

*Supplementary Information*

DFT investigation of Cu(I)-catalyzed addition of 1,4-pentadiene to acetophenone:  
mechanism and selectivity for the synthesis of a chiral tertiary alcohol with a 1,3-  
diene unit

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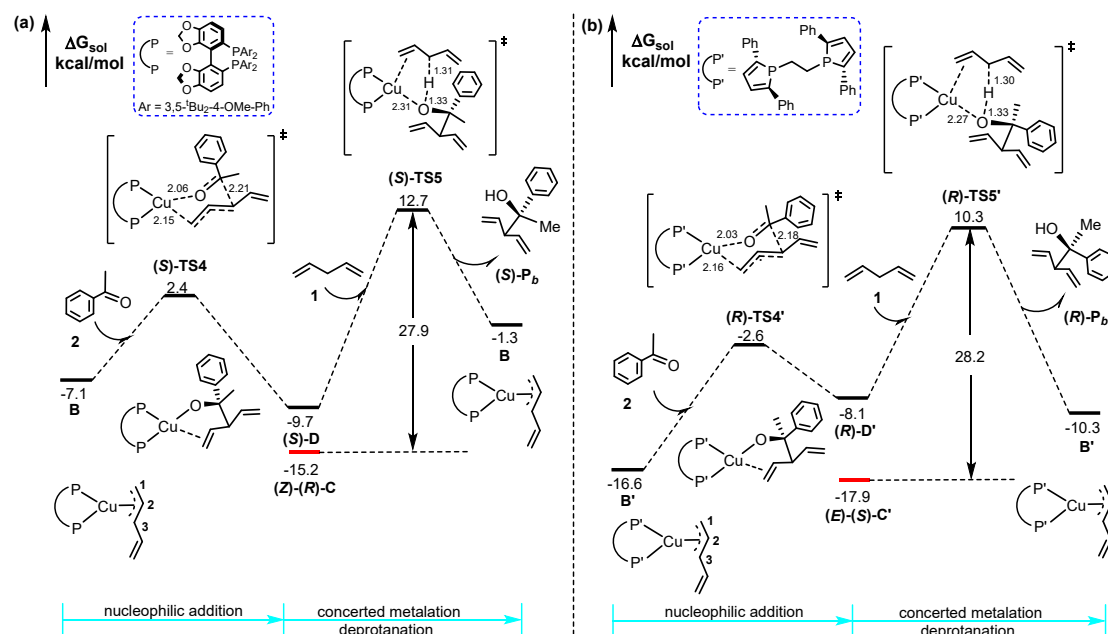
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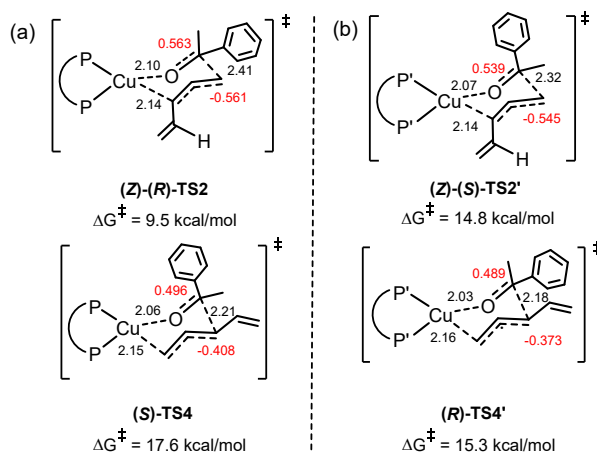
I. Formation of branched products ( <b>S</b> )- <b>P<sub>b</sub></b> and ( <b>R</b> )- <b>P<sub>b</sub></b> with the ligands ( <i>R</i> )-DTBM-SEGPHOS) and ( <i>R,R</i> )-Ph-BPE, respectively.....	S3
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I. Formation of branched products (**S**)-**P<sub>b</sub>** and (**R**)-**P<sub>b</sub>** with the ligands (*R*)-DTBM-SEGPPOS) and (*R,R*)-Ph-BPE, respectively



**Fig. S1.** Calculated Gibbs energy profiles for the formation of (a) (*S*)-type branched product (**S**)-**P<sub>b</sub>** with the (*R*)-DTBM-SEGPPOS ligand and (b) (*R*)-type branched product (**R**)-**P<sub>b</sub>** with the (*R,R*)-Ph-BPE ligand. Bond distances are in Å.

II. NBO analyses for (**S**)-**TS4** and (**R**)-**TS4'**



**Fig. S2** NBO analyses for (a) the regioselectivity-determining transition states (**Z**)-(**R**)-**TS2** and (**S**)-**TS4**, as well as (b) (**Z**)-(**S**)-**TS2'** and (**R**)-**TS4'**. Energy barriers associated

with these transition states are given in kcal mol<sup>-1</sup>, bond distances are in Å (black color), and electron charges are in *e* (red color).

### III. Calculated energies and imaginary frequencies

Stationary point	Thermal correction to Gibbs free energy at M06 (gas) /Lanl2dz/6-31G(d,p) (in a.u.) (1)	Single-point energy at M06 (SMD-N,N-Dimethylformamide) /SDD/6-311+G(d,p) (in a.u.) (2)	Gibbs free energies (G) (in a.u.) (3)=(1)+(2)	Imaginary frequencies (cm <sup>-1</sup> )
1,4-pentadiene	0.082563	-195.1857521	-195.10319	
acetophenone	0.10523	-384.7253913	-384.62016	
1,3,5-trimethylbenzene	0.149524	-350.0048127	-349.85529	
A	1.643751	-4709.779846	-4708.1361	
TS1	1.751219	-4904.938789	-4903.1876	-1262.64
B	1.578049	-4554.973289	-4553.3952	
A'	0.706405	-2546.16928	-2545.4629	
TS1'	0.809339	-2741.329967	-2740.5206	-1141.61
B'	0.638406	-2391.375315	-2390.7369	
(Z)-(R)-TS2	1.706872	-4939.710242	-4938.0034	-185.25
(E)-(R)-TS2	1.710468	-4939.706518	-4937.996	-213.49
(Z)-(R)-C	1.715543	-4939.733988	-4938.0184	
(E)-(R)-C	1.713454	-4939.731048	-4938.0176	
(Z)-(R)-TS3	1.815053	-5134.899636	-5133.0846	-1557.94
(E)-(R)-TS3	1.818883	-5134.901594	-5133.0827	-1524.80
(Z)-(R)-P <sub>1</sub>	0.215713	-579.9288337	-579.71312	
(E)-(R)-P <sub>1</sub>	0.213536	-579.9302665	-579.71673	
(Z)-(S)-TS2	1.711333	-4939.711488	-4938.0002	-189.21

<b>(E)-(S)-TS2</b>	1.70895	-4939.704368	-4937.9954	-241.24
<b>(Z)-(S)-C</b>	1.717562	-4939.731061	-4938.0135	
<b>(E)-(S)-C</b>	1.720558	-4939.727121	-4938.0066	
<b>(Z)-(S)-TS3</b>	1.818623	-5134.900071	-5133.0814	-1528.06
<b>(E)-(S)-TS3</b>	1.821816	-5134.902608	-5133.0808	-1534.86
<b>(Z)-(S)-P<sub>l</sub></b>	0.216135	-579.9305953	-579.71446	
<b>(E)-(S)-P<sub>l</sub></b>	0.214027	-579.9312622	-579.71724	
<b>(Z)-(S)-TS2'</b>	0.770109	-2776.095858	-2775.3257	-247.64
<b>(E)-(S)-TS2'</b>	0.771234	-2776.095368	-2775.3241	-170.59
<b>(Z)-(S)-C'</b>	0.773792	-2776.122435	-2775.3486	
<b>(E)-(S)-C'</b>	0.773893	-2776.123241	-2775.3493	
<b>(Z)-(S)-TS3'</b>	0.877526	-2971.294132	-2970.4166	-1567.91
<b>(E)-(S)-TS3'</b>	0.878669	-2971.294874	-2970.4162	-1521.85
<b>(Z)-(R)-TS2'</b>	0.770683	-2776.094303	-2775.3236	-287.10
<b>(E)-(R)-TS2'</b>	0.771537	-2776.093598	-2775.3221	-195.92
<b>(Z)-(R)-C'</b>	0.776345	-2776.125628	-2775.3493	
<b>(E)-(R)-C'</b>	0.774571	-2776.120021	-2775.3455	
<b>(Z)-(R)-TS3'</b>	0.879137	-2971.29303	-2970.4139	-1502.14
<b>(E)-(R)-TS3'</b>	0.878349	-2970.4148	-2970.4148	-1465.92
<b>(R)-TS4</b>	1.712708	-4939.709733	-4937.997	-305.88
<b>(R)-D</b>	1.714023	-4939.721706	-4938.0077	
<b>(R)-TS5</b>	1.819424	-5134.885907	-5133.0665	-1583.03
<b>(R)-P<sub>b</sub></b>	0.214505	-579.9185107	-579.70401	
<b>(S)-TS4</b>	1.714997	-4939.705526	-4937.9905	-308.56
<b>(S)-D</b>	1.712741	-4939.722464	-4938.0097	
<b>(S)-TS5</b>	1.819414	-5134.889728	-5133.0703	-1572.15
<b>(S)-P<sub>b</sub></b>	0.21389	-579.9181915	-579.7043	
<b>(S)-TS4'</b>	0.77335	-2776.092779	-2775.3194	-327.09
<b>(S)-D'</b>	0.775196	-2776.108221	-2775.333	
<b>(S)-TS5'</b>	0.88091	-2971.277347	-2970.3964	-1512.59
<b>(R)-TS4'</b>	0.7733	-2776.098152	-2775.3249	-324.04
<b>(R)-D'</b>	0.775499	-2776.109158	-2775.3337	

