	0.40305200	-4.36422800
C	-1.90498300	5.63502000	-1.90747700
H	-3.29951300	6.11266200	-0.33401900
H	-0.47464900	4.87178600	-3.32949800
C	-4.02201600	1.46464500	3.96627900
H	-2.10469300	1.26237900	4.93372300
H	-5.77585800	1.68854800	2.72734300
O	-4.47296400	-2.23119200	-3.69113400
C	-4.58544200	-3.35679200	-2.80637100
C	-3.66055700	-2.14764100	2.75851500
O	-5.09046000	-1.37716300	1.18962600
C	-1.32667700	-2.38802700	2.42541500
P	0.09891500	-1.57994500	0.12277000
H	-1.97445900	6.61076300	-2.37960900
H	-4.58314300	1.45369900	4.89638600
H	-4.01709800	-4.19640400	-3.21689100
H	-5.64147900	-3.61344100	-2.67581500
C	-2.43998800	-2.52824000	3.27140800
O	-4.89029500	-2.18067200	3.35665800
C	-5.82220600	-1.67787000	2.38556700
H	-0.36628400	-2.70638400	2.80531500
C	1.32966600	-2.69811000	0.89610200
C	-0.29954100	-2.32766700	-1.49664300

H	-2.34018900	-2.92211700	4.27623700
H	-6.57140100	-2.44571500	2.16940800
H	-6.28297400	-0.76310600	2.76861600
C	1.85830500	-3.81902500	0.24619000
C	1.87448700	-2.30780300	2.13243500
C	-0.06989000	-1.56931800	-2.65132500
C	-0.86696700	-3.60528900	-1.60753500
C	2.91174700	-4.53503900	0.81865200
H	1.48257100	-4.11430800	-0.72643300
C	2.90024100	-3.04485800	2.71896100
C	-0.40949700	-2.07909100	-3.90450400
H	0.34387800	-0.56980000	-2.55239600
C	-1.18596800	-4.12113800	-2.86248800
H	-1.07448800	-4.18501000	-0.71339200
C	3.43004900	-4.15561800	2.05559000
H	3.34609300	-5.37172900	0.28112800
H	3.31003800	-2.73113000	3.67465000
C	-0.96523600	-3.35570200	-4.01134700
H	-0.24809500	-1.47821400	-4.79447100
H	-1.61706200	-5.11497000	-2.94366500
H	4.25816400	-4.70702800	2.48997600
H	-1.23089500	-3.75264300	-4.98676900
H	1.52367000	-1.39674800	2.60921000
C	2.61048300	2.63573600	-1.46107900
C	2.62985300	1.28520800	-1.43301200
C	2.78549800	0.47253100	-0.21988800
Pd	0.69033500	0.64628700	0.22638100
C	2.41500300	3.47288600	-2.68261300
H	1.50371100	4.06936800	-2.55733800
H	2.26507500	2.84196700	-3.56850700
C	3.56979500	4.46700000	-2.94590300
H	3.74410500	5.04878600	-2.03168100
H	4.49203500	3.91296300	-3.15427400
C	3.23786900	5.39170500	-4.09328600
C	2.30239300	6.42319800	-3.92025500
C	3.79881200	5.20693500	-5.36200000
C	1.93864300	7.24616500	-4.98597500
H	1.85788000	6.58073200	-2.94004600
C	3.43980600	6.02994100	-6.43222100
H	4.52402400	4.41048700	-5.51150700
C	2.50735300	7.05190600	-6.24785100
H	1.21539300	8.04235000	-4.83122200
H	3.88938700	5.87228400	-7.40892000
H	2.22721900	7.69370200	-7.07841300

C	3.42386300	-0.88099600	-0.42857000
H	3.43571100	-1.43309900	0.50890600
H	2.83677400	-1.47864300	-1.13673400
C	4.88054200	-0.83403700	-0.94913800
H	5.48847500	-0.21143700	-0.28131500
H	4.90533000	-0.36478200	-1.94026700
C	5.42841100	-2.23976200	-1.00259300
C	6.20325700	-2.75208800	0.04504900
C	5.07062600	-3.10180300	-2.04853400
C	6.60879800	-4.08768200	0.05234000
H	6.48111200	-2.09794600	0.86811900
C	5.47077200	-4.43816500	-2.04628000
H	4.46503000	-2.72009300	-2.86765200
C	6.24110200	-4.93751400	-0.99270600
H	7.21132500	-4.46458000	0.87460800
H	5.18346200	-5.08983000	-2.86729200
H	6.55602800	-5.97737400	-0.98992800
H	3.24328700	1.02501800	0.60213300
H	2.71713700	3.17003300	-0.51800400
H	2.49635900	0.74056500	-2.37126200
C	0.73828800	3.97086700	2.80803500
C	1.55577600	3.12821900	3.58275800
C	1.81896600	2.05615100	2.72982300
N	0.52149400	3.45031600	1.58739100
H	0.30486200	4.92905800	3.07236300
H	1.91243500	3.27836300	4.59308000
H	2.41306200	1.16426200	2.88597800
N	1.19866700	2.27438600	1.54190100
INT9'			
P	-1.46242800	0.81491300	-0.63054200
C	-2.68789100	-0.38661600	-1.28955400
C	-0.90156100	1.70871200	-2.12648600
C	-2.51308600	1.97973300	0.31140600
C	-3.44036100	-1.17185800	-0.36612200
C	-2.84183600	-0.57818300	-2.66533300
C	-1.32779200	2.99768100	-2.46509200
C	0.04336600	1.06132500	-2.94022500
C	-2.11400700	2.37307800	1.59466300
C	-3.73417100	2.44088200	-0.20268200
C	-4.29862700	-2.10251500	-0.91429600
C	-3.35723700	-0.99207300	1.10748200
C	-3.71572600	-1.54477300	-3.19446200
H	-2.27069600	0.02696600	-3.35710600
C	-0.82508100	3.62500200	-3.60775000
H	-2.04181500	3.51868200	-1.83728900

C	0.52719200	1.68082000	-4.09027200
H	0.41307600	0.07941500	-2.65787000
C	-2.91402000	3.22922500	2.35051200
H	-1.19061000	1.98379900	2.00470800
C	-4.52692900	3.30746100	0.54907400
H	-4.06925200	2.11081300	-1.18123100
C	-4.42394800	-2.30282800	-2.28811900
O	-5.11136700	-2.97729900	-0.24337300
C	-4.38889900	-0.34681500	1.76645800
C	-2.24091200	-1.37475100	1.90496000
H	-3.81770200	-1.69213400	-4.26334100
C	0.09510300	2.96754700	-4.42459600
H	-1.15447700	4.62963400	-3.85638000
H	1.25529300	1.16884000	-4.71226300
C	-4.11859300	3.70227400	1.82674400
H	-2.60006800	3.51612300	3.34975600
H	-5.46788800	3.66651200	0.14207300
O	-5.31818600	-3.30848600	-2.52969200
C	-5.72684900	-3.80156500	-1.24316700
C	-4.33793200	-0.01357600	3.11667800
O	-5.56187700	0.10501100	1.22146500
C	-2.19549800	-1.01976200	3.25995300
P	-0.72445300	-2.06117200	1.12756000
H	0.48232200	3.45742100	-5.31310600
H	-4.74267400	4.36968300	2.41395200
H	-5.38128200	-4.83297600	-1.12583100
H	-6.81441800	-3.72886400	-1.15542900
C	-3.24312100	-0.32907100	3.89362700
O	-5.47790600	0.65633300	3.47363100
C	-6.26813700	0.76913600	2.27947900
H	-1.32244600	-1.28004100	3.84751100
C	-0.02477700	-3.19980100	2.38327800
C	-1.28224200	-3.25375700	-0.15224200
H	-3.18917900	-0.05505400	4.94094600
H	-7.23389000	0.27872500	2.43453900
H	-6.38750200	1.82591600	2.02423600
C	-0.81585700	-3.87834200	3.32492400
C	1.34794900	-3.47482100	2.31296000
C	-0.78489400	-3.10953600	-1.45238100
C	-2.14075800	-4.32214800	0.14403700
C	-0.23837700	-4.80699500	4.18966600
H	-1.87926800	-3.67489300	3.39209800
C	1.91942800	-4.40870100	3.17843300
C	-1.16036200	-4.00648700	-2.45353100

H	-0.11364100	-2.28538700	-1.67525300
C	-2.50964400	-5.22054500	-0.85485500
H	-2.52497000	-4.44836500	1.15074000
C	1.13182900	-5.07316300	4.11888800
H	-0.85866200	-5.32259500	4.91749300
H	2.98650700	-4.60133300	3.12078100
C	-2.02547900	-5.06040500	-2.15715600
H	-0.77999500	-3.87901500	-3.46265800
H	-3.17090000	-6.04954400	-0.61774600
H	1.58110200	-5.79408400	4.79619700
H	-2.31915000	-5.75879100	-2.93538900
H	1.96880500	-2.96011800	1.58914500
C	1.18373800	2.01794500	0.41044400
C	2.29553700	1.97149900	-0.55808300
C	3.59876500	1.79602200	-0.28380900
Pd	0.38039600	0.02338300	0.54268700
C	4.67713400	1.73651500	-1.32224600
H	5.22004300	0.78332000	-1.24281400
H	4.23949900	1.76900700	-2.32852700
C	5.70156600	2.88804800	-1.17975600
H	5.16990900	3.84270800	-1.27247500
H	6.12772700	2.85737600	-0.16886500
C	6.80347200	2.80381300	-2.20794900
C	7.94255400	2.02110500	-1.97566200
C	6.68679000	3.45937400	-3.44070000
C	8.93859100	1.89778900	-2.94531000
H	8.04743300	1.50611700	-1.02341500
C	7.67983200	3.34022100	-4.41446400
H	5.80842100	4.07078000	-3.63513800
C	8.81056400	2.55811100	-4.16957300
H	9.81615400	1.28914400	-2.74409200
H	7.57245100	3.86061600	-5.36255000
H	9.58631200	2.46605600	-4.92465300
H	3.92624500	1.67525400	0.74723900
C	1.51555600	2.51262800	1.81309400
H	0.72107300	2.25065500	2.52140800
H	2.41758700	2.03116700	2.19405500
C	1.69835300	4.04675900	1.84725200
H	2.53692900	4.31390500	1.19421400
H	0.79965900	4.52042900	1.43116400
C	1.93396100	4.54399400	3.25042600
C	3.22423300	4.57590200	3.79625600
C	0.85618700	4.91712300	4.06518100
C	3.43339200	4.97225400	5.11790900