<b>(R)-TS5'</b>	0.878218	-2971.279454	-2970.4012	-1539.79
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#### IV. Cartesian coordinates of all the structures

##### 1,4-pentadiene

C	-0.00000800	-0.26960900	0.68067500
C	-1.24370100	-0.40756500	-0.14600100
H	-0.00006800	0.69744900	1.20559600
H	-0.00019500	-1.05275500	1.45952000
C	-2.21513300	0.49718000	-0.21441300
H	-1.32531400	-1.32846600	-0.73133600
H	-3.09928100	0.34750300	-0.83096900
H	-2.16505100	1.42953300	0.34944000
C	1.24384900	-0.40766000	-0.14569400
H	1.32588900	-1.32887200	-0.73049400
C	2.21501500	0.49733300	-0.21452100
H	2.16462100	1.42995500	0.34886600
H	3.09926800	0.34757500	-0.83090200

##### acetophenone

C	1.81859500	1.27104000	-0.00001900
C	0.43048100	1.19361700	-0.00004100
C	-0.20643500	-0.05101300	-0.00002300
C	0.56874000	-1.21461500	0.00002800
C	1.95322000	-1.13836600	0.00002600
C	2.58019400	0.10654100	0.00000700
H	2.30731900	2.24385400	-0.00001600
H	-0.15529000	2.11185000	-0.00007500
H	0.05234300	-2.17243700	0.00005100
H	2.55007600	-2.04882500	0.00004800
H	3.66723900	0.16982100	0.00002800
C	-1.69100900	-0.20201900	-0.00001300
O	-2.20527100	-1.30519800	-0.00005300
C	-2.53985800	1.04466500	0.00005800
H	-3.59323000	0.75237800	0.00015400
H	-2.33483900	1.66292400	0.88410700
H	-2.33501100	1.66292200	-0.88401200

##### 1,3,5-trimethylbenzene

C	-1.37752500	0.13602500	-0.01404100
C	-0.57483300	1.28122600	-0.00511500
C	0.80677500	1.12519100	0.00465200
C	1.39740500	-0.14262200	0.00653400
C	0.57125900	-1.26108500	0.00179100
C	-0.82188300	-1.13884400	-0.00716000

H	-2.46455700	0.24669500	-0.02544900
H	1.44597200	2.01146300	0.00853400
H	1.01927400	-2.25774600	0.00288500
C	2.89111100	-0.28168500	-0.00308800
H	3.31818200	0.04526100	-0.96170900
H	3.35807300	0.33261700	0.77850200
H	3.20011600	-1.32175500	0.15751100
C	-1.68984000	-2.36243200	0.00624500
H	-1.36146300	-3.09861300	-0.73958200
H	-1.65896800	-2.86432300	0.98377600
H	-2.73782000	-2.11534700	-0.20302600
C	-1.20184000	2.64403900	0.00482300
H	-1.95432300	2.74699500	-0.78860100
H	-1.71453300	2.84251600	0.95661700
H	-0.45373000	3.43336600	-0.13730800

**A**

P	1.77387500	0.07928200	-0.20211800
C	1.17850500	1.53482600	-1.15108700
C	2.98548900	-0.76492900	-1.27896900
C	2.82157200	0.87073200	1.06663600
C	0.20980500	2.36114100	-0.51297800
C	1.59686100	1.80314400	-2.45303700
C	2.54328800	-1.35938700	-2.46446200
C	4.30295900	-0.95036600	-0.89133000
C	3.68446800	1.90368300	0.72632100
C	2.75617500	0.44523900	2.39112900
C	-0.20365700	2.20485500	0.91050400
C	-0.27597200	3.40607300	-1.26903000
C	1.08638500	2.87851800	-3.19544800
H	2.34652800	1.16076600	-2.91404000
C	3.37631600	-2.16167500	-3.23821100
H	1.51341300	-1.18453800	-2.77754900
C	5.19455300	-1.75821900	-1.60948100
H	4.64956100	-0.46514400	0.01804300
C	4.56327600	2.47956300	1.64809400
H	3.67941500	2.26398400	-0.30268300
C	3.61002500	0.96463000	3.36433400
H	2.02474700	-0.31961200	2.64967100
C	-1.13985100	1.25084400	1.40320300
C	0.36372900	3.03214500	1.85891400
C	0.14005100	3.65599900	-2.57378900
H	1.42057600	3.08858400	-4.20880100
C	4.67389300	-2.42744500	-2.73021100

C	4.58071300	1.90252500	2.93554000
P	-1.79729600	-0.01035800	0.24659500
C	-1.39001900	1.15005000	2.77253300
C	0.08103700	2.93905600	3.21776200
C	-3.22654800	-0.77564300	1.09805400
C	-2.57910200	0.97747000	-1.08871700
C	-0.78677700	1.99772600	3.71349600
H	-2.08382600	0.38981300	3.12781700
C	-4.25054400	-0.07143800	1.73868900
C	-3.33792200	-2.15410200	0.97657800
C	-3.49650100	1.99146500	-0.84956900
C	-2.24401600	0.67424400	-2.40460600
H	-0.99693100	1.92001000	4.77753800
C	-5.32954600	-0.72113100	2.32776700
H	-4.18337700	1.01120800	1.79943000
C	-4.43382000	-2.87117700	1.47955400
H	-2.53135400	-2.68837800	0.47400800
C	-4.18356500	2.64381000	-1.87865900
H	-3.69066000	2.28097200	0.18009600
C	-2.85118200	1.30959700	-3.48710800
H	-1.47357900	-0.07720700	-2.56862700
C	-5.36606800	-2.13782700	2.23583400
C	-3.89270900	2.22412900	-3.19679000
C	-1.54954200	4.98939600	-2.12056100
H	-2.48472400	4.54000100	-2.50681500
H	-1.66035500	6.06489900	-1.94863300
O	-1.19211300	4.34868700	-0.90500900
O	-0.50388500	4.75864500	-3.04952200
H	1.75884300	5.49608400	3.03128800
C	1.70761100	4.40505000	2.95080700
H	2.69441800	3.94057800	3.13392100
O	0.77291600	3.90271000	3.89105300
O	1.25389800	4.04488100	1.65554500
O	5.42150500	-3.37882400	-3.38815300
O	5.56373200	2.25702100	3.83303400
O	-4.59560700	2.73319500	-4.26733700
O	-6.38337300	-2.77638400	2.90995900
C	6.77747700	1.56845300	3.60831900
H	7.45439800	1.84087500	4.42512500
H	6.62520800	0.47828800	3.60928500
H	7.24033500	1.85064900	2.64997200
C	3.42528200	0.60200800	4.84568800
C	5.38637600	3.69015500	1.16279400
C	6.64832800	-1.81179300	-1.10038500



C	5.39157300	-4.64305300	-2.75414000
H	5.83267800	-5.36191000	-3.45349100
H	5.97640200	-4.64847500	-1.82240600
H	4.36211200	-4.94880300	-2.51711300
C	2.92837400	-2.65007100	-4.62485100
C	-5.22319900	3.70976100	-1.47382000
C	-2.34554000	1.05424300	-4.91610400
C	-5.84569900	2.12479300	-4.52048000
H	-6.66271900	2.64304800	-3.99716800
H	-6.03500300	2.19147600	-5.59824000
H	-5.84612700	1.06716900	-4.21989000
C	-6.47249100	0.08750000	2.96406500
C	-4.51295500	-4.36921100	1.12425400
C	-5.97646200	-3.39367900	4.11385000
H	-6.88797500	-3.65795100	4.66166500
H	-5.39601200	-4.30781800	3.93064600
H	-5.36918400	-2.71259500	4.72848100
C	-0.24267200	-6.21101400	1.05132700
C	-0.41499700	-5.69185800	-0.23016700
C	-0.28911800	-4.32143800	-0.48220600
C	-0.00289200	-3.41136900	0.55242000
C	0.17394000	-3.94688300	1.84162200
C	0.06302500	-5.31909600	2.07946500
H	-0.65684800	-6.37385100	-1.05187400
H	0.20266400	-5.70766900	3.09325800
C	0.50538200	-3.02177400	2.98078400
H	0.50266300	-3.52987800	3.95590700
H	1.50440200	-2.57752300	2.83813100
H	-0.20592700	-2.17993000	3.03355400
C	-0.43650200	-7.67282500	1.32905800
H	0.17568800	-8.00868200	2.17673800
H	-1.48439100	-7.90056200	1.58146200
H	-0.17547500	-8.28998400	0.45892200
C	-0.43707100	-3.81322600	-1.89225400
H	-0.81658500	-4.58189400	-2.58162400
H	-1.12082900	-2.94686100	-1.93909400
H	0.53428900	-3.46445000	-2.27944400
Cu	0.09653000	-1.48514300	0.20569100
C	6.72123800	-2.66000300	0.17542400
H	7.74920500	-2.66975500	0.56685000
H	6.06317000	-2.26099700	0.95982900
H	6.42204300	-3.70082700	-0.00648400
C	7.67182300	-2.32950900	-2.11768000
H	8.68074800	-2.15491500	-1.71750100

H	7.58800300	-3.40010700	-2.32055600
H	7.59123200	-1.79956400	-3.07517400
C	7.10696500	-0.38390200	-0.75002400
H	7.02699400	0.28155800	-1.62113300
H	6.53523600	0.06724000	0.07162400
H	8.15939700	-0.40307200	-0.43360400
C	1.55435200	-2.08634000	-4.99569400
H	0.75372200	-2.46472500	-4.34307600
H	1.53720600	-0.98715600	-4.96101100
H	1.30746700	-2.38684200	-6.02317200
C	2.82901400	-4.17728700	-4.72663300
H	2.35566500	-4.45009500	-5.68083700
H	3.81173700	-4.65796800	-4.70092000
H	2.21017600	-4.59389400	-3.91888700
C	3.92207200	-2.12888700	-5.67382800
H	4.93519500	-2.50381700	-5.49503100
H	3.60802600	-2.45089200	-6.67749700
H	3.95087600	-1.02982600	-5.66727500
C	6.41496000	3.23453500	0.12061000
H	5.93250900	2.74059800	-0.73429100
H	6.97560900	4.09945200	-0.26244100
H	7.14210900	2.52731500	0.54498300
C	6.10615300	4.48157800	2.25923100
H	6.95323300	3.94858700	2.70059600
H	6.50231300	5.40617400	1.81545800
H	5.42673700	4.76337400	3.07358000
C	4.43107300	4.69515300	0.49087700
H	3.85525100	4.27306100	-0.34112100
H	3.70763500	5.09495600	1.21361900
H	5.01090000	5.54043300	0.09480200
C	4.61918300	-0.16852000	5.42216200
H	5.50852500	0.46101600	5.52266700
H	4.36679900	-0.54041300	6.42557700
H	4.86912200	-1.03987700	4.79935500
C	3.20881600	1.89279100	5.64885800
H	2.31673600	2.42929500	5.29294100
H	3.05149000	1.64924200	6.70975000
H	4.07165400	2.56525800	5.57786000
C	2.18614200	-0.27445000	5.05321900
H	1.27221300	0.19336000	4.65685400
H	2.29260900	-1.26590700	4.59007600
H	2.03897100	-0.43255300	6.13018400
C	-3.54893800	-5.17672400	2.00173900
H	-3.53220200	-6.22677600	1.67114800

H	-2.52206900	-4.79269700	1.93031900
H	-3.83844300	-5.16649400	3.06111100
C	-4.07167100	-4.55794200	-0.34106200
H	-4.65489900	-3.91711100	-1.01740700
H	-3.00432500	-4.36070700	-0.49695000
H	-4.23845500	-5.60370300	-0.63477500
C	-5.92513000	-4.96245100	1.20338900
H	-6.31110100	-5.07028300	2.22039200
H	-6.64482800	-4.35596400	0.63713100
H	-5.90608600	-5.96652500	0.75702500
C	-6.68606000	-0.24313700	4.44748600
H	-7.38120800	0.48454300	4.89036600
H	-7.12034300	-1.23548200	4.59293200
H	-5.74186500	-0.18344600	5.00821300
C	-6.20599500	1.59426200	2.89474700
H	-5.30630900	1.88536600	3.45670100
H	-6.10004600	1.95426100	1.86173700
H	-7.05785100	2.12892700	3.33548500
C	-7.76667700	-0.18574000	2.18523100
H	-8.03699500	-1.24705800	2.21658800
H	-8.59643600	0.39531600	2.61458600
H	-7.65428300	0.11213700	1.13275000
C	-5.46401000	4.80491500	-2.52104700
H	-5.88251000	4.44126700	-3.46045900
H	-6.16574200	5.54202700	-2.10637000
H	-4.53500000	5.33901200	-2.76590800
C	-4.77140000	4.44981600	-0.20101200
H	-4.79216400	3.81978800	0.69716700
H	-3.75476500	4.85510300	-0.29823100
H	-5.45607100	5.28660000	-0.00893200
C	-6.54805700	3.00611900	-1.14443800
H	-6.98732400	2.50761500	-2.01725900
H	-6.39748900	2.23618700	-0.37343100
H	-7.28288700	3.73138100	-0.76503000
C	-1.90672700	2.38167900	-5.55099700
H	-1.52827300	2.19961900	-6.56779700
H	-2.73567000	3.09323400	-5.61725900
H	-1.09777700	2.84908500	-4.97059100
C	-1.12367800	0.12963100	-4.91738000
H	-0.29638800	0.53328100	-4.31387900
H	-1.35982500	-0.88027900	-4.54984600
H	-0.75916600	0.02284800	-5.94836600
C	-3.40455700	0.38533900	-5.80095500
H	-4.21971400	1.06775500	-6.05554100

H	-2.94573600	0.05972100	-6.74554500
H	-3.82788900	-0.50380500	-5.31189600

**TS1**

P	1.73225800	0.33458600	0.22970200
C	0.97747400	0.91568200	1.81206600
C	2.92205400	1.63057700	-0.28444700
C	2.89406100	-0.93222000	0.89951000
C	0.02375700	0.04543400	2.41152200
C	1.30135800	2.12788000	2.42097300
C	2.54134300	2.96167200	-0.48084600
C	4.18590000	1.24419400	-0.70850800
C	3.62994700	-0.61185100	2.04012600
C	3.10075400	-2.15913300	0.28346300
C	-0.23428400	-1.32217300	1.88975400
C	-0.56471100	0.49492900	3.57290300
C	0.69748300	2.55322800	3.61461400
H	2.06093300	2.76672000	1.97212700
C	3.35104400	3.87127200	-1.15816000
H	1.56783200	3.28605200	-0.11938800
C	5.05207800	2.09899400	-1.39808800
H	4.50916000	0.22228300	-0.51908600
C	4.63705000	-1.43523400	2.52465900
H	3.40265000	0.32095400	2.54979000
C	4.10857100	-3.04382300	0.71198600
H	2.45569000	-2.42721600	-0.55509400
C	-0.97153300	-1.62824500	0.71352400
C	0.39586700	-2.38814100	2.50231600
C	-0.24742800	1.71583800	4.15720700
H	0.96131400	3.49678000	4.08675300
C	4.55960700	3.37878200	-1.70969400
C	4.92947400	-2.59816400	1.76985000
P	-1.73397100	-0.26798200	-0.24201100
C	-0.93153700	-2.91729100	0.17396100
C	0.36138100	-3.68020600	1.99472500
C	-3.30669400	-0.89803500	-0.95233300
C	-2.55571700	0.79578500	1.01124900
C	-0.28121800	-3.97731500	0.81694200
H	-1.37733000	-3.10483000	-0.80296800
C	-3.87596000	-2.15695200	-0.79510600
C	-4.05432200	0.09021300	-1.57760300
C	-3.57744700	0.26238800	1.78076400
C	-2.31264000	2.16291100	1.06324400
H	-0.26101200	-4.97804700	0.39152100

C	-5.10257800	-2.48506200	-1.37452600
H	-3.35372100	-2.89989100	-0.20355300
C	-5.32387900	-0.13711400	-2.10495900
H	-3.63475200	1.09739300	-1.63082000
C	-4.45126600	1.05223800	2.52704200
H	-3.73212600	-0.81430400	1.74968400
C	-3.11057100	3.01733500	1.82666900
H	-1.47450900	2.55409700	0.48828600
C	-5.77046700	-1.47360800	-2.10170000
C	-4.23765200	2.44710400	2.47007100
C	-1.97077200	0.86373500	5.22908600
H	-2.90785800	1.30258900	4.83931700
H	-2.11524100	0.42165300	6.21997100
O	-1.51372500	-0.13117400	4.32579000
O	-0.97681100	1.87304600	5.29755200
H	1.80336700	-4.02229700	4.67845500
C	1.81431400	-3.62861800	3.65663300
H	2.84763800	-3.51738300	3.27903600
O	1.09145400	-4.50318300	2.80250600
O	1.16548400	-2.36600600	3.62907800
O	5.25353000	4.20021300	-2.56902700
O	6.05117400	-3.30641500	2.13907000
O	-5.12916300	3.31324900	3.06563700
O	-6.88665200	-1.82725900	-2.82772700
C	7.17290700	-3.05803600	1.31723600
H	8.03662800	-3.51963500	1.80836500
H	7.05509200	-3.50019500	0.31771500
H	7.35555300	-1.97862100	1.20013300
C	4.22283400	-4.41961100	0.02272000
C	5.32868600	-1.11460300	3.85833100
C	6.45791800	1.54118600	-1.69121900
C	5.04324700	3.87491500	-3.93001500
H	5.58579200	4.62002100	-4.52168300
H	5.42703800	2.87311100	-4.17704200
H	3.97528100	3.90628300	-4.19569200
C	2.96473900	5.35661700	-1.23641800
C	-5.58397200	0.31067300	3.26105900
C	-2.72080600	4.49379100	2.00273500
C	-6.26076500	3.61618700	2.27453000
H	-7.02466800	2.82683000	2.33277200
H	-6.69155400	4.54457700	2.66654000
H	-5.98643400	3.76152900	1.21894400
C	-5.71682700	-3.87376200	-1.14398800
C	-6.09797900	1.10671300	-2.57489300