H	4.06946800	4.28577100	3.17624700
C	1.05928400	5.31438100	5.38761100
H	-0.15064200	4.89660500	3.65252200
C	2.35070900	5.34325900	5.91894900
H	4.44191700	4.99377900	5.52221200
H	0.21087800	5.60408200	6.00213200
H	2.51249900	5.65404700	6.94733500
H	0.37677500	2.63357000	0.00276800
H	2.00799500	2.06029200	-1.60472400
C	2.57264200	-0.48169600	2.75291800
C	3.83906300	-1.06003200	2.85315000
C	4.12548100	-1.46232900	1.53740600
N	2.17143500	-0.54217200	1.46422000
H	1.94326200	-0.03384100	3.51031200
H	4.44923500	-1.16814700	3.73957800
H	5.00637600	-1.96247500	1.15190200
N	3.11176200	-1.15211400	0.70425000
TS8			
P	-1.75434200	1.29744000	-0.42617500
C	-2.68552000	-0.00949400	-1.32622700
C	-1.61873000	2.65725300	-1.64826300
C	-2.98206900	1.88167900	0.80295200
C	-3.13906300	-1.15851500	-0.61045500
C	-2.86933800	0.06924100	-2.71041200
C	-2.31890100	3.86314200	-1.52537900
C	-0.69855700	2.50670700	-2.69996000
C	-2.55751200	2.16935800	2.10644800
C	-4.33665400	2.02426600	0.46855500
C	-3.73078300	-2.15025200	-1.36838500
C	-3.05700100	-1.34444300	0.86646900
C	-3.46702300	-0.96291500	-3.45462000
H	-2.54040900	0.95128800	-3.24327400
C	-2.10921000	4.89575700	-2.44306700
H	-3.02161700	4.00223900	-0.71168400
C	-0.50107100	3.53201100	-3.62165100
H	-0.13522400	1.58270900	-2.79194200
C	-3.47732200	2.58862600	3.06804200
H	-1.50965900	2.04488300	2.36091800
C	-5.25089600	2.46073400	1.42654300
H	-4.67481300	1.78344900	-0.53450200
C	-3.87584300	-2.07427600	-2.75174500
O	-4.22727400	-3.34554600	-0.91770600
C	-4.21023000	-1.22054100	1.61927500
C	-1.87321500	-1.68629000	1.58562300
H	-3.59058800	-0.88898900	-4.52886600

C	-1.20504100	4.73293900	-3.49255900
H	-2.65505100	5.82839600	-2.33368000
H	0.20867100	3.39869700	-4.43284600
C	-4.82397100	2.73635400	2.72926900
H	-3.14167900	2.79643100	4.07971500
H	-6.29739000	2.57763500	1.15909000
O	-4.46341200	-3.21707900	-3.22112100
C	-4.64044700	-4.07422500	-2.08163000
C	-4.23645800	-1.37010000	3.00445300
O	-5.47282500	-0.94125200	1.16197100
C	-1.91223500	-1.83795000	2.97644000
P	-0.25777200	-1.59948800	0.73214000
H	-1.04359800	5.53763500	-4.20370300
H	-5.54043900	3.06406000	3.47708600
H	-4.01032700	-4.96143000	-2.19629600
H	-5.69686700	-4.34105100	-1.98822700
C	-3.09841200	-1.68329000	3.71632100
O	-5.51296200	-1.18460800	3.46652400
C	-6.28896100	-0.77547400	2.32965800
H	-0.99614200	-2.05329100	3.51186400
C	0.89059500	-2.67202800	1.66599800
C	-0.47000200	-2.54489700	-0.82903900
H	-3.11319300	-1.80095600	4.79373500
H	-7.17387600	-1.41079500	2.24612300
H	-6.55570400	0.28123800	2.43585900
C	0.49916700	-3.87784700	2.26880300
C	2.24237700	-2.30411500	1.67530300
C	-0.06386700	-1.94964700	-2.02847600
C	-0.99089700	-3.84639800	-0.84742400
C	1.44846800	-4.69931500	2.87458100
H	-0.54602700	-4.16903200	2.28056900
C	3.19024300	-3.13265100	2.27702300
C	-0.19191500	-2.63805400	-3.23599600
H	0.33273400	-0.93826500	-2.00693700
C	-1.11101500	-4.53605600	-2.05211900
H	-1.31784200	-4.31430900	0.07488000
C	2.79644300	-4.32928400	2.87672300
H	1.13609900	-5.62714900	3.34538300
H	4.23388000	-2.83223600	2.28831100
C	-0.71684700	-3.93082700	-3.24969900
H	0.11250300	-2.16246900	-4.16372200
H	-1.51008400	-5.54666900	-2.05823800
H	3.53435100	-4.96995800	3.35124400
H	-0.81893000	-4.46713000	-4.18862900

H	2.54233500	-1.35544400	1.24765400
C	0.96230900	2.73221500	0.40440900
C	1.95197700	2.14584700	-0.50954600
C	3.00210500	1.37351700	-0.12528800
Pd	0.22553700	0.73469300	0.63359100
C	3.91032300	0.66255100	-1.08161500
H	3.89396800	-0.41689700	-0.87135600
H	3.56437100	0.78870100	-2.11590000
C	5.37784300	1.14232200	-0.96922400
H	5.42017200	2.21080400	-1.21112500
H	5.70104900	1.03749400	0.07390600
C	6.29660100	0.36247800	-1.87827400
C	6.81849800	-0.87367400	-1.47299800
C	6.60100900	0.82548200	-3.16461600
C	7.62407200	-1.62653700	-2.32791900
H	6.59162700	-1.24513500	-0.47612400
C	7.40718500	0.07679500	-4.02410600
H	6.20378400	1.78363000	-3.49188900
C	7.92148600	-1.15292000	-3.60808200
H	8.02301900	-2.58055700	-1.99389500
H	7.63615000	0.45526400	-5.01675100
H	8.55132300	-1.73593300	-4.27417200
H	3.20844800	1.23899400	0.93692800
C	1.41429000	3.39197000	1.69076300
H	0.54662200	3.57344000	2.33570800
H	2.08682300	2.74087700	2.24769800
C	2.12842400	4.73703800	1.41973400
H	2.97604400	4.54705800	0.74866600
H	1.45136300	5.42234000	0.89419100
C	2.61635100	5.37033100	2.70007900
C	3.69393800	4.80520500	3.39875600
C	1.98590600	6.49440300	3.24641200
C	4.13035800	5.35015300	4.60544100
H	4.18860400	3.92635100	2.99188600
C	2.41968100	7.04529200	4.45479500
H	1.14723000	6.94219000	2.71795000
C	3.49431700	6.47490500	5.13855200
H	4.96739100	4.89792200	5.13067500
H	1.91794500	7.91994000	4.86048500
H	3.83391000	6.90144400	6.07834600
H	0.24074100	3.35412100	-0.12427200
H	1.74901400	2.24120100	-1.57622000
C	0.45276700	0.43861500	3.77579100
C	1.33616500	0.34950600	4.85466200

C	2.60028700	0.41552200	4.24745800
N	1.16143800	0.54398200	2.62838400
H	-0.62815300	0.43044200	3.75902200
H	1.09709800	0.25719000	5.90575900
H	3.58151400	0.38361700	4.70786700
N	2.48712500	0.53209700	2.91083900
(E)-(S)-TS9			
P	-1.41547900	1.17547500	-1.30096100
C	-2.61555300	-0.16194700	-1.67364200
C	-1.47655600	2.27789800	-2.75744600
C	-2.18211600	2.08447200	0.08245300
C	-2.95075700	-1.08737800	-0.64037800
C	-3.09456000	-0.35048400	-2.97296800
C	-2.13373000	3.51206300	-2.76474600
C	-0.73578200	1.88822500	-3.88749200
C	-1.37934400	2.43204700	1.17737800
C	-3.54827500	2.40011900	0.09619000
C	-3.77732100	-2.13185600	-1.00860600
C	-2.51843000	-0.97490700	0.78233300
C	-3.90903600	-1.44290600	-3.32259500
H	-2.83326300	0.36312500	-3.74453700
C	-2.05233100	4.34534400	-3.88256900
H	-2.68947200	3.83709300	-1.89298600
C	-0.67748800	2.70926200	-5.01095500
H	-0.18932200	0.94861400	-3.87078000
C	-1.93455800	3.09075700	2.27394400
H	-0.32571100	2.16909400	1.16880200
C	-4.09742100	3.07473100	1.18582700
H	-4.18032100	2.10495400	-0.73572900
C	-4.22951900	-2.32375500	-2.31282100
O	-4.24611400	-3.13696700	-0.20461100
C	-3.44401700	-0.57335800	1.72714900
C	-1.21881200	-1.30022800	1.27989600
H	-4.26642800	-1.58294500	-4.33623500
C	-1.33137400	3.94522100	-5.00671800
H	-2.53778800	5.31561800	-3.86283100
H	-0.10252700	2.39805800	-5.87807100
C	-3.29306300	3.41447100	2.27776800
H	-1.30923800	3.34862900	3.12313200
H	-5.15330000	3.32996700	1.18598100
O	-4.98942700	-3.45987500	-2.37810600
C	-5.02451400	-3.99877400	-1.04722800
C	-3.14470600	-0.43641100	3.08151400
O	-4.75447300	-0.24122900	1.50869000
C	-0.93796400	-1.18398700	2.64444100

P	0.12340500	-1.66583200	0.08205300
H	-1.26442900	4.59863700	-5.87126700
H	-3.72574300	3.92974700	3.13023100
H	-4.58074200	-4.99796600	-1.05136300
H	-6.05856300	-4.01975600	-0.68924700
C	-1.89538200	-0.74249800	3.57560200
O	-4.25025900	-0.00242700	3.75952800
C	-5.27561000	0.19445800	2.77241900
H	0.04820800	-1.44130400	3.01016400
C	1.48118800	-2.42422800	1.04947300
C	-0.54215200	-2.99799000	-0.97001500
H	-1.66128500	-0.65301100	4.63005700
H	-6.15006600	-0.40862400	3.03124000
H	-5.52071400	1.25905200	2.71437700
C	1.82307300	-3.77906300	0.94871000
C	2.28151700	-1.57573500	1.83533300
C	-0.41614500	-2.88003100	-2.36014100
C	-1.20303900	-4.10772600	-0.42345000
C	2.93603700	-4.27689600	1.63085700
H	1.23342600	-4.44568300	0.33032100
C	3.38373300	-2.07690000	2.52348900
C	-0.95253400	-3.85817900	-3.19738600
H	0.07943000	-2.00701400	-2.77548200
C	-1.72193300	-5.09256800	-1.26225200
H	-1.32603300	-4.18942600	0.65206200
C	3.71558900	-3.43119800	2.42031100
H	3.19425400	-5.32770100	1.53802000
H	3.99064400	-1.40933600	3.12757000
C	-1.60452600	-4.96480600	-2.64929100
H	-0.86790800	-3.75332800	-4.27472000
H	-2.22430800	-5.95546700	-0.83462100
H	4.58242500	-3.82050600	2.94574400
H	-2.02373500	-5.72551900	-3.30109600
H	2.04471700	-0.51734500	1.89539900
C	2.13129200	2.36086500	-1.18557900
C	2.63100100	1.21630500	-1.81488700
C	2.90349700	0.03979600	-1.06145900
Pd	0.75449900	0.31675900	-0.97268100
C	1.68139400	3.60045000	-1.87839000
H	1.05305800	3.36593600	-2.74337600
H	2.60076300	4.08688900	-2.24376600
C	0.97319500	4.56508100	-0.91532900
H	0.04948400	4.11273500	-0.53569700
H	1.64746400	4.70126300	-0.06000100