C	-6.60629600	-1.95567800	-4.20721700
H	-7.53768500	-2.25935800	-4.69738400
H	-6.26012500	-1.00698300	-4.64464900
H	-5.83179900	-2.71713500	-4.38798700
C	0.09930200	-3.85739900	-3.29525200
C	1.33961100	-3.22937700	-3.15208800
C	1.44753000	-1.83766700	-3.14824100
C	0.30786100	-1.01060000	-3.29204600
C	-0.91234000	-1.66423200	-3.58752500
C	-1.01690500	-3.05757900	-3.54127100
H	2.23589700	-3.84892200	-3.03751300
H	-1.99194200	-3.53195500	-3.70046000
C	-2.09331500	-0.85373600	-4.04022300
H	-1.98825300	-0.61164700	-5.10990200
H	-3.04940600	-1.38441000	-3.91548400
H	-2.15095800	0.10445400	-3.50645100
C	-0.01453700	-5.35086100	-3.21306100
H	-1.06370600	-5.67482000	-3.21891900
H	0.48843400	-5.84736000	-4.05549500
H	0.45276700	-5.73987900	-2.29568900
C	2.80419100	-1.18966900	-3.07970400
H	3.54617100	-1.79933800	-2.54498300
H	3.19727200	-1.01571500	-4.09414000
H	2.75597200	-0.20766500	-2.58745400
Cu	0.08135400	0.27551400	-1.65249900
C	0.91326200	1.44805100	-4.61080400
C	2.15674900	1.43348300	-5.39441300
C	2.26819300	1.26699700	-6.71592800
H	3.07601900	1.52272500	-4.79796800
H	3.23601200	1.21522100	-7.21044400
H	1.38721800	1.17188000	-7.35204100
C	0.91611800	2.19356800	-3.37470800
H	1.90058700	2.44308600	-2.95934700
C	-0.16537100	2.36802200	-2.55808200
H	-1.18221600	2.22743800	-2.93498900
H	-0.07710100	2.93970500	-1.63181300
H	0.69087200	0.29383100	-4.07788700
H	0.00018800	1.55568900	-5.21436200
C	-5.88559900	-4.66250100	-2.44908600
H	-6.16088600	-5.70202800	-2.21970900
H	-6.67515000	-4.24836100	-3.08291100
H	-4.94620700	-4.68606700	-3.02166500
C	-7.08005200	-3.71572500	-0.45762400
H	-7.76988600	-3.11943100	-1.06439500

H	-7.53446100	-4.70330200	-0.28954000
H	-6.96522200	-3.22804000	0.52166000
C	-4.84081600	-4.72925500	-0.22337200
H	-3.85368000	-4.93921700	-0.66279300
H	-4.68890200	-4.26217300	0.76017800
H	-5.33597400	-5.69482800	-0.05401600
C	-5.39121400	1.73976500	-3.77973100
H	-5.92970700	2.64182400	-4.10446300
H	-4.35815900	2.03275900	-3.54729100
H	-5.34993900	1.04659700	-4.63227200
C	-7.57080700	0.87822400	-2.93040400
H	-8.04581500	1.85874400	-3.07887300
H	-7.71436000	0.31097000	-3.85557000
H	-8.10873200	0.36026600	-2.12736900
C	-6.11022100	2.11487400	-1.40664600
H	-6.63730400	1.68718600	-0.54070100
H	-5.10856900	2.41187000	-1.06588100
H	-6.64168600	3.02881800	-1.71018200
C	2.81521400	-4.99969100	-0.19713900
H	2.30568300	-5.15552200	0.76456200
H	2.17525700	-4.37393500	-0.83116000
H	2.90307400	-5.97623900	-0.69562200
C	4.89625100	-4.27545900	-1.34763600
H	4.98872500	-5.25995300	-1.82929700
H	4.30916700	-3.63232400	-2.01636000
H	5.90309600	-3.84253900	-1.27741300
C	4.96416300	-5.48179500	0.84662800
H	4.79974400	-6.46213600	0.37762600
H	6.04496900	-5.32887000	0.90470300
H	4.57581000	-5.53264400	1.87319100
C	6.82803000	-0.83436200	3.69952100
H	7.23249400	-0.44592700	4.64534900
H	7.39376000	-1.73648200	3.44725200
H	7.00985300	-0.07436900	2.92480300
C	4.70712800	0.11872900	4.52047700
H	4.88690100	1.03649900	3.94278400
H	3.62250400	0.00701200	4.66608300
H	5.16248700	0.26074700	5.50990700
C	5.12388800	-2.28837600	4.82626900
H	5.64557200	-2.08849100	5.77371700
H	4.05523900	-2.40848700	5.05834500
H	5.50729200	-3.22954500	4.41615400
C	7.04795800	1.01866400	-0.36672200
H	7.14638300	1.83404000	0.36368100

H	6.44448700	0.22676500	0.09662600
H	8.04978900	0.60257800	-0.54744300
C	6.35963500	0.37194400	-2.68042200
H	7.36333600	-0.01809100	-2.90459900
H	5.76072700	-0.45960000	-2.28050800
H	5.89898900	0.68219600	-3.62952500
C	7.47812500	2.55467100	-2.22049500
H	7.28377600	2.87184100	-3.24946400
H	7.52683400	3.45199500	-1.59248700
H	8.47074100	2.08197400	-2.21460800
C	4.10067000	6.19655000	-0.63499300
H	5.03840600	6.06153300	-1.18386900
H	3.83365800	7.26300800	-0.66695300
H	4.27061500	5.92385300	0.41641900
C	1.70675900	5.65068900	-0.41453400
H	0.81366200	5.15643000	-0.82455600
H	1.81781500	5.35115600	0.63815700
H	1.51328700	6.73180200	-0.42919400
C	2.68117500	5.82404300	-2.66940500
H	2.26398400	6.84116100	-2.64682700
H	3.58976600	5.85792600	-3.27864300
H	1.94460200	5.17306300	-3.16291800
C	-1.39652100	4.81181800	1.29855600
H	-0.56948900	4.17931800	1.65467900
H	-1.47165900	4.70694000	0.20567100
H	-1.12349000	5.85591000	1.50543800
C	-3.76271800	5.46238700	1.42851100
H	-4.02920000	5.19235000	0.39554100
H	-4.67532200	5.49772800	2.03021100
H	-3.34747100	6.48010500	1.40830600
C	-2.51820000	4.77733300	3.49822500
H	-3.43347900	4.59694000	4.07248800
H	-1.72062800	4.14186500	3.90999300
H	-2.22318400	5.82701600	3.64415600
C	-6.18016000	1.06714000	4.45373500
H	-6.70410900	1.98536700	4.18155100
H	-6.90063600	0.41390400	4.96536000
H	-5.40326800	1.34008500	5.18175400
C	-6.68514800	-0.03215900	2.24527300
H	-6.26537900	-0.56675200	1.37803500
H	-7.44787000	-0.67528500	2.70949700
H	-7.19226800	0.86367000	1.86349800
C	-5.06066200	-1.02438300	3.82789200
H	-4.86191000	-1.77158300	3.04853400



H	-4.13532100	-0.89485500	4.40641100
H	-5.82058900	-1.45989200	4.49046000
<b>B</b>			
P	1.79433400	0.28162600	0.12140400
C	1.02579900	0.46791800	1.77342600
C	2.97318200	1.65846800	-0.13791600
C	2.95258400	-1.11306400	0.35975100
C	0.04614000	-0.50570500	2.12911700
C	1.25325000	1.58352000	2.57501600
C	2.50808300	2.96723300	-0.29956200
C	4.29903600	1.38819100	-0.43866000
C	3.70928700	-1.21125200	1.53005700
C	3.21563600	-1.97246000	-0.69574000
C	-0.13670700	-1.77646500	1.37078700
C	-0.67708600	-0.23313100	3.26913600
C	0.51798200	1.81877900	3.74688900
H	2.01263700	2.30545500	2.27401700
C	3.31283500	3.97037600	-0.83290700
H	1.47026000	3.18321800	-0.04887400
C	5.16769900	2.34588000	-0.97232800
H	4.67722600	0.38256300	-0.28060900
C	4.81575400	-2.05283700	1.61657600
H	3.43147800	-0.58316400	2.37485800
C	4.29314700	-2.87298400	-0.66410800
H	2.57046300	-1.92825200	-1.57662400
C	-0.91481500	-1.93141700	0.19049400
C	0.57566500	-2.89384100	1.76338400
C	-0.45598700	0.89920100	4.05031600
H	0.69533800	2.68832900	4.37541800
C	4.61440800	3.60292900	-1.26169100
C	5.15122500	-2.78861800	0.45015200
P	-1.66814800	-0.46440600	-0.58919300
C	-0.87820100	-3.12527700	-0.53438800
C	0.56561300	-4.09108300	1.05482400
C	-3.14695600	-1.02784600	-1.51482800
C	-2.60556700	0.43513900	0.70859400
C	-0.14509500	-4.23927600	-0.11022500
H	-1.40967000	-3.18903800	-1.48243900
C	-3.86011200	-2.20177600	-1.27883900
C	-3.76871900	0.00363700	-2.20586500
C	-3.70729100	-0.14489600	1.31831200
C	-2.32915200	1.77568200	0.94308900
H	-0.11844200	-5.16304600	-0.68237900

C	-5.13377600	-2.40623700	-1.80879500
H	-3.41355500	-2.96442200	-0.64831300
C	-5.09215000	-0.07744400	-2.64195400
H	-3.22517100	0.94398100	-2.31849900
C	-4.61572500	0.58807700	2.08352700
H	-3.89199000	-1.20277100	1.14511800
C	-3.16348600	2.56668900	1.73401400
H	-1.44229600	2.19562700	0.46944700
C	-5.70806900	-1.34157800	-2.54368100
C	-4.35217200	1.97059900	2.22196900
C	-2.27690200	-0.09469800	4.77523100
H	-3.15489700	0.39881100	4.31611100
H	-2.55222300	-0.66234800	5.66944800
O	-1.68550400	-0.96621300	3.82236300
O	-1.31260600	0.88847900	5.11069400
H	2.25251600	-4.76903800	3.53317000
C	2.12444000	-4.22079900	2.59420700
H	3.09719900	-3.96894700	2.13259100
O	1.36527500	-4.99788900	1.68437200
O	1.40314900	-3.02261000	2.84162700
O	5.32904100	4.52238600	-1.99773400
O	6.36549300	-3.43721500	0.44577800
O	-5.24208600	2.79219300	2.87956700
O	-6.91889200	-1.56601100	-3.15877300
C	7.35288300	-2.75840500	-0.30385800
H	8.29421000	-3.29758100	-0.15180200
H	7.11892600	-2.74095900	-1.37892900
H	7.47148800	-1.71731500	0.03721000
C	4.40723000	-3.87504400	-1.82777000
C	5.60732500	-2.18248200	2.93099500
C	6.63017900	1.89784000	-1.14973100
C	5.28510700	4.25623100	-3.38591800
H	5.78144100	5.09415600	-3.88771000
H	5.81045400	3.32413000	-3.64420000
H	4.24912400	4.17532900	-3.74774500
C	2.81074600	5.42060700	-0.90083900
C	-5.84620100	-0.16936800	2.61772500
C	-2.74853300	4.00233900	2.08964600
C	-6.32882800	3.25892500	2.10726800
H	-7.16388200	2.54382100	2.09998600
H	-6.68025200	4.19007200	2.56665600
H	-6.02925000	3.46296400	1.06875100
C	-5.89820300	-3.70487000	-1.50712600
C	-5.76480600	1.25152700	-3.03460400

C	-6.80651600	-1.72760400	-4.55801200
H	-7.81349900	-1.93299000	-4.93683900
H	-6.41701700	-0.82302700	-5.04831800
H	-6.14273700	-2.56787900	-4.81127700
Cu	0.11019100	0.63057800	-1.46174800
C	0.61036600	0.17105800	-3.71460500
C	1.65299800	-0.77074000	-4.02063000
C	1.51345800	-1.99271900	-4.57328000
H	2.66649800	-0.42745000	-3.76104700
H	2.36940900	-2.62913600	-4.78979300
H	0.53157600	-2.37679800	-4.85383900
C	0.88122800	1.45607500	-3.21838300
H	1.94241100	1.69523100	-3.05631100
C	-0.05570900	2.38849300	-2.72154900
H	-1.09695400	2.33437700	-3.05102000
H	0.29180800	3.37272200	-2.40841400
H	-0.41647600	-0.08051400	-4.00531500
C	-6.22989300	-4.48616500	-2.78537700
H	-6.60400500	-5.48577300	-2.52174600
H	-7.00698400	-3.99341000	-3.37694600
H	-5.33666200	-4.61926100	-3.41255400
C	-7.19642500	-3.38378800	-0.75355400
H	-7.83875200	-2.70157400	-1.32044700
H	-7.75844900	-4.31102200	-0.56793700
H	-6.97931900	-2.92604000	0.22322100
C	-5.08104100	-4.64149800	-0.61245600
H	-4.14646200	-4.96883700	-1.09064200
H	-4.83018200	-4.18135500	0.35425700
H	-5.67480100	-5.54006400	-0.39810800
C	-5.14721500	1.81500200	-4.31806700
H	-5.58082800	2.79949300	-4.54559400
H	-4.05962400	1.94113700	-4.23016600
H	-5.33648200	1.16001600	-5.17999400
C	-7.28742500	1.19389400	-3.19229800
H	-7.66232900	2.22103700	-3.30636800
H	-7.61734300	0.63409400	-4.07242900
H	-7.76927100	0.75445700	-2.30948600
C	-5.51125500	2.24211700	-1.87646400
H	-5.89841600	1.83338000	-0.92963400
H	-4.44888400	2.47229000	-1.72370800
H	-6.02702300	3.19209600	-2.07869700
C	3.01511700	-4.49742900	-2.04843600
H	2.65137200	-4.96661500	-1.12157100
H	2.26559200	-3.77074500	-2.38756800

H	3.08135100	-5.27471000	-2.82285500
C	4.82781700	-3.14922600	-3.11113400
H	4.81354100	-3.84581700	-3.96253100
H	4.14556700	-2.32065900	-3.34506200
H	5.84408500	-2.73708400	-3.03583700
C	5.35397300	-5.05361600	-1.57699200
H	5.22273600	-5.78284700	-2.38893000
H	6.41189500	-4.77656600	-1.56110400
H	5.12474300	-5.56079500	-0.63075300
C	7.01694400	-1.58852400	2.81879900
H	7.48722100	-1.57077700	3.81275100
H	7.66208000	-2.18178300	2.16250200
H	6.98834600	-0.55383900	2.44796900
C	4.89395200	-1.45130400	4.07143600
H	4.88480600	-0.36216100	3.92698200
H	3.85548500	-1.79248500	4.19172100
H	5.42387900	-1.65065400	5.01271000
C	5.72687700	-3.65518300	3.34984400
H	6.35286600	-3.72889300	4.25097000
H	4.74500400	-4.07793100	3.60361900
H	6.18185600	-4.26951300	2.56676100
C	7.10848300	1.31443700	0.19333400
H	7.06555100	2.07349100	0.98705100
H	6.51047500	0.45400500	0.52162700
H	8.15152200	0.97546400	0.10379800
C	6.71055600	0.79572400	-2.21559500
H	7.74432800	0.42828500	-2.30466400
H	6.06835400	-0.06293100	-1.96652700
H	6.39887800	1.16405700	-3.20306600
C	7.63046000	3.00546500	-1.49425500
H	7.51481000	3.40246700	-2.50705600
H	7.56206800	3.84562100	-0.79275900
H	8.64593800	2.58941100	-1.42630000
C	3.78508000	6.32600200	-0.13448000
H	4.79135500	6.29566900	-0.56513000
H	3.43022500	7.36673700	-0.16344200
H	3.84796400	6.02191800	0.92007400
C	1.44134900	5.56455300	-0.23301600
H	0.65483500	5.01819000	-0.77376700
H	1.44981200	5.21577600	0.80979500
H	1.15546000	6.62522700	-0.22443000
C	2.65854200	5.92708500	-2.34038500
H	2.13347600	6.89319800	-2.33719700
H	3.62652600	6.08361800	-2.82583300

H	2.06444900	5.22693000	-2.94687100
C	-1.37888000	4.34510700	1.49496800
H	-0.59460600	3.64941400	1.82589100
H	-1.39416100	4.34424800	0.39444700
H	-1.08970200	5.35425700	1.81965700
C	-3.72595500	5.05841400	1.55742900
H	-3.94567700	4.89334300	0.49198600
H	-4.66735000	5.07560200	2.11321400
H	-3.27664900	6.05725700	1.65352000
C	-2.63650700	4.12238500	3.61628700
H	-3.60107500	3.93988400	4.10321600
H	-1.90849800	3.39941400	4.01334500
H	-2.29700300	5.13240300	3.88993700
C	-6.44515300	0.42007800	3.90030000
H	-6.87503900	1.41550800	3.77498400
H	-7.24331900	-0.24380300	4.26074700
H	-5.68838300	0.49139700	4.69447900
C	-6.90295100	-0.22675700	1.50348300
H	-6.48061500	-0.68584700	0.59512600
H	-7.76643000	-0.83115000	1.82110400
H	-7.27480500	0.76703000	1.22408200
C	-5.47787100	-1.62555400	2.95929700
H	-5.26231000	-2.23374700	2.07049900
H	-4.60608700	-1.68717000	3.62605500
H	-6.32695800	-2.10438100	3.46523800

**A'**

C	-2.34944500	-1.77631800	-1.60300200
C	-0.09223600	-1.19882500	-3.05073500
C	-1.11660400	-2.11964600	-3.70927800
C	-2.46785800	-1.71971300	-3.13555300
H	-2.32528300	-2.83874400	-1.30293400
H	-0.26302200	-0.17882300	-3.43436600
H	-1.07946300	-2.04366300	-4.80570500
H	-0.91642600	-3.17260200	-3.45216000
H	-2.71495800	-0.68856800	-3.43841100
H	-3.29108800	-2.35953100	-3.48404100
C	1.36856200	-1.50800700	-3.18351700
C	2.29551500	-0.47771300	-2.97750000
C	1.85567900	-2.79162300	-3.44270700
C	3.66252000	-0.72429200	-3.00460000
H	1.92605100	0.53383500	-2.78930000
C	3.22584800	-3.04031500	-3.47658000
H	1.16110500	-3.61066300	-3.62829700