C	0.66165000	5.90860800	-1.52997900
C	1.68500600	6.67781800	-2.10676100
C	-0.64076600	6.42049200	-1.52527500
C	1.39930300	7.91760800	-2.67890100
H	2.70403500	6.29515700	-2.08830100
C	-0.92831900	7.66305700	-2.09557500
H	-1.43648500	5.83975600	-1.06578400
C	0.09211400	8.41410700	-2.68056700
H	2.20170000	8.50255600	-3.12138500
H	-1.94711500	8.04256600	-2.08128900
H	-0.12636400	9.38052100	-3.12724000
C	3.46314000	-1.21368200	-1.67769900
H	3.04915100	-2.09079400	-1.16936900
H	3.16927100	-1.28715600	-2.73204800
C	5.00440500	-1.28452500	-1.56141500
H	5.27820100	-1.13181400	-0.50967900
H	5.45243600	-0.46266200	-2.13105500
C	5.53087100	-2.61568800	-2.04037700
C	5.42425700	-3.74897500	-1.22108400
C	6.08125800	-2.76374800	-3.31876700
C	5.85717600	-4.99712300	-1.66778600
H	4.99874600	-3.64723400	-0.22586800
C	6.51758700	-4.01161500	-3.76981500
H	6.17224700	-1.89270900	-3.96346500
C	6.40632700	-5.13289500	-2.94574200
H	5.77017900	-5.86356200	-1.01731700
H	6.94701900	-4.10633600	-4.76351700
H	6.74730800	-6.10372900	-3.29431900
H	3.16994100	0.18813400	-0.01446300
H	2.19525700	2.40181700	-0.10356900
H	2.68116300	1.18514300	-2.90275700
C	5.30946800	3.84618200	0.38397600
C	6.32745800	4.64292200	-0.15951900
C	5.75065300	5.12713500	-1.34333200
N	4.22059400	3.86538200	-0.41468500
H	5.30830400	3.27122900	1.30567800
H	7.31591100	4.83864400	0.23807800
H	6.17970700	5.78630500	-2.09202300
N	4.49534700	4.65192100	-1.48931800
(E)-(S)-INT10			
P	-1.15874800	1.20638300	-1.53858100
C	-2.51029200	-0.00329200	-1.84966200
C	-1.18643400	2.31543200	-3.00249800
C	-1.83153400	2.19759200	-0.14708900
C	-2.91029600	-0.87356600	-0.78886100

C	-3.03074500	-0.17811600	-3.13533500
C	-1.74683800	3.59777700	-3.02072700
C	-0.48805000	1.86303200	-4.13616300
C	-1.02410100	2.37025100	0.98579500
C	-3.12765800	2.73059100	-0.15057100
C	-3.83625300	-1.84501400	-1.12277900
C	-2.47906200	-0.77442500	0.63961900
C	-3.95011700	-1.19678200	-3.44696900
H	-2.71703600	0.49089600	-3.92770100
C	-1.62116000	4.40693300	-4.15239400
H	-2.24915800	3.99164000	-2.14694100
C	-0.38279000	2.66172400	-5.27240100
H	-0.01012800	0.88662400	-4.11219200
C	-1.49872400	3.07071300	2.09426600
H	-0.03316800	1.92390500	0.99429400
C	-3.59324300	3.45597600	0.94620800
H	-3.77678000	2.56632200	-1.00499900
C	-4.33152700	-2.02192200	-2.41223700
O	-4.39425300	-2.77649700	-0.28326900
C	-3.37584400	-0.25176700	1.55362700
C	-1.24096800	-1.24503900	1.18098600
H	-4.34052400	-1.32248200	-4.45053200
C	-0.94746700	3.94114100	-5.28079600
H	-2.03628900	5.40897100	-4.13517300
H	0.15593300	2.29588500	-6.14196900
C	-2.78163900	3.62344100	2.07208400
H	-0.87139800	3.18344300	2.97362100
H	-4.59358100	3.87970800	0.92805900
O	-5.20903600	-3.07557400	-2.43431300
C	-5.23847900	-3.59935500	-1.09804300
C	-3.10718500	-0.13795000	2.91554200
O	-4.63190200	0.23538500	1.29084200
C	-0.99391300	-1.14767800	2.55334500
P	0.09564000	-1.74124200	0.01519800
H	-0.84806900	4.57437800	-6.15784700
H	-3.15134300	4.17577100	2.93121100
H	-4.85100700	-4.62265100	-1.10288200
H	-6.26264400	-3.56070400	-0.71422700
C	-1.92069900	-0.58708000	3.45198200
O	-4.17640800	0.43421300	3.55583600
C	-5.12998400	0.75295300	2.53060000
H	-0.05485300	-1.51454800	2.95002800
C	1.34500000	-2.64385900	1.01915800
C	-0.70767200	-3.04155800	-0.99553300

H	-1.71147800	-0.51686100	4.51344300
H	-6.08701300	0.27768000	2.76403500
H	-5.22800100	1.84042400	2.45435800
C	1.58637600	-4.01983200	0.90613300
C	2.21038500	-1.87266600	1.81651500
C	-0.59943600	-2.95486000	-2.38942600
C	-1.45780600	-4.08063500	-0.42614400
C	2.65758900	-4.61018700	1.58228900
H	0.94926300	-4.63326500	0.27961500
C	3.26510400	-2.46454600	2.50682300
C	-1.23593100	-3.89015700	-3.20558200
H	-0.03877400	-2.13125000	-2.82292500
C	-2.07696300	-5.02679000	-1.24182700
H	-1.56881800	-4.13751100	0.65249700
C	3.49520000	-3.83914800	2.38837600
H	2.83562400	-5.67651600	1.47505500
H	3.91865400	-1.85229100	3.12169600
C	-1.97342500	-4.92831300	-2.63253700
H	-1.16306500	-3.80449900	-4.28574600
H	-2.64696100	-5.83618900	-0.79390000
H	4.32704900	-4.30075000	2.91244900
H	-2.47020300	-5.65698100	-3.26664900
H	2.06373300	-0.79814500	1.87208700
C	2.78783000	2.74962400	-0.93682100
C	2.74219700	1.37332700	-1.57059300
C	3.10610400	0.22178000	-0.85580800
Pd	0.90680600	0.19725500	-1.03602900
C	1.70318500	3.70941200	-1.42862700
H	0.74341300	3.24244700	-1.20974600
H	1.76292900	3.80912500	-2.51691700
C	1.74828300	5.09715300	-0.77007100
H	1.79500300	4.97389900	0.32042300
H	2.66126400	5.61920900	-1.07536300
C	0.52906200	5.91142700	-1.13556200
C	0.54200700	6.77385900	-2.23836400
C	-0.66211100	5.77298000	-0.41033600
C	-0.60304800	7.48210600	-2.60748800
H	1.45841100	6.88843700	-2.81251400
C	-1.81074600	6.47429100	-0.77742800
H	-0.69344000	5.10128800	0.44200100
C	-1.78548900	7.33363800	-1.87889400
H	-0.57194900	8.14965300	-3.46458200
H	-2.72328100	6.34528200	-0.20185400
H	-2.67710700	7.88522400	-2.16444600

C	3.73283000	-1.01314600	-1.45741600
H	3.28942400	-1.91112800	-1.01297100
H	3.53296500	-1.05879300	-2.53531400
C	5.25956900	-1.07300600	-1.21437800
H	5.44009600	-0.93975500	-0.13924300
H	5.74720200	-0.23555600	-1.72713200
C	5.83899900	-2.39085700	-1.66747900
C	5.63770400	-3.54673100	-0.89795300
C	6.52571800	-2.50820800	-2.88158000
C	6.11176900	-4.78481800	-1.33027200
H	5.10134600	-3.47186900	0.04512000
C	7.00388300	-3.74610700	-3.31785400
H	6.68685200	-1.62049400	-3.48887400
C	6.79791400	-4.88920900	-2.54361800
H	5.94698200	-5.66875300	-0.71953800
H	7.53781600	-3.81648600	-4.26183500
H	7.16940600	-5.85283200	-2.88112400
H	3.31226100	0.34650400	0.20981600
H	2.69742700	2.64258500	0.15039800
H	2.83922500	1.37426300	-2.65644400
C	5.17880500	3.30310500	-0.29271000
C	6.26353700	3.84426100	-0.96365300
C	5.75417400	4.17317300	-2.23783600
N	4.12497200	3.34098200	-1.14706600
H	5.07481300	2.90283500	0.70543500
H	7.26451400	3.98818300	-0.58371400
H	6.26859900	4.62797900	-3.07479000
N	4.45943700	3.85972100	-2.34957200
(E)-(S)-3			
C	-5.44448000	0.88536000	1.04029500
C	-6.10934900	0.04384000	1.91605800
C	-5.08596400	-0.72797700	2.50631600
N	-4.12045200	0.59678200	1.14627300
H	-5.80611500	1.64998000	0.36854800
H	-7.17269000	0.00162300	2.10172700
H	-5.17136000	-1.50758500	3.25211100
N	-3.88070100	-0.39446600	2.03521700
C	-3.00894200	1.15727100	0.36473400
C	-3.13066400	0.73596500	-1.11030500
H	-4.02699800	1.19630300	-1.54618100
H	-2.27276500	1.14787600	-1.65442600
C	-3.19156700	-0.78882400	-1.30395000
H	-2.27674800	-1.23885100	-0.89935600
H	-4.02638000	-1.19087100	-0.71996100
C	-3.35475500	-1.15704300	-2.75935000