C	4.13428000	-2.01198700	-3.25052600
H	4.36273900	0.09235200	-2.83132100
H	3.58366400	-4.04786900	-3.68377100
H	5.20452100	-2.20917300	-3.27505900
C	-3.48975200	-1.10288900	-0.88735500
C	-4.60572900	-1.86081000	-0.52095700
C	-3.48995000	0.26650800	-0.60916500
C	-5.69049400	-1.27175900	0.12019400
H	-4.61336500	-2.93216500	-0.73376200
C	-4.56748400	0.85625400	0.04530500
H	-2.62767000	0.88692900	-0.86771900
C	-5.67005800	0.08968400	0.41320300
H	-6.55058100	-1.87887800	0.40018500
H	-4.52752900	1.92201900	0.27178900
H	-6.51156000	0.55209900	0.92682800
P	-0.63435700	-1.08422700	-1.23660900
C	0.90442700	-1.26685100	2.94710400
C	3.24586300	-0.49101200	1.76037400
C	3.26457800	-0.78750500	3.26806900
C	2.18374900	-1.82218400	3.56299400
H	0.64615800	-0.33677800	3.48192700
H	3.76198600	-1.31876500	1.24252700
H	4.25821900	-1.12044900	3.59880300
H	3.03363800	0.13651500	3.82171800
H	2.45417600	-2.78269500	3.09512200
H	2.07015000	-2.00983600	4.64038200
C	3.87530900	0.80806200	1.32155200
C	4.75550700	1.51919400	2.13765400
C	3.61086400	1.31045300	0.04300500
C	5.34736300	2.69846000	1.69069000
H	4.99123800	1.15475000	3.13677400
C	4.20153300	2.48225800	-0.40900000
H	2.91913900	0.77056400	-0.60736700
C	5.07385400	3.18519000	0.41818100
H	6.02636300	3.24046300	2.34723400
H	3.96976400	2.85247600	-1.40793700
H	5.53249100	4.11000800	0.07285900
C	-0.32817200	-2.11644500	2.85620700
C	-1.53765200	-1.48221800	2.54405400
C	-0.31803600	-3.50519200	2.98779200
C	-2.70027800	-2.21184300	2.34089100
H	-1.55666300	-0.39489400	2.44539600
C	-1.48556500	-4.24177100	2.78657100
H	0.60553600	-4.02362000	3.24600200

C	-2.67448300	-3.60157100	2.45234600
H	-3.62436000	-1.69237100	2.08615900
H	-1.46071400	-5.32554800	2.89222800
H	-3.58298300	-4.17952800	2.28805500
P	1.43676000	-0.66359600	1.25148200
C	0.17709100	-2.56499200	-0.44471200
C	1.50580700	-2.22052800	0.22409100
H	0.31552800	-3.37875600	-1.17281300
H	-0.54197900	-2.92533300	0.30600600
H	1.86364500	-3.06690800	0.83129000
H	2.27642300	-2.02753900	-0.54169700
Cu	0.03889200	0.86351600	0.23547800
C	-2.38656600	4.33424100	0.84988600
C	-1.72761700	3.11350100	1.03579900
C	-0.83560500	2.60932500	0.07158300
C	-0.64704200	3.39473000	-1.08384100
C	-1.30586600	4.61253200	-1.25640100
C	-2.18926700	5.10154000	-0.29456200
H	-3.06858200	4.70341600	1.62239900
H	-1.12580900	5.20301700	-2.16035300
C	-2.01781600	2.32774300	2.28559600
H	-1.09072800	1.92353000	2.72065500
H	-2.51789200	2.93437800	3.05379300
H	-2.67875600	1.46975700	2.06951500
C	0.28426500	2.91107600	-2.16274900
H	1.28183700	2.68840900	-1.75040300
H	-0.09136600	1.97692800	-2.61522400
H	0.40782700	3.64367000	-2.97276000
C	-2.90539800	6.40466500	-0.49803300
H	-2.23019900	7.18069100	-0.88452700
H	-3.72739300	6.31081600	-1.22329000
H	-3.33960300	6.77602400	0.43941200

**TS1'**

C	-3.02414900	-0.75870000	1.82264400
C	-0.45216600	-0.94403700	2.76785300
C	-1.58573800	-1.32065100	3.72459100
C	-2.73556100	-1.83667400	2.87719300
H	-3.44259000	0.11776800	2.34811100
H	0.00654900	-1.87207800	2.39210500
H	-1.24169500	-2.05253600	4.46931700
H	-1.93420500	-0.43803400	4.28385200
H	-2.45267200	-2.77596000	2.37438900
H	-3.63901000	-2.05096800	3.46630500

C	0.65421600	-0.08849300	3.31821700
C	1.93854500	-0.20579500	2.77188100
C	0.46092400	0.82966400	4.35520000
C	2.99324100	0.55886700	3.25704800
H	2.11078800	-0.91499700	1.96130200
C	1.51373900	1.60898200	4.82861200
H	-0.51994800	0.93776100	4.81759900
C	2.78617500	1.47654900	4.28390900
H	3.98764300	0.42726600	2.82776200
H	1.33709700	2.31626000	5.63781200
H	3.61217500	2.07628300	4.66239000
C	-4.01401800	-1.19595900	0.77943500
C	-5.36474000	-0.87817300	0.94432000
C	-3.64444400	-1.96067600	-0.32904600
C	-6.31833900	-1.29915100	0.02308500
H	-5.66707000	-0.28163000	1.80739900
C	-4.59064300	-2.37161400	-1.26208100
H	-2.59513900	-2.22178000	-0.47461900
C	-5.93244500	-2.04114900	-1.09010200
H	-7.36587400	-1.03992800	0.17109200
H	-4.27317600	-2.95209100	-2.12792100
H	-6.67391600	-2.36414400	-1.81885600
P	-1.30890400	-0.22587900	1.22692800
C	-0.90532200	2.90659800	-1.79110700
C	1.70937800	3.15110800	-0.98893500
C	1.25210900	3.96920700	-2.19546900
C	-0.22543900	4.25763400	-1.99660500
H	-0.88088000	2.36911700	-2.75372200
H	1.66653200	3.81205800	-0.10495900
H	1.85065200	4.88482600	-2.30463800
H	1.38660400	3.38174300	-3.11908500
H	-0.34662700	4.89196200	-1.10455100
H	-0.67223200	4.80195200	-2.84067100
C	3.09737700	2.57451100	-1.05547200
C	3.93588000	2.76380600	-2.15502000
C	3.59722200	1.87020700	0.04455900
C	5.23646200	2.26455100	-2.15519600
H	3.58309900	3.31732200	-3.02376800
C	4.89216100	1.37179600	0.04770300
H	2.96068700	1.71785800	0.91869600
C	5.72091900	1.56694300	-1.05491200
H	5.87415200	2.42808900	-3.02264600
H	5.25713200	0.82207000	0.91570400
H	6.73818000	1.17882000	-1.05378800



C	-2.32081000	2.90446100	-1.29142300
C	-3.13659500	1.79995800	-1.56297300
C	-2.85152600	3.93943900	-0.51611700
C	-4.42272900	1.70891500	-1.04824900
H	-2.74905200	0.99387700	-2.18508400
C	-4.14125700	3.85181800	0.00331900
H	-2.25548400	4.82606800	-0.30218100
C	-4.92690000	2.73145400	-0.24778900
H	-5.02916900	0.83174900	-1.27055700
H	-4.53146700	4.66832900	0.60949400
H	-5.93245500	2.65790900	0.16462600
P	0.29697400	1.90416000	-0.70523800
C	-1.38557700	1.59802200	1.58675600
C	-0.19550200	2.37724800	1.03352400
H	-1.47370000	1.76488600	2.67157300
H	-2.32099600	1.95300100	1.13075900
H	-0.38648300	3.46053800	1.09339300
H	0.69771700	2.17693500	1.64890100
Cu	0.05813200	-0.51080200	-0.79535700
C	3.60916800	-2.81198500	1.02848500
C	3.78621400	-1.96812100	-0.06651200
C	2.72106600	-1.63489300	-0.90723700
C	1.40789300	-2.09988800	-0.64753900
C	1.27070300	-3.04152800	0.40447300
C	2.34541700	-3.37519500	1.22622600
H	4.78094900	-1.56188200	-0.27167200
H	2.20053300	-4.08091000	2.05020300
C	-0.03768300	-3.75525600	0.58541900
H	-0.14441300	-4.55659000	-0.16274600
H	-0.13265500	-4.22184300	1.57715000
H	-0.88661000	-3.07356900	0.43236200
C	4.72559300	-3.08505000	1.99054500
H	4.78164400	-4.14765300	2.26294500
H	5.69835300	-2.78907400	1.57709200
H	4.58044300	-2.52437800	2.92754100
C	2.98579400	-0.83784700	-2.15126300
H	3.99881700	-0.41547600	-2.16947500
H	2.87408800	-1.48476900	-3.03704600
H	2.26407500	-0.01669900	-2.27264100
C	0.11718000	-3.03451300	-2.96014000
C	0.95341900	-3.95926300	-3.73101400
C	0.97410800	-5.28902300	-3.59722500
H	1.64704700	-3.49263600	-4.44046800
H	1.65770000	-5.91538700	-4.16591500

H	0.29763100	-5.80021700	-2.90983200
C	-0.16426300	-1.72121400	-3.47105700
H	0.54115900	-1.33313700	-4.21564600
C	-1.03810700	-0.83982200	-2.90770400
H	-1.86576000	-1.19008800	-2.28291600
H	-1.13982300	0.16303300	-3.32386500
H	0.76023000	-2.61841100	-1.90381900
H	-0.73115200	-3.51399100	-2.44565200