C	-4.63088900	-1.25068400	-3.33031900
C	-2.23878500	-1.36284500	-3.58040100
C	-4.78952500	-1.54216300	-4.68574900
H	-5.50588500	-1.09664200	-2.70275300
C	-2.39153700	-1.65559400	-4.93663300
H	-1.24218200	-1.29628900	-3.14991800
C	-3.66876600	-1.74551900	-5.49411500
H	-5.78735700	-1.61525400	-5.10974800
H	-1.51394700	-1.81699200	-5.55674800
H	-3.78998200	-1.97609000	-6.54875500
C	-2.93765600	2.65388600	0.51812100
H	-3.78960000	3.22051900	0.14025500
C	-1.89922600	3.29925800	1.05218500
H	-1.04888800	2.71992100	1.41708900
C	-1.78051600	4.79068800	1.16840600
H	-2.71280300	5.27201000	0.84931500
H	-1.62085200	5.07130600	2.21894500
C	-0.60446300	5.35112600	0.33326200
H	0.32263600	4.85545500	0.64752300
H	-0.76493300	5.08962900	-0.71924600
C	-0.46723800	6.84760500	0.48379200
C	0.28433400	7.39548100	1.53173200
C	-1.13070400	7.71952300	-0.38895300
C	0.37232900	8.77750900	1.70395300
H	0.80770600	6.73096600	2.21557000
C	-1.04588200	9.10267300	-0.22168500
H	-1.71576500	7.30866500	-1.20863600
C	-0.29355300	9.63649300	0.82670200
H	0.96376300	9.18367100	2.52000500
H	-1.56401800	9.76301800	-0.91176200
H	-0.22381200	10.71268400	0.95705600
H	-2.11805400	0.70059400	0.80297800
(E)-(R)-TS9			
P	-1.65745200	1.57729700	0.13583500
C	-2.60033700	0.44422200	-0.95918700
C	-1.83673000	3.25514200	-0.57865500
C	-2.62664600	1.58600200	1.68563300
C	-2.89271100	-0.87900300	-0.50337200
C	-2.87812600	0.81373200	-2.27792800
C	-2.67725900	4.23941600	-0.04259200
C	-0.98674100	3.59272300	-1.64672500
C	-1.95451800	1.39936400	2.89959100
C	-4.02198000	1.73573000	1.68488900
C	-3.47417400	-1.72031400	-1.43396800
C	-2.68275800	-1.38944600	0.88453800

C	-3.44307400	-0.07823600	-3.20758300
H	-2.65085000	1.82140700	-2.60542100
C	-2.67066400	5.53300900	-0.57002700
H	-3.32455300	4.00856000	0.79544800
C	-0.99053700	4.87979600	-2.17853500
H	-0.30012800	2.84949700	-2.04291800
C	-2.66482900	1.36161000	4.09975700
H	-0.87762700	1.26513400	2.89655500
C	-4.72786300	1.71794100	2.88645100
H	-4.55353000	1.84669300	0.74484900
C	-3.72549400	-1.34777900	-2.75294800
O	-3.87168200	-3.01720300	-1.23743100
C	-3.78518200	-1.55769900	1.70149400
C	-1.42880600	-1.77980400	1.44728000
H	-3.64863400	0.22117500	-4.22886900
C	-1.83207400	5.85556800	-1.63705200
H	-3.31840900	6.29021900	-0.13774700
H	-0.31436300	5.12743100	-2.99068200
C	-4.05096900	1.52449900	4.09474800
H	-2.13387000	1.21331600	5.03477000
H	-5.80633500	1.84840900	2.88068700
O	-4.27875700	-2.39828800	-3.43521900
C	-4.34375000	-3.49116000	-2.50619000
C	-3.70295500	-2.02520600	3.01193000
O	-5.09048100	-1.27820600	1.39275600
C	-1.36025600	-2.26894900	2.75483100
P	0.10149000	-1.45268000	0.49579900
H	-1.82093300	6.86529800	-2.03625600
H	-4.60483900	1.49808000	5.02855900
H	-3.69425500	-4.29958300	-2.85456400
H	-5.38123900	-3.82310400	-2.40605800
C	-2.49922000	-2.39642900	3.57009600
O	-4.94912400	-2.04547200	3.57702000
C	-5.85498700	-1.56295600	2.57220600
H	-0.40000700	-2.56015400	3.16336500
C	1.43341600	-2.36704600	1.35901900
C	-0.17149600	-2.32733500	-1.08390900
H	-2.43241300	-2.76893700	4.58577500
H	-6.59509300	-2.33691000	2.34705000
H	-6.33023700	-0.64390000	2.92642500
C	1.96926800	-3.57198900	0.88773900
C	2.01495000	-1.75268700	2.48171300
C	0.13748800	-1.66598600	-2.28007400
C	-0.72333200	-3.61580900	-1.12722800

C	3.06352600	-4.15484000	1.53141600
H	1.54900600	-4.04833700	0.00952200
C	3.09603200	-2.34348400	3.13127900
C	-0.10795500	-2.28316200	-3.50641700
H	0.54564500	-0.65999500	-2.23936700
C	-0.94820000	-4.23864700	-2.35405900
H	-0.99402200	-4.12031100	-0.20481500
C	3.62641700	-3.54619200	2.65355000
H	3.47855100	-5.08256900	1.14857700
H	3.53484100	-1.85912300	3.99855400
C	-0.64967000	-3.56985100	-3.54453800
H	0.11848900	-1.75889200	-4.42992800
H	-1.36487700	-5.24150700	-2.38133200
H	4.47950100	-3.99958300	3.14955700
H	-0.84070400	-4.05063000	-4.49945400
H	1.62626000	-0.79993500	2.83104700
C	1.72899900	3.06862600	0.40982700
C	2.33839600	2.03012500	-0.31608100
C	2.75885700	0.80394300	0.24432100
Pd	0.56327100	0.81299700	0.24199200
C	3.51626600	-0.21728400	-0.55894800
H	3.21961800	-1.22726000	-0.25952500
H	3.27458200	-0.11514500	-1.62399500
C	5.04498900	-0.08583100	-0.36467100
H	5.36798800	0.90119700	-0.71410300
H	5.26226600	-0.13340700	0.71059900
C	5.78247900	-1.18690500	-1.08615100
C	5.83360300	-2.47694400	-0.53830900
C	6.37231800	-0.96768500	-2.33661500
C	6.45823400	-3.52006200	-1.22144400
H	5.37583800	-2.66122700	0.43059500
C	7.00058600	-2.00886700	-3.02379700
H	6.33980600	0.02818400	-2.77218200
C	7.04504700	-3.28908100	-2.46870900
H	6.49000500	-4.51275900	-0.77975900
H	7.45682300	-1.81879400	-3.99161800
H	7.53466100	-4.09955200	-3.00147500
H	2.94577200	0.76994600	1.31808800
C	1.67549300	3.18619400	1.91302900
H	1.22717300	2.28903600	2.36036400
H	2.69699700	3.24209500	2.30554400
C	0.87278100	4.42489400	2.34173400
H	1.41015700	5.30329200	1.96813300
H	-0.10359100	4.40503400	1.84245800

C	0.67460200	4.48789800	3.83541500
C	-0.57853100	4.22548600	4.40207000
C	1.75041500	4.76064800	4.69269400
C	-0.75564600	4.22349300	5.78717500
H	-1.42094300	4.01563300	3.74986400
C	1.57879400	4.76265700	6.07721000
H	2.72823300	4.97538800	4.26785400
C	0.32420100	4.49064600	6.63041900
H	-1.73746500	4.01459900	6.20412700
H	2.42357600	4.97908000	6.72569300
H	0.19055100	4.49191300	7.70867400
H	1.17598500	3.79775300	-0.16273000
H	2.40811200	2.16625200	-1.39239200
C	4.31177500	4.46696200	-1.87825900
C	5.26346900	4.08276000	-0.90613100
N	3.32723600	4.73797900	0.05476100
H	4.42397800	4.49353800	-2.95833600
H	6.28642200	3.76028300	-1.05585000
C	4.57868500	4.27378900	0.29378800
H	4.91881900	4.10464800	1.31080200
N	3.15992500	4.84522700	-1.30448800
(E)-(R)-INT10			
P	-1.50591400	1.49870600	0.52715900
C	-2.58002600	0.38146700	-0.46959600
C	-1.88379000	3.17445600	-0.14559800
C	-2.29693200	1.42171800	2.18522800
C	-2.85108400	-0.94824300	-0.01837700
C	-2.97784200	0.78094000	-1.75022700
C	-3.11241700	3.83956500	-0.02173300
C	-0.84747600	3.80062400	-0.85183000
C	-1.47002200	1.16764200	3.28649400
C	-3.67730900	1.55137000	2.38977800
C	-3.54516700	-1.75413200	-0.90423100
C	-2.49874600	-1.52264400	1.31637100
C	-3.65335100	-0.07606400	-2.63745800
H	-2.75659400	1.78972100	-2.07934300
C	-3.29578400	5.09848700	-0.59129000
H	-3.92965700	3.38478400	0.52356400
C	-1.02919800	5.06084700	-1.42362800
H	0.10361400	3.28474900	-0.94203500
C	-2.00506700	1.06404000	4.56961800
H	-0.40602400	1.03197000	3.11917900
C	-4.21140900	1.47930900	3.67597300
H	-4.34502600	1.66482700	1.54307400
C	-3.92268600	-1.34761600	-2.18099800

O	-3.94834300	-3.04994200	-0.69600900
C	-3.50798300	-1.72177700	2.24000900
C	-1.19947500	-1.97027300	1.71024500
H	-3.94911400	0.24952700	-3.62835200
C	-2.25546000	5.71237900	-1.29379000
H	-4.25215600	5.60291300	-0.48402900
H	-0.21061200	5.53315800	-1.95903900
C	-3.37660500	1.23385800	4.76941800
H	-1.35321100	0.85150100	5.41214100
H	-5.28149500	1.59811300	3.82244200
O	-4.56910100	-2.37171200	-2.82518600
C	-4.54697000	-3.48733900	-1.92237700
C	-3.29444200	-2.26878400	3.50295500
O	-4.83478900	-1.40273500	2.09480200
C	-1.00163300	-2.53842600	2.97197200
P	0.22418600	-1.58806100	0.61469800
H	-2.40099800	6.69546200	-1.73276600
H	-3.79568300	1.16032900	5.76881900
H	-3.94060800	-4.28910400	-2.35482200
H	-5.57140400	-3.81893100	-1.72804800
C	-2.04630200	-2.69437800	3.90117600
O	-4.47389000	-2.30336300	4.20166400
C	-5.47299100	-1.75639700	3.32806100
H	-0.00925900	-2.87095700	3.25305100
C	1.61792900	-2.59499500	1.26440200
C	-0.24791700	-2.40480300	-0.95710800
H	-1.87762300	-3.12997900	4.87950500
H	-6.24189600	-2.51182000	3.13553600
H	-5.90073300	-0.85934900	3.78547800
C	2.07563900	-3.78052400	0.67420300
C	2.34042700	-2.05423100	2.34313600
C	-0.07763900	-1.69094300	-2.15074100
C	-0.81084100	-3.68847200	-0.99800000
C	3.22244200	-4.41545300	1.15863600
H	1.55078400	-4.20326000	-0.17488400
C	3.47276100	-2.69719000	2.83734400
C	-0.46644600	-2.24959500	-3.36840500
H	0.33510800	-0.68645600	-2.10773900
C	-1.17953100	-4.25483600	-2.21781400
H	-0.97730500	-4.23417200	-0.07419200
C	3.92066200	-3.88085800	2.24181400
H	3.57105400	-5.32766400	0.68255000
H	4.01539800	-2.26810600	3.67491400
C	-1.01522100	-3.53318600	-3.40375500