**B'**

C	2.64463800	2.19841500	0.20355400
C	0.15843700	3.12368000	-0.48977100
C	1.15798800	4.16607600	-0.00015900
C	2.53228300	3.62154700	-0.37199500
H	2.79820700	2.28033500	1.29311900
H	0.19461600	3.11148100	-1.59255200
H	0.96404400	5.15544800	-0.43900800
H	1.09861700	4.28155700	1.09433000
H	2.62699400	3.57277400	-1.46933200
H	3.35717500	4.25107700	-0.00984300
C	-1.27972500	3.18596600	-0.06855800
C	-2.21874700	2.44645500	-0.80276600
C	-1.71252700	3.86280400	1.07287200
C	-3.53865600	2.34836800	-0.38254800
H	-1.89334500	1.91321700	-1.70042100
C	-3.04056400	3.77556300	1.48961300
H	-1.01119800	4.46475600	1.65111600
C	-3.95311100	3.00769200	0.77356400
H	-4.24511400	1.74920000	-0.95687100
H	-3.35870600	4.31136900	2.38308400
H	-4.98773300	2.92765100	1.10581300
C	3.76787600	1.38754300	-0.37998700
C	4.97960000	1.28125500	0.30512400
C	3.64081400	0.74698500	-1.61559600
C	6.03647400	0.54506700	-0.22218100
H	5.08777900	1.77367300	1.27348700
C	4.69126900	0.00502600	-2.14337300
H	2.69680200	0.81571400	-2.16094900
C	5.89245800	-0.10112200	-1.44633400
H	6.97300300	0.47026100	0.32867300
H	4.56899300	-0.49431800	-3.10436300
H	6.71351800	-0.68595600	-1.85733700
P	0.92191900	1.46306500	-0.01809900
C	-0.30190800	-2.45783200	1.44355500

C	-2.86394200	-1.49634900	1.19222000
C	-2.68196600	-2.97982700	1.55212800
C	-1.37258900	-3.09591000	2.32444300
H	-0.14408900	-3.10944700	0.56740400
H	-3.10736700	-0.95380900	2.12195800
H	-3.54747100	-3.35060400	2.11846700
H	-2.62490400	-3.57709900	0.62683000
H	-1.47001300	-2.54945300	3.27685800
H	-1.12059800	-4.13610900	2.57488700
C	-3.92964200	-1.20505300	0.17558200
C	-3.74152300	-1.49718600	-1.17876100
C	-5.13885900	-0.63169800	0.57200100
C	-4.73344500	-1.21641800	-2.11080300
H	-2.79172700	-1.92114500	-1.51103000
C	-6.13802400	-0.35417900	-0.35670500
H	-5.29401200	-0.39176800	1.62542700
C	-5.93599900	-0.64282100	-1.70290000
H	-4.56159000	-1.44044700	-3.16280500
H	-7.07468100	0.09342600	-0.02678800
H	-6.71224700	-0.42240700	-2.43386800
C	1.04037200	-2.11321200	2.01641400
C	2.11348100	-1.94973200	1.13002800
C	1.25022400	-1.85755400	3.37322000
C	3.34927300	-1.50462500	1.58104100
H	1.97250900	-2.18175400	0.07208600
C	2.49170400	-1.41495200	3.82744400
H	0.44086200	-1.99990000	4.08997300
C	3.53977300	-1.22179300	2.93239400
H	4.16535100	-1.37808800	0.86994600
H	2.63737000	-1.22055500	4.88940900
H	4.50754500	-0.86854600	3.28709700
P	-1.13517900	-0.93524600	0.70244600
C	0.42911300	1.20784200	1.75902500
C	-0.87782900	0.43874500	1.93297800
H	0.38004400	2.16990000	2.29272800
H	1.26171800	0.63962200	2.20134000
H	-0.96372700	0.05251300	2.96055300
H	-1.73784200	1.10816000	1.76828000
Cu	-0.20467000	-0.15964900	-1.26722500
C	0.71569100	-2.50208400	-2.51404000
C	1.96769600	-3.16607200	-2.28988400
C	2.14093200	-4.38881600	-1.75224800
H	2.85937700	-2.58861000	-2.56735900
H	3.12824600	-4.81934100	-1.60454700

H	1.28715100	-5.00225600	-1.45906300
C	0.60910900	-1.25628900	-3.09287400
H	1.56041000	-0.78420800	-3.37590200
C	-0.56985400	-0.45312800	-3.24928100
H	-1.52622700	-0.98160000	-3.32680200
H	-0.49266400	0.40910300	-3.91338500
H	-0.20251000	-3.03556500	-2.23494400

**(Z)-(R)-TS2**

P	-1.69552100	-0.86331700	0.13170200
C	-0.91241000	-2.29373400	0.96971400
C	-2.92970200	-1.56053900	-1.01690500
C	-2.67345200	-0.05355200	1.44030300
C	0.15490600	-2.00852400	1.86724500
C	-1.22289400	-3.60911800	0.62798600
C	-2.49556900	-2.38391500	-2.05107300
C	-4.24420000	-1.09749300	-1.04398600
C	-3.58940700	-0.74151900	2.22385800
C	-2.44790100	1.29995800	1.67891400
C	0.43560200	-0.67090500	2.46839400
C	0.87076800	-3.10418600	2.30593900
C	-0.48894800	-4.70343100	1.10550900
H	-2.05781700	-3.80155900	-0.04336800
C	-3.31409800	-2.74054300	-3.12511400
H	-1.46950800	-2.75453400	-2.03171100
C	-5.08502300	-1.33126000	-2.13096400
H	-4.59658500	-0.49321100	-0.21250500
C	-4.37743600	-0.09784400	3.18407500
H	-3.69748200	-1.81535800	2.06760300
C	-3.19510200	2.00972700	2.61575800
H	-1.66708300	1.79493600	1.10046400
C	1.29532300	0.33685700	1.94426300
C	-0.12490900	-0.40032700	3.70102700
C	0.57116400	-4.41032600	1.92663500
H	-0.73615100	-5.72706400	0.83375500
C	-4.56270700	-2.09020600	-3.20352300
C	-4.22887300	1.30432400	3.27839000
P	1.79744500	0.19162600	0.17824600
C	1.57442300	1.47999100	2.69233500
C	0.14550500	0.75806400	4.42293800
C	2.98824300	1.54921300	-0.09885400
C	2.82658000	-1.31417300	0.18047400
C	1.01391100	1.71216200	3.95663200
H	2.24171200	2.23367500	2.27827900

C	4.31198600	1.34155500	-0.45773300
C	2.49583500	2.85388800	-0.08418300
C	3.90419700	-1.46585500	1.04211900
C	2.51194700	-2.34385200	-0.70094000
H	1.24099500	2.60746200	4.53081000
C	5.18925700	2.39104200	-0.75147000
H	4.66319900	0.31932200	-0.55309500
C	3.33030300	3.95442700	-0.27086000
H	1.42990400	2.99911400	0.08559600
C	4.76965700	-2.56241200	0.97032100
H	4.08493100	-0.68170200	1.77780000
C	3.30864800	-3.48082800	-0.81239700
H	1.60778300	-2.23466400	-1.29798600
C	4.69180600	3.70132400	-0.57294700
C	4.50043400	-3.50464700	-0.04689700
C	2.47395000	-4.43117900	3.02357700
H	3.30644100	-4.40582000	2.29246100
H	2.80684500	-4.79649600	4.00041000
O	1.93528600	-3.12555500	3.16081200
O	1.44318200	-5.26793300	2.52791000
H	-1.57522900	-0.87976100	6.37265600
C	-1.47918400	-0.32212900	5.43543900
H	-2.45159900	0.10089400	5.11305700
O	-0.54202100	0.72785300	5.60121600
O	-0.98468300	-1.18098700	4.41970700
O	-5.30763900	-2.16192000	-4.35825700
O	-5.09922800	2.04011900	4.05090300
O	5.40784500	-4.50407600	-0.31952500
O	5.49680000	4.80265700	-0.76790700
C	-6.32440100	2.30945100	3.40138700
H	-6.86931100	3.02237800	4.02965200
H	-6.16300000	2.75059300	2.40627800
H	-6.93447800	1.40199200	3.28133100
C	-2.83942200	3.46590000	2.95148700
C	-5.30535000	-0.98051000	4.04347900
C	-6.53620000	-0.82632500	-2.10536600
C	-4.81461900	-1.30119000	-5.36819000
H	-5.53536100	-1.32995500	-6.19258200
H	-4.71884200	-0.26801700	-4.99965900
H	-3.83048000	-1.62357500	-5.74021500
C	-2.77189900	-3.81727600	-4.08364300
C	5.92012700	-2.61924300	1.99640100
C	2.86352100	-4.66642800	-1.68200700
C	6.47160500	-4.07083000	-1.14378400

H	7.15328600	-3.39102300	-0.61046500
H	7.02857500	-4.96504700	-1.44430100
H	6.10010200	-3.55265300	-2.04029400
C	6.60059000	2.02635600	-1.25656600
C	2.74422200	5.37301200	-0.18624000
C	6.44320600	5.12293000	0.22630000
H	6.41459300	6.20650000	0.39773400
H	6.22343700	4.61027200	1.17405200
H	7.46055700	4.86256000	-0.09905600
Cu	-0.15155300	0.37870900	-1.12853300
C	-1.67220500	2.83337200	-1.92322500
O	-0.66437700	2.41272100	-1.29699200
C	-1.61662400	4.18498400	-2.54035500
C	-2.76660300	4.94960100	-2.76522600
C	-0.37260700	4.73654200	-2.87552100
C	-2.67578000	6.22432500	-3.31549100
H	-3.74586300	4.55427300	-2.49975400
C	-0.28280800	6.00313000	-3.43092500
H	0.52100000	4.13654900	-2.69520600
C	-1.43637500	6.75456700	-3.65461100
H	-3.58208300	6.80586000	-3.47936900
H	0.69274400	6.41077000	-3.69421500
H	-1.36522300	7.74965300	-4.09103300
C	-3.02404300	2.22466300	-1.64520300
H	-3.43409600	2.63495200	-0.70504500
H	-3.75229500	2.39854500	-2.44498200
H	-2.91230800	1.14457100	-1.51118600
C	1.26208300	5.34292700	0.20333400
H	0.63892100	4.77012500	-0.49502000
H	1.12173700	4.92113200	1.21093100
H	0.87435000	6.37089700	0.21503300
C	3.44457600	6.21757100	0.88727300
H	3.51706700	5.66932500	1.83841800
H	4.44690600	6.53153800	0.58765200
H	2.86258500	7.13124500	1.07489100
C	2.86923500	6.06497800	-1.54850400
H	2.40219600	7.06088400	-1.51142800
H	3.91740300	6.18090100	-1.84381800
H	2.35633600	5.48180600	-2.32565700
C	7.08478900	2.97930500	-2.35682300
H	7.20105000	4.01233400	-2.02256900
H	8.05453900	2.63249500	-2.74087100
H	6.37428900	2.98614800	-3.19535800
C	6.61297800	0.62276500	-1.88904700