H	-0.34764000	-1.68178500	-4.28656000
H	-1.60305000	-5.25517500	-2.24273600
H	4.81286400	-4.37551200	2.61464900
H	-1.31822700	-3.96958100	-4.35119900
H	2.01696600	-1.11281200	2.77959800
C	2.46440400	3.29420400	0.87045100
C	2.42998600	2.09174400	-0.04669300
C	2.90867400	0.81087500	0.26513000
Pd	0.70975000	0.70209800	0.41592300
C	3.47060800	-0.14747300	-0.75832400
H	3.16258200	-1.17111600	-0.52238500
H	3.07415100	0.08052100	-1.75566500
C	5.01687100	-0.12181700	-0.80358800
H	5.35862700	0.85307700	-1.17124800
H	5.39265100	-0.22817400	0.22322700
C	5.56156900	-1.23812200	-1.66083200
C	5.55142000	-2.55608900	-1.17973500
C	6.02400800	-1.00553700	-2.96106300
C	5.99174500	-3.61175300	-1.97691400
H	5.18957500	-2.75345200	-0.17366000
C	6.46835200	-2.05994800	-3.76278400
H	6.03634100	0.01094400	-3.34773500
C	6.45312100	-3.36716200	-3.27349000
H	5.97620200	-4.62581900	-1.58581400
H	6.82671700	-1.85908700	-4.76890500
H	6.79820400	-4.18827900	-3.89564900
H	3.25576600	0.62383100	1.28222800
C	2.44299600	2.97928900	2.37322400
H	1.64972600	2.24439700	2.55015700
H	3.39120900	2.51019900	2.66220400
C	2.19322000	4.22463600	3.24726300
H	2.35685200	3.94825100	4.29583400
H	2.92999900	4.99643800	2.99902800
C	0.79075000	4.76461600	3.07670400
C	0.51015200	5.78873600	2.16208300
C	-0.27230700	4.19180200	3.78638600
C	-0.80219400	6.21871900	1.95833600
H	1.32575200	6.22413200	1.59136300
C	-1.58558000	4.61415800	3.58162300
H	-0.06976300	3.39487600	4.49668800
C	-1.85360300	5.63090100	2.66346600
H	-1.00632900	6.99909800	1.23169100
H	-2.39567600	4.13561900	4.12439500
H	-2.87517100	5.95445900	2.48835600

H	1.61798700	3.94107100	0.63617600
H	2.37521700	2.35969100	-1.10319500
C	4.72314500	5.91162600	0.08568000
C	5.68429700	4.88791600	0.22182900
N	3.63882300	4.13493500	0.55186600
H	4.87492700	6.95642500	-0.15315000
H	6.75667100	4.95658500	0.10970000
C	4.94263600	3.75710000	0.52315500
H	5.23180400	2.73245300	0.70259100
N	3.48320200	5.45291300	0.28622600
(E)-(R)-3			
C	-1.22932100	-0.27223000	1.62917200
C	0.09636600	-0.66486000	1.57471200
C	0.54187900	-0.21464600	0.31291700
N	-1.50474800	0.35739000	0.45701300
H	-1.98517800	-0.38760900	2.39252400
H	0.65175800	-1.20325400	2.32855200
H	1.52084700	-0.32165700	-0.13617200
N	-0.42727900	0.40993400	-0.36132800
C	-2.75755500	1.01498100	0.08429600
H	-3.52691400	0.55018400	0.71531700
C	-3.09992600	0.72326100	-1.38606000
H	-4.02223200	1.26006100	-1.63729300
H	-2.30440600	1.13579400	-2.01290900
C	-3.27364200	-0.77558400	-1.68172800
H	-2.37785500	-1.30634400	-1.34191600
H	-4.12046200	-1.16594100	-1.10324200
C	-3.48801300	-1.03062100	-3.15453800
C	-4.77344700	-1.18417700	-3.68725500
C	-2.39177600	-1.06977200	-4.02747900
C	-4.96230100	-1.37545700	-5.05764700
H	-5.63286000	-1.15695500	-3.02114800
C	-2.57504800	-1.25995700	-5.39705900
H	-1.38917800	-0.94967000	-3.62331900
C	-3.86289400	-1.41384600	-5.91712400
H	-5.96726500	-1.49708900	-5.45278300
H	-1.71342400	-1.29151000	-6.05840100
H	-4.00743200	-1.56493300	-6.98318400
C	-2.73126600	2.49918000	0.36580300
H	-3.68396500	3.00315100	0.20024100
C	-1.67124400	3.20093900	0.76881200
H	-0.72020800	2.69035900	0.91339800
C	-1.67091000	4.68401700	1.00094400
H	-2.68848600	5.08515400	0.91951200
H	-1.32239600	4.90488700	2.01975300

C	-0.75000400	5.42749700	0.00392600
H	0.26070600	5.00634200	0.07027000
H	-1.10900700	5.23355600	-1.01370700
C	-0.71065200	6.91326500	0.27084600
C	0.24678900	7.46296300	1.13330300
C	-1.66572900	7.76702700	-0.29675600
C	0.25252700	8.82880100	1.42097300
H	0.99624400	6.81327900	1.57968200
C	-1.66505200	9.13332700	-0.01250100
H	-2.41358500	7.35480300	-0.97041000
C	-0.70473400	9.66916700	0.84861600
H	1.00641300	9.23703400	2.08868100
H	-2.41132400	9.77996300	-0.46610400
H	-0.70031500	10.73295500	1.06876000
INT8c			
P	-3.16717300	0.23070800	-1.03889900
C	-4.27409400	-1.20080000	-1.35990500
C	-3.17986400	1.17888600	-2.60848900
C	-4.13521800	1.27784300	0.10660800
C	-4.50978000	-2.12291000	-0.29897000
C	-4.79636500	-1.45249900	-2.63280000
C	-3.61117700	2.51020300	-2.66681600
C	-2.57132800	0.61219700	-3.74281400
C	-3.43229200	2.11469700	0.98371900
C	-5.53711100	1.28397700	0.11040600
C	-5.25075400	-3.24526000	-0.62089500
C	-4.08209200	-1.96144500	1.12147000
C	-5.53378400	-2.61188400	-2.93335600
H	-4.63150300	-0.73562900	-3.42628300
C	-3.41921500	3.26639400	-3.82541400
H	-4.06870800	2.96829300	-1.79704700
C	-2.41346900	1.35685400	-4.90950500
H	-2.20597300	-0.40986600	-3.70021200
C	-4.12811100	2.94723700	1.86158600
H	-2.34759400	2.07641400	0.99968800
C	-6.22828700	2.11888000	0.98797500
H	-6.08230000	0.63058100	-0.56270500
C	-5.73467900	-3.50179100	-1.90147200
O	-5.61238700	-4.26524400	0.22115600
C	-5.03002900	-1.60248300	2.05985500
C	-2.79215800	-2.30299700	1.63355300
H	-5.92396000	-2.79371000	-3.92824900
C	-2.82344900	2.69353900	-4.94796100
H	-3.71387000	4.31092200	-3.84159800
H	-1.94574700	0.90358800	-5.77905700

C	-5.52470600	2.94984000	1.86584200
H	-3.57741400	3.58208300	2.54965600
H	-7.31490500	2.12153900	0.98728500
O	-6.40703000	-4.69452300	-1.91512700
C	-6.29181400	-5.23381400	-0.58846700
C	-4.77468900	-1.57138400	3.43223100
O	-6.34491500	-1.27832600	1.83382700
C	-2.56206900	-2.30952900	3.01091900
P	-1.41454300	-2.50247700	0.43877200
H	-2.66376400	3.28914000	-5.84115700
H	-6.06555700	3.59563400	2.55204500
H	-5.70117000	-6.15433400	-0.62354200
H	-7.29079200	-5.41187900	-0.18045700
C	-3.55290800	-1.95036800	3.94327200
O	-5.90954000	-1.19762900	4.10266500
C	-6.83049600	-0.77449400	3.08439600
H	-1.58270100	-2.57489700	3.38554700
C	0.01397000	-3.14994200	1.38245000
C	-1.96241100	-3.87809300	-0.63299000
H	-3.35571300	-1.95669800	5.00896600
H	-7.81526900	-1.19744800	3.28795300
H	-6.85373300	0.32152000	3.04676400
C	0.62562800	-4.36559600	1.04195200
C	0.62888300	-2.31870800	2.33661700
C	-1.93604900	-3.70519400	-2.02159900
C	-2.45411600	-5.07462900	-0.09158500
C	1.82905800	-4.74065600	1.64392600
H	0.17771600	-5.01335500	0.29664300
C	1.82223000	-2.70597600	2.94183900
C	-2.40784600	-4.71254800	-2.86339600
H	-1.57232900	-2.76438200	-2.42496200
C	-2.90701000	-6.08797300	-0.93497500
H	-2.48961000	-5.20550600	0.98569900
C	2.43179800	-3.91233100	2.59238300
H	2.29757300	-5.67961300	1.36241600
H	2.29647300	-2.03728000	3.65276600
C	-2.89356400	-5.90404500	-2.32116600
H	-2.40392600	-4.56493400	-3.93925500
H	-3.27660700	-7.01801200	-0.51217200
H	3.38062600	-4.19218900	3.04000300
H	-3.26290100	-6.68813800	-2.97570000
H	0.20485500	-1.35079800	2.57019400
Pd	-0.90913700	-0.45743400	-0.55950900
C	0.65030900	0.12529900	-2.04506700

C	0.37103100	1.29548200	-1.32521400
C	1.10441500	-1.05329000	-1.39089100
H	1.06727500	-1.95658600	-1.99978500
C	-0.26200100	2.49951100	-1.95025800
H	-1.05423700	2.87118600	-1.29127500
H	-0.73622600	2.23184300	-2.89569500
C	0.71558500	3.66922900	-2.21367200
H	1.13953500	4.01688500	-1.26385800
H	1.54832700	3.31957700	-2.83517600
C	-0.03177200	4.78051300	-2.91267500
C	-0.86771000	5.64033600	-2.18769500
C	0.00162100	4.90112500	-4.30689200
C	-1.65528000	6.59015400	-2.83882400
H	-0.90610300	5.55685500	-1.10392100
C	-0.78147200	5.85167200	-4.96389100
H	0.64016100	4.23520900	-4.88252300
C	-1.61704600	6.69734900	-4.23161600
H	-2.29724700	7.24828600	-2.25945600
H	-0.73973400	5.93093700	-6.04698500
H	-2.22812700	7.43787100	-4.74008800
C	2.08055500	-1.10188800	-0.24588300
H	2.09396700	-2.11951400	0.14686600
H	1.76104600	-0.44637600	0.56744600
C	3.53286400	-0.72006600	-0.61690900
H	3.89258900	-1.33135100	-1.45397000
H	3.55536900	0.32720300	-0.94357900
C	4.40580300	-0.92486200	0.59940400
C	4.24981200	-0.09196600	1.71763400
C	5.29390800	-2.00224000	0.68553500
C	4.96445900	-0.33314800	2.89014300
H	3.53720300	0.72672200	1.67165800
C	6.01334600	-2.24673700	1.85817200
H	5.41502000	-2.66200300	-0.17064500
C	5.84924900	-1.41330800	2.96582000
H	4.82714500	0.31933000	3.74851400
H	6.69929900	-3.08851700	1.90594500
H	6.40520200	-1.60238800	3.88007200
H	0.83130800	1.43529300	-0.34582800
C	0.97281500	1.27441000	3.17470500
C	-0.22380600	0.98328100	3.85171700
C	-1.10703600	0.65255100	2.81780100
N	0.81494400	1.12924300	1.84390000
H	0.28407000	0.05060200	-3.06801800
H	1.92953100	1.58470000	3.58182900

H	-0.42112700	1.01665900	4.91548400
H	-2.14811000	0.36564900	2.86623400
N	-0.47553100	0.74077200	1.62334600
(Z)-(S)-TS9			
C	0.42698200	-2.59605400	0.02068300
C	-0.60944200	-1.93430300	-0.65940700
C	-1.49138000	-1.02130000	-0.00071100
Pd	0.46587200	-0.04695400	-0.15061400
H	0.59576300	-2.37821000	1.06780900
C	-1.96477800	-1.19977800	1.41638700
H	-2.29948000	-0.23687400	1.80819800
H	-1.15686000	-1.55114000	2.06142600
C	-3.13207400	-2.20785300	1.54502700
H	-3.94869900	-1.91769200	0.87125000
H	-2.76903200	-3.19489100	1.24269600
C	-3.61406100	-2.22997700	2.97519600
C	-2.91397800	-2.96783500	3.94059100
C	-4.69640900	-1.44264100	3.38564700
C	-3.28659500	-2.90937900	5.28395600
H	-2.06833400	-3.57768400	3.63746300
C	-5.07419600	-1.38575900	4.72880400
H	-5.24350900	-0.86221700	2.64563400
C	-4.36622500	-2.11700700	5.68510700
H	-2.73288800	-3.48869300	6.01862100
H	-5.91942700	-0.77084900	5.02782500
H	-4.65748500	-2.07581500	6.73142400
C	1.48557100	-3.39318200	-0.68850600
H	1.68263000	-2.95864300	-1.67363700
H	1.09578000	-4.40220000	-0.85538600
C	2.77667900	-3.45227300	0.14120200
H	3.00094200	-2.44498400	0.50535000
H	2.57554300	-4.05322900	1.03719700
C	3.99288400	-3.96257400	-0.59543100
C	3.91271300	-4.97852400	-1.55570600
C	5.24929300	-3.39855100	-0.33018700
C	5.05134500	-5.41385100	-2.23612800
H	2.95132700	-5.42968200	-1.78300200
C	6.39014100	-3.82900500	-1.00733500
H	5.32711200	-2.60068500	0.40407200
C	6.29535400	-4.83920600	-1.96782200
H	4.96505200	-6.20081000	-2.98073800
H	7.35148100	-3.37109900	-0.78908800
H	7.18103500	-5.17598700	-2.49958400
P	2.59938300	0.37222200	-1.07086500
C	2.53389100	2.07700400	-1.76107700

C	2.93727500	-0.70862000	-2.51064900
C	4.10987800	0.34795700	-0.04587400
C	2.53694000	3.17772300	-0.85247100
C	2.31444800	2.29309700	-3.12449400
C	1.85754600	-0.98699200	-3.36917100
C	4.16252900	-1.34588000	-2.73424300
C	4.00277000	-0.10601200	1.27529900
C	5.35043000	0.79005200	-0.52689800
C	2.33321900	4.42671400	-1.40806800
C	2.79680600	3.07589600	0.61120600
C	2.08164000	3.57550900	-3.65565100
H	2.32042000	1.45081800	-3.80512500
C	2.01338900	-1.85952800	-4.44347100
H	0.89100400	-0.52854400	-3.17780000
C	4.31024200	-2.23863300	-3.79778300
H	4.99681500	-1.18024600	-2.06591900
C	5.12494500	-0.13394300	2.10300200
H	3.03307400	-0.41514600	1.65343900
C	6.47561700	0.74295000	0.29520700
H	5.43247400	1.17546700	-1.53850800
C	2.09044300	4.62705300	-2.76538000
O	2.31942900	5.63050700	-0.75391000
C	4.03022700	3.46652400	1.09607800
C	1.84253400	2.65274700	1.58522600
H	1.90874300	3.72706400	-4.71501100
C	3.24209900	-2.49269800	-4.65639000
H	1.17251400	-2.06149000	-5.10067200
H	5.25636300	-2.75219400	-3.93149700
C	6.36373800	0.28331700	1.61103800
H	5.03131700	-0.47722600	3.12862700
H	7.43835600	1.06919000	-0.08798300
O	1.90113200	5.96047900	-3.01138300
C	1.99062900	6.62035900	-1.73823100
C	4.36641300	3.42941500	2.44774500
O	5.09822900	3.92282600	0.36766400
C	2.18304600	2.64796400	2.94125300
P	0.23236100	1.97789700	1.00396600
H	3.35800300	-3.19172800	-5.47948700
H	7.23959100	0.25712800	2.25258300
H	1.02159300	7.06530700	-1.49311600
H	2.78322100	7.37319400	-1.77422600
C	3.45570500	3.03229200	3.40198300
O	5.65700700	3.85180500	2.61722700
C	6.17599600	4.09048400	1.29891300

H	1.44885300	2.33874900	3.67361800
C	-0.76507000	1.76533800	2.52057600
C	-0.49967000	3.36791400	0.07298800
H	3.70451800	3.01580500	4.45681000
H	6.55351400	5.11454700	1.23703200
H	6.95821800	3.35674900	1.08131800
C	-1.95402900	2.46881700	2.75146100
C	-0.40283500	0.72859500	3.39940500
C	-1.00237500	3.11785700	-1.21075000
C	-0.51191500	4.67539000	0.57919700
C	-2.76634900	2.13488000	3.83847900
H	-2.25755900	3.26218200	2.07688200
C	-1.20794500	0.40843300	4.48877400
C	-1.50764600	4.16321800	-1.98349800
H	-0.96631200	2.10556900	-1.60389800
C	-1.03435700	5.71622800	-0.18752200
H	-0.10328800	4.87794700	1.56457200
C	-2.39845800	1.10622200	4.70607400
H	-3.69473300	2.67578900	3.99835700
H	-0.93278900	-0.41492800	5.13982500
C	-1.52559900	5.46258500	-1.47180500
H	-1.87956300	3.96563200	-2.98438600
H	-1.04907900	6.72628900	0.21202900
H	-3.04733200	0.82526300	5.52875100
H	-1.91882600	6.27743700	-2.07277300
H	0.49004500	0.14145500	3.20267800
H	-0.69910100	-2.08749000	-1.73372600
H	-2.21672600	-0.53028600	-0.65154400
C	0.07713600	-4.89339700	3.49560900
C	-0.68054800	-5.93602700	2.93889900
C	-0.90546200	-5.50584500	1.62427800
N	0.28410800	-3.91532500	2.58738600
H	0.47704600	-4.80225200	4.50038100
H	-1.01447500	-6.85213100	3.40959000
H	-1.44731500	-5.99245100	0.82064000
N	-0.32571100	-4.30061500	1.43694500
(Z)-(S)-INT10			
C	0.61936100	-2.99376400	0.51952000
C	-0.34228800	-2.14524000	-0.29481500
C	-1.43817500	-1.46761500	0.26374300
Pd	0.23298100	-0.00746600	-0.11185400
H	0.89613400	-2.48126200	1.44306100
C	-1.82714300	-1.48846100	1.71822000
H	-2.24842400	-0.51716000	1.98894200
H	-0.94266300	-1.61915100	2.34937600

C	-2.85592100	-2.57109200	2.12533700
H	-3.77177400	-2.44809600	1.53378700
H	-2.45467300	-3.56601600	1.91068500
C	-3.15500800	-2.41756700	3.59771500
C	-2.24689300	-2.90031300	4.55189400
C	-4.26570300	-1.68955400	4.04003100
C	-2.44576000	-2.65808100	5.91158700
H	-1.37603500	-3.45608600	4.21299800
C	-4.46955600	-1.44591000	5.39973200
H	-4.97085500	-1.29999500	3.30929500
C	-3.55790300	-1.92758400	6.34128900
H	-1.73313600	-3.04039200	6.63799600
H	-5.33826200	-0.87823300	5.72288600
H	-3.71347100	-1.73935600	7.40009700
C	1.89057600	-3.32301900	-0.26874700
H	2.33024400	-2.37873500	-0.58678200
H	1.62380000	-3.85907400	-1.18905800
C	2.94674300	-4.12181400	0.50900800
H	3.14113000	-3.62291200	1.46611200
H	2.56278900	-5.12132100	0.74289000
C	4.22584300	-4.21314100	-0.29138100
C	4.38259500	-5.18594500	-1.28699800
C	5.24889200	-3.27384400	-0.10973300
C	5.52829800	-5.21860500	-2.08324400
H	3.59656300	-5.92197000	-1.44036600
C	6.39548700	-3.29998400	-0.90473000
H	5.14097600	-2.50848800	0.65179300
C	6.53948900	-4.27233500	-1.89695800
H	5.63223900	-5.98272800	-2.84904000
H	7.17312800	-2.55737000	-0.74692800
H	7.43261100	-4.29719800	-2.51534400
P	2.32171200	0.36121200	-1.13554400
C	2.43873300	2.06676800	-1.81314100
C	2.65883500	-0.73625800	-2.57142500
C	3.80178300	0.22556400	-0.06122900
C	2.47172900	3.16140700	-0.89658800
C	2.32245300	2.30334600	-3.18617200
C	1.57085300	-1.01403600	-3.41828600
C	3.86928200	-1.40656600	-2.78653300
C	3.61128000	-0.23551400	1.24890100
C	5.08576600	0.60719900	-0.47380800
C	2.41604700	4.42328800	-1.45864600
C	2.64372400	3.04429000	0.58169100
C	2.23280800	3.60114300	-3.72318400

H	2.29773700	1.46187600	-3.86832300
C	1.70160100	-1.91590200	-4.47194600
H	0.61438600	-0.53296000	-3.22994600
C	3.99130800	-2.33210600	-3.82545700
H	4.71012000	-1.24825300	-2.12408900
C	4.68619300	-0.31645000	2.13380300
H	2.60795300	-0.49983200	1.57161400
C	6.16646500	0.49839100	0.40136600
H	5.23612400	1.00202300	-1.47394000
C	2.27888900	4.64609400	-2.82661700
O	2.47193000	5.62525000	-0.79928700
C	3.88381300	3.34836500	1.11315300
C	1.62339800	2.70253600	1.52299700
H	2.13866400	3.76912800	-4.79010300
C	2.91363200	-2.58399300	-4.67386800
H	0.85352400	-2.11371600	-5.12162700
H	4.92743600	-2.86608800	-3.95176400
C	5.96731000	0.04350900	1.70845100
H	4.52490200	-0.65800900	3.15191900
H	7.16164400	0.78023300	0.06859300
O	2.22650000	5.99350100	-3.07614200
C	2.29062900	6.63948800	-1.79523400
C	4.17053200	3.29617900	2.47418600
O	5.00829900	3.72217700	0.41990000
C	1.91888400	2.68521300	2.88977700
P	-0.01529700	2.11264300	0.89904900
H	3.00992300	-3.30543900	-5.48034000
H	6.80723800	-0.02448900	2.39368400
H	1.34913500	7.16510600	-1.60888000
H	3.14389300	7.32400400	-1.77522100
C	3.19948000	2.97461700	3.39616200
O	5.48565600	3.61998900	2.68744200
C	6.05715600	3.84188600	1.38892100
H	1.13791300	2.44192300	3.59856300
C	-1.10902600	2.17030100	2.37694400
C	-0.55684300	3.51588300	-0.14986500
H	3.40786000	2.94741200	4.45973000
H	6.47912200	4.85035300	1.34466300
H	6.81790100	3.07937300	1.19480700
C	-2.18528100	3.05748600	2.51243300
C	-0.94114100	1.16452100	3.34645600
C	-0.99815800	3.23420900	-1.44928700
C	-0.48735900	4.84920100	0.27887800
C	-3.06531900	2.94238800	3.59224600

H	-2.34760500	3.83170600	1.77110500
C	-1.81261900	1.05460500	4.42729700
C	-1.36067100	4.26913900	-2.31166300
H	-1.02487400	2.19995500	-1.78195500
C	-0.87006700	5.88209600	-0.57592900
H	-0.12308000	5.07714700	1.27610100
C	-2.88256700	1.94468000	4.55044200
H	-3.89950600	3.63347600	3.67765700
H	-1.68501500	0.25103600	5.14610600
C	-1.29917900	5.59414900	-1.87494200
H	-1.68324700	4.04296000	-3.32376100
H	-0.82423600	6.91206100	-0.23273800
H	-3.57834100	1.84373900	5.37800600
H	-1.58135900	6.40137200	-2.54486400
H	-0.14152600	0.43943700	3.22796600
H	-0.36422800	-2.37865200	-1.35881800
H	-2.23748600	-1.18072300	-0.42102600
C	-0.56037100	-5.75719500	2.39248700
C	-1.09497700	-6.15282100	1.14881700
C	-0.72440400	-5.14038700	0.27722800
N	0.09148300	-4.59191700	2.30010700
H	-0.62468500	-6.25943700	3.34896000
H	-1.67164800	-7.03671400	0.91798300
H	-0.90864800	-4.99491500	-0.77683900
N	-0.02466100	-4.23194600	1.00145700
(Z)-(S)-3			
C	-4.55782300	-0.73236800	1.53639300
C	-4.43598900	-1.93839100	2.20589900
C	-3.08405400	-2.30325200	2.03000800
N	-3.33569100	-0.44437800	1.01965500
H	-5.39448500	-0.06251700	1.40484800
H	-5.20722700	-2.46664300	2.74730600
H	-2.56517900	-3.17747200	2.40135700
N	-2.41823900	-1.39807400	1.30638800
C	-2.96590000	0.68568300	0.15669600
C	-3.49465700	0.47173800	-1.26905500
H	-4.59247500	0.46696500	-1.24636800
H	-3.19880000	1.33679500	-1.87583700
C	-2.98799800	-0.81993400	-1.92944900
H	-1.89237100	-0.79111300	-1.97816900
H	-3.25101500	-1.67519000	-1.29832100
C	-3.56685900	-1.00085400	-3.31272600
C	-4.77511600	-1.68604600	-3.49531700
C	-2.93688000	-0.44764200	-4.43498900
C	-5.34048800	-1.81636100	-4.76466100

H	-5.27299600	-2.12341300	-2.63279800
C	-3.49738400	-0.57521200	-5.70684800
H	-1.99614800	0.08367900	-4.30927500
C	-4.70259600	-1.26034000	-5.87575000
H	-6.27604200	-2.35546600	-4.88669500
H	-2.99126300	-0.14347800	-6.56607200
H	-5.13885700	-1.36345600	-6.86528300
C	-3.44312900	2.00601500	0.73174800
H	-4.14961000	2.56045800	0.11639300
C	-3.06449200	2.51833500	1.90702300
H	-3.47814200	3.48180300	2.20136500
C	-2.09694900	1.90358100	2.87806200
H	-2.60716200	1.75060300	3.83987000
H	-1.76709600	0.91848200	2.53713300
C	-0.85421300	2.79656800	3.12399300
H	-0.17630200	2.25719500	3.79646000
H	-0.32353200	2.93320600	2.17464300
C	-1.19848700	4.14290100	3.71796800
C	-1.47705500	4.26501300	5.08634200
C	-1.28942400	5.28700300	2.91515600
C	-1.83604900	5.49493600	5.63813300
H	-1.40744300	3.38654900	5.72408700
C	-1.64937700	6.52057200	3.46167700
H	-1.07625000	5.20763900	1.85194700
C	-1.92405800	6.62848100	4.82606800
H	-2.04349200	5.56993700	6.70212000
H	-1.71238200	7.39666300	2.82197100
H	-2.20128800	7.58758400	5.25424800
H	-1.87213100	0.65060400	0.13857500
(Z)-(R)-TS9			
P	-2.01041300	1.28071400	-0.66906600
C	-2.48641600	-0.35302500	-1.37373800
C	-2.13774700	2.46581000	-2.06219100
C	-3.36967100	1.71090800	0.47023700
C	-2.77581700	-1.43603900	-0.48604100
C	-2.37992600	-0.58473800	-2.74879200
C	-3.16783900	3.40715300	-2.18556400
C	-1.09889700	2.46682700	-3.01062400
C	-3.04003700	2.14941000	1.75885900
C	-4.71785000	1.58020000	0.10528200
C	-2.92890400	-2.67780800	-1.07380400
C	-2.98753500	-1.31111900	0.98455100
C	-2.53063300	-1.86417800	-3.31431800
H	-2.17013600	0.24347400	-3.41397500
C	-3.16641400	4.31880200	-3.24421100

H	-3.96751300	3.43941900	-1.45467300
C	-1.10972800	3.36435300	-4.07590200
H	-0.27690000	1.76410400	-2.90391800
C	-4.04693400	2.45132000	2.67602900
H	-1.99401800	2.22484200	2.04166000
C	-5.72180700	1.89837700	1.01837500
H	-4.97879600	1.21278600	-0.88236500
C	-2.79340600	-2.89924900	-2.44369100
O	-3.23579900	-3.85808600	-0.44675000
C	-4.27501300	-1.34933200	1.48449300
C	-1.94537900	-1.19475300	1.94920100
H	-2.44554200	-2.02484400	-4.38293500
C	-2.14488200	4.29623200	-4.19376700
H	-3.96830800	5.04709300	-3.32383700
H	-0.30406100	3.34655400	-4.80396900
C	-5.38752500	2.32737500	2.30614400
H	-3.78486100	2.77483400	3.67879300
H	-6.76457400	1.80504100	0.72844700
O	-3.00007300	-4.22371600	-2.72178000
C	-3.11262200	-4.87812300	-1.44763700
C	-4.56805400	-1.23065000	2.84173500
O	-5.43801000	-1.46311200	0.76864000
C	-2.24858500	-1.09674600	3.31019900
P	-0.21928000	-1.02268600	1.35361900
H	-2.14801600	5.00579600	-5.01585300
H	-6.17166000	2.55953900	3.02069000
H	-2.20415300	-5.46006400	-1.25796200
H	-4.00712900	-5.50419300	-1.43923700
C	-3.57232400	-1.10621100	3.78585100
O	-5.92407300	-1.25699800	3.02745400
C	-6.50581900	-1.43028700	1.72610700
H	-1.44353900	-1.00350300	4.02871600
C	0.77080200	-1.07079300	2.89472800
C	0.10979000	-2.59717000	0.48716000
H	-3.79686800	-1.01781400	4.84255000
H	-7.05208200	-2.37861200	1.69390900
H	-7.16127700	-0.58290700	1.50850600
C	1.34756400	-2.23553800	3.41609800
C	0.99671600	0.15454500	3.54378500
C	0.83248200	-2.54654100	-0.71281600
C	-0.32765000	-3.83563300	0.97794500
C	2.15149400	-2.17056300	4.55587500
H	1.19742400	-3.18841000	2.92207700
C	1.79248200	0.21694500	4.68498100

C	1.14230900	-3.72029400	-1.39974200
H	1.13964500	-1.58005800	-1.10285300
C	-0.00650700	-5.00981400	0.29732200
H	-0.92483100	-3.87737100	1.88354900
C	2.37722700	-0.94770200	5.18946500
H	2.61299100	-3.07618300	4.93814400
H	1.98201500	1.17591700	5.15615100
C	0.73047200	-4.95371400	-0.89008400
H	1.70461400	-3.67241600	-2.32724300
H	-0.33462300	-5.96819800	0.68966900
H	3.01745000	-0.89856500	6.06506400
H	0.97636200	-5.86968000	-1.41938000
H	0.56454300	1.06459000	3.13668600
C	1.08390100	2.87418400	-0.34770400
C	2.12799400	1.91514000	-0.42370700
C	2.73600700	1.28843100	0.67687300
Pd	0.15332700	0.98497800	0.15343100
C	3.59942900	0.06712500	0.46303100
H	3.01399400	-0.68450300	-0.07955900
H	4.43245000	0.33480200	-0.19755200
C	4.15079800	-0.56095900	1.75094700
H	4.84937500	0.13263300	2.22176300
H	3.32508700	-0.71217800	2.44844800
C	4.82178100	-1.88313800	1.47062400
C	6.21552200	-2.00696700	1.50317700
C	4.05864200	-3.01205600	1.13499700
C	6.83365900	-3.22591100	1.21256300
H	6.81459600	-1.13618000	1.75908800
C	4.67023100	-4.22997200	0.84071800
H	2.97625800	-2.93288700	1.10094600
C	6.06315600	-4.34185100	0.88007100
H	7.91729900	-3.30323000	1.24576000
H	4.05859300	-5.09053500	0.58146400
H	6.54295600	-5.29022100	0.65376200
C	0.85578400	3.75257100	0.85999300
H	-0.15577500	4.17388400	0.82145300
H	0.92182300	3.17359000	1.78763500
C	1.89582000	4.89870400	0.94750600
H	2.89227400	4.44499800	0.95161300
H	1.80806500	5.53084300	0.05477000
C	1.68507000	5.71613300	2.19847600
C	2.24275800	5.28644800	3.41270500
C	0.88955500	6.86861800	2.18951300
C	2.00590300	6.00104300	4.58796200

H	2.86650800	4.39273400	3.41751600
C	0.65355800	7.58425400	3.36548600
H	0.45500000	7.20949400	1.25184300
C	1.21133600	7.15091800	4.57009300
H	2.44900800	5.66264200	5.52141800
H	0.03792200	8.47983400	3.34010700
H	1.03190300	7.70729400	5.48632700
H	0.75620700	3.29870400	-1.29381700
H	2.43425600	1.58040300	-1.41461200
C	6.48903500	2.41511300	2.47267300
C	5.45683300	2.52303100	3.42357500
H	7.55554500	2.33974600	2.64269000
H	5.52895900	2.54184000	4.50627400
N	4.47794900	2.58574800	1.47484100
H	2.46387000	1.55561700	1.68736800
N	4.25658400	2.60799000	2.81967900
C	5.80522200	2.45224800	1.25297100
H	6.19395300	2.39653300	0.24181600
(Z)-(R)-INT10			
P	-2.14599500	1.41143800	-0.51948400
C	-2.51342300	-0.17328100	-1.40164400
C	-2.35740200	2.71011500	-1.80833200
C	-3.59183900	1.62449600	0.58659800
C	-2.73024000	-1.36063900	-0.63270000
C	-2.36184600	-0.26174100	-2.78896800
C	-3.47646200	3.54697900	-1.91303600
C	-1.28189800	2.90937700	-2.69267500
C	-3.35227300	1.95983600	1.92524400
C	-4.91157600	1.42843300	0.15319400
C	-2.76254700	-2.54740000	-1.34041800
C	-2.98772300	-1.40177700	0.83634100
C	-2.39078500	-1.48849300	-3.47942100
H	-2.20397900	0.64291800	-3.36350700
C	-3.52520600	4.54631900	-2.88804400
H	-4.30940400	3.43008500	-1.22964200
C	-1.34013000	3.89248500	-3.67849500
H	-0.39534100	2.28901100	-2.59530800
C	-4.41454700	2.09731200	2.81935300
H	-2.32729200	2.08372900	2.26384700
C	-5.97393400	1.58789200	1.04167800
H	-5.10384800	1.13253200	-0.87351600
C	-2.57916900	-2.62272400	-2.72030700
O	-2.98739400	-3.80569300	-0.83865800
C	-4.28241600	-1.56267000	1.29118100
C	-1.97473100	-1.33798700	1.83694300

H	-2.27100100	-1.53578700	-4.55595400
C	-2.46398300	4.71747100	-3.77735700
H	-4.39782800	5.19055300	-2.95110300
H	-0.50356300	4.02423400	-4.35895900
C	-5.72650100	1.91535500	2.37781300
H	-4.21797600	2.33946500	3.85963600
H	-6.99402100	1.44738700	0.69480000
O	-2.66817400	-3.92961000	-3.12840200
C	-2.72179500	-4.70681500	-1.92152600
C	-4.61381600	-1.60324700	2.64377700
O	-5.42098800	-1.66936500	0.53337600
C	-2.31656300	-1.39658100	3.19113500
P	-0.24648500	-1.03915500	1.28556200
H	-2.50631800	5.49383800	-4.53584600
H	-6.55419900	2.02215900	3.07297800
H	-1.75300300	-5.19282000	-1.75665400
H	-3.53326000	-5.43357300	-1.99498600
C	-3.64948100	-1.52279700	3.62440200
O	-5.97108300	-1.72874400	2.78629400
C	-6.50942700	-1.79766900	1.45720500
H	-1.53526700	-1.34068600	3.93906300
C	0.68223400	-1.07707600	2.87420900
C	0.18726800	-2.61541600	0.45162900
H	-3.90413200	-1.55649800	4.67763400
H	-6.99745600	-2.76726000	1.31136800
H	-7.20979200	-0.97133800	1.30893500
C	1.24594100	-2.22758400	3.43955600
C	0.83487100	0.15101800	3.54044800
C	0.98980800	-2.54852000	-0.69617500
C	-0.24686200	-3.86709900	0.91162500
C	1.95742700	-2.14997000	4.63902500
H	1.14440700	-3.18522200	2.94232200
C	1.53170100	0.22653500	4.74490900
C	1.38738700	-3.71434400	-1.35134500
H	1.29643100	-1.57453100	-1.06750600
C	0.15824400	-5.03375700	0.26286400
H	-0.90695200	-3.92434500	1.77174200
C	2.10031600	-0.92624200	5.29476900
H	2.40567300	-3.04755800	5.05501400
H	1.64677100	1.18479800	5.24274000
C	0.98094100	-4.95927800	-0.86588200
H	2.01339800	-3.65145600	-2.23642400
H	-0.17165600	-6.00038100	0.63315300
H	2.65901100	-0.86765700	6.22423500

H	1.29462600	-5.86882500	-1.37024200
H	0.40856300	1.04806400	3.09673600
C	1.41101000	2.77929100	-0.14283500
C	2.21123400	1.62950200	-0.07348800
C	3.09189500	1.22394300	1.09170000
Pd	0.06649900	1.03391700	0.20287600
C	3.59822700	-0.21303300	0.91232300
H	2.72315500	-0.83700100	0.72188300
H	4.21962100	-0.26321200	0.00794200
C	4.37838600	-0.76481200	2.10966600
H	5.24760500	-0.12933400	2.31153200
H	3.74020000	-0.70593700	2.99968100
C	4.83319300	-2.19457300	1.90393500
C	6.16564000	-2.56260400	2.12784100
C	3.93477200	-3.18900600	1.48730400
C	6.59015200	-3.88160600	1.94960300
H	6.87836100	-1.80500500	2.44521100
C	4.35300900	-4.50639300	1.30331200
H	2.89928800	-2.93482300	1.29677600
C	5.68449200	-4.86002600	1.53614400
H	7.62975100	-4.14230900	2.12986200
H	3.63470400	-5.25245900	0.97388100
H	6.01329400	-5.88577000	1.39336900
C	1.24828800	3.76461200	0.99109200
H	0.22937300	4.17120500	0.98749300
H	1.37884700	3.26017200	1.95482000
C	2.24464500	4.94867300	0.91749200
H	3.26445500	4.55441000	0.87774200
H	2.07355900	5.50109000	-0.01480700
C	2.09177800	5.87058600	2.10312100
C	2.60405400	5.49492600	3.35450500
C	1.39966400	7.08311400	1.99999700
C	2.43060600	6.31444800	4.46968600
H	3.14364800	4.55526300	3.44070700
C	1.22545000	7.90698600	3.11462100
H	0.99660800	7.38519600	1.03581700
C	1.74100400	7.52494300	4.35422600
H	2.83791000	6.01077900	5.43071700
H	0.68884000	8.84674300	3.01341300
H	1.60875300	8.16474300	5.22248200
H	1.17705100	3.17156000	-1.13150700
H	2.49934000	1.17348000	-1.02195500
C	6.02279600	3.39426400	0.95311300
C	5.62066600	3.38489800	2.30463200

H	6.85323200	3.91999300	0.50472100
H	6.06221100	3.90095700	3.14717300
N	4.23160300	2.14723600	1.26119800
H	2.56003600	1.30201200	2.03953700
N	4.53458900	2.62503300	2.48987400
C	5.10042500	2.58038100	0.31389600
H	4.99094800	2.29253200	-0.72110300
(Z)-(R)-3			
C	1.72058500	-0.97486600	-3.19344900
C	1.70186600	-1.46670900	-4.48749900
C	0.78698800	-0.63237300	-5.16475900
N	0.86159400	0.07678300	-3.15931500
H	2.26524100	-1.28187200	-2.31235600
H	2.26508700	-2.30090900	-4.87921300
H	0.47780800	-0.66987800	-6.20136800
N	0.27669700	0.30199200	-4.35726000
C	0.50648600	0.90688100	-2.00762800
H	1.05708900	0.47451800	-1.16530500
C	-0.99870100	0.79029100	-1.71005900
H	-1.21756200	1.41867500	-0.84245900
H	-1.56192000	1.19997200	-2.55436600
C	-1.45072200	-0.65081900	-1.42126400
H	-1.35246400	-1.25038400	-2.33283100
H	-0.78253600	-1.09368700	-0.67125100
C	-2.87385300	-0.68349700	-0.91727600
C	-3.14548000	-0.62967200	0.45670700
C	-3.95173300	-0.70386400	-1.81150300
C	-4.45952500	-0.59365600	0.92628900
H	-2.31918500	-0.61267900	1.16321800
C	-5.26737200	-0.66827200	-1.34671600
H	-3.75549400	-0.74821800	-2.88024700
C	-5.52594500	-0.61153100	0.02469800
H	-4.65040700	-0.55827200	1.99559500
H	-6.09080900	-0.68734700	-2.05542000
H	-6.54950300	-0.58595600	0.38753500
C	0.94309800	2.34011500	-2.22889200
H	1.10608400	2.61777600	-3.26687600
C	1.09922800	3.24595100	-1.25793600
H	1.39442300	4.25674200	-1.53906800
C	0.83177500	3.01916700	0.20389500
H	0.70826700	1.95243400	0.41697900
H	1.68325500	3.35961400	0.80778500
C	-0.44239700	3.76799400	0.67955300
H	-0.23808000	4.84557900	0.69634700
H	-1.23955600	3.60994000	-0.05498500

C	-0.90431600	3.28804200	2.03446500
C	-0.26446600	3.70531400	3.20908200
C	-1.95219400	2.36330500	2.13623400
C	-0.65876700	3.20906000	4.45256200
H	0.54721400	4.42673700	3.14784300
C	-2.34939300	1.86350400	3.37735600
H	-2.46529100	2.03269400	1.23707100
C	-1.70232100	2.28417300	4.54089100
H	-0.15361100	3.54672400	5.35343900
H	-3.16775000	1.15067800	3.43288200
H	-2.01056200	1.89915200	5.50880100