H	6.46132900	-0.18291600	-1.15559000
H	5.85001200	0.51815700	-2.67190900
H	7.59560500	0.45086800	-2.34924700
C	7.60467100	1.97582400	-0.09655300
H	7.26838100	1.26418800	0.67045300
H	8.58463600	1.63479000	-0.46229400
H	7.75271400	2.94272800	0.39366300
C	5.37938500	-2.27613400	3.39665200
H	4.92730200	-1.28036900	3.46176900
H	4.62333700	-2.99941300	3.72740300
H	6.20593800	-2.30319300	4.11986200
C	6.60048300	-3.98583500	2.14225700
H	7.21222400	-4.26884600	1.28165100
H	7.26674200	-3.95348000	3.01603200
H	5.86945800	-4.78824200	2.30664600
C	6.97229000	-1.56170400	1.63785800
H	7.42539100	-1.74167300	0.65264000
H	6.52534300	-0.55680700	1.61707200
H	7.78124600	-1.55658900	2.38287500
C	2.81587700	-5.93365400	-0.81681500
H	2.11146600	-5.81168300	0.01909200
H	2.47608600	-6.78744700	-1.42128700
H	3.80111200	-6.17760900	-0.40474700
C	1.45410500	-4.44878100	-2.24666300
H	0.70769400	-4.28712800	-1.45205000
H	1.41211300	-3.60161800	-2.94805600
H	1.15232700	-5.34567200	-2.80615400
C	3.78964200	-4.89285700	-2.88351400
H	3.93009300	-3.96239700	-3.45336800
H	4.76961500	-5.27505500	-2.58245300
H	3.34337100	-5.63410400	-3.56188200
C	-2.27963000	-5.00271500	-3.23081600
H	-1.45977500	-4.73718700	-2.55099900
H	-3.09994800	-5.41676900	-2.62716400
H	-1.90588500	-5.80088500	-3.88787300
C	-3.80737100	-4.40927100	-5.04625600
H	-4.70543200	-4.74908400	-4.51516800
H	-4.12471000	-3.71743400	-5.83176100
H	-3.35954300	-5.28061000	-5.54478800
C	-1.58570400	-3.27518300	-4.89047600
H	-0.76255100	-2.94533400	-4.24075500
H	-1.19209400	-4.05942700	-5.55364600
H	-1.86850800	-2.41682000	-5.51553200
C	-7.48637100	-2.02595600	-2.21832200

H	-8.53114200	-1.68380100	-2.18132400
H	-7.33823200	-2.56845800	-3.15788900
H	-7.33073600	-2.72561300	-1.38495600
C	-6.83621700	0.17145300	-3.23124700
H	-6.85876300	-0.30792100	-4.21410100
H	-7.82302400	0.62781000	-3.06625700
H	-6.09370500	0.98275800	-3.25037400
C	-6.85635200	-0.11129400	-0.78829600
H	-6.69389900	-0.75587200	0.08713200
H	-6.25925100	0.80366300	-0.65774500
H	-7.91466500	0.18222000	-0.78907500
C	-4.53627100	-2.23741800	4.49158400
H	-4.21549600	-2.87313900	3.65877100
H	-3.63960700	-1.97735600	5.07056200
H	-5.18386300	-2.85149000	5.13238200
C	-5.80598700	-0.32453200	5.33653800
H	-6.53093600	0.47809200	5.17583900
H	-6.30025100	-1.09214200	5.94869400
H	-4.97686700	0.09172000	5.92459400
C	-6.50645300	-1.44321800	3.20841300
H	-7.12662700	-0.60098200	2.87236700
H	-6.18229900	-1.99305700	2.31289900
H	-7.14657600	-2.11260400	3.80152600
C	-2.55588700	3.57307600	4.45733900
H	-1.73321500	2.90452300	4.75005900
H	-2.26109400	4.60214600	4.71003300
H	-3.43705200	3.31299700	5.05459500
C	-3.95057400	4.45030200	2.56629700
H	-4.83568900	4.34736400	3.20139900
H	-3.58417800	5.48051300	2.68034800
H	-4.24987300	4.32137700	1.51537400
C	-1.57141300	3.91589300	2.21548900
H	-0.70613600	3.27766700	2.45058600
H	-1.69152900	3.93677900	1.12159600
H	-1.32405800	4.93876000	2.53225600
C	0.09117500	0.00616600	-3.22116400
C	-1.15752600	0.51157400	-3.66402800
C	-1.46312100	1.78762700	-4.08287800
H	0.16635000	-1.08860400	-3.16827300
H	-1.99665800	-0.18881900	-3.56000800
H	-0.67942800	2.47834500	-4.38961900
H	-2.45755700	2.00786800	-4.47168800
C	1.35160200	0.70434300	-3.42961100
C	2.57379000	0.14662600	-3.49093500



H	1.28290800	1.79528300	-3.49993300
H	3.46882100	0.75457800	-3.61058700
H	2.71680000	-0.93463500	-3.41114000

**(E)-(R)-TS2**

P	-1.58902800	-0.90145100	0.05625600
C	-0.73758100	-2.28439400	0.90701900
C	-2.82515500	-1.66856700	-1.04497400
C	-2.55655500	-0.12651800	1.39602200
C	0.28920300	-1.94437500	1.83098800
C	-1.00227100	-3.61781900	0.59693100
C	-2.39087400	-2.47319700	-2.09447400
C	-4.16473100	-1.28670000	-1.00972000
C	-3.40208600	-0.85871700	2.21870800
C	-2.40349700	1.23967500	1.61794900
C	0.54318700	-0.58367000	2.38909300
C	1.01005000	-3.00807200	2.33641000
C	-0.26654500	-4.67761500	1.14467700
H	-1.80942100	-3.85318800	-0.09462000
C	-3.24339900	-2.89854900	-3.11686100
H	-1.34385400	-2.78356900	-2.11993500
C	-5.03890600	-1.57084900	-2.05718400
H	-4.51109000	-0.69824000	-0.16485600
C	-4.19042300	-0.25411400	3.20380100
H	-3.45698900	-1.93792400	2.07364200
C	-3.16495800	1.91515700	2.56906600
H	-1.68116500	1.77986500	1.00731800
C	1.33921100	0.44394400	1.80629500
C	0.03301900	-0.30842300	3.64234500
C	0.75034900	-4.33297000	2.00010000
H	-0.48296000	-5.71529700	0.90150200
C	-4.52770100	-2.31624400	-3.14332200
C	-4.12478200	1.15567000	3.28134900
P	1.81933200	0.24171100	0.03754900
C	1.59545600	1.61908200	2.51272800
C	0.28278400	0.87717400	4.32548300
C	2.95995500	1.62225000	-0.30724100
C	2.89949100	-1.22943900	0.12020400
C	1.08022400	1.85969200	3.79450400
H	2.21152800	2.38993900	2.05311800
C	4.28405600	1.45868900	-0.68802000
C	2.41613100	2.90702300	-0.30335400
C	3.95591800	-1.28941100	1.01837800
C	2.65052700	-2.32119700	-0.70693300

H	1.28911200	2.78063900	4.33395600
C	5.10561600	2.53880000	-1.03140800
H	4.67988300	0.44956600	-0.76080200
C	3.20628900	4.03708600	-0.49915300
H	1.34741700	3.01032000	-0.11668500
C	4.86400600	-2.35398000	1.03417400
H	4.08925800	-0.46008300	1.71356100
C	3.49278200	-3.42945500	-0.73031100
H	1.77654600	-2.27737400	-1.35216700
C	4.56700000	3.83055200	-0.83932200
C	4.66025100	-3.36332500	0.06986100
C	2.59827200	-4.27207500	3.18763200
H	3.46873400	-4.26499700	2.50315100
H	2.88281500	-4.58735300	4.19649400
O	2.03528900	-2.97128500	3.23648600
O	1.60898300	-5.14812800	2.67554100
H	-1.29578300	-0.78127700	6.37990800
C	-1.25063800	-0.24351300	5.42758900
H	-2.24641500	0.13790900	5.12716700
O	-0.34850000	0.84372900	5.53506200
O	-0.75951800	-1.10835300	4.41574800
O	-5.32292300	-2.44921700	-4.25812500
O	-5.00309900	1.84666700	4.08519900
O	5.61392300	-4.34005100	-0.11807500
O	5.32934300	4.95890000	-1.04526900
C	-6.27182400	2.03750700	3.49324300
H	-6.79627300	2.78937000	4.09314400
H	-6.18067800	2.39926400	2.45779400
H	-6.86683600	1.11177500	3.48698500
C	-2.88955300	3.39926700	2.86140900
C	-5.03128600	-1.18348300	4.10243500
C	-6.50610400	-1.12231600	-1.97859100
C	-4.92101600	-1.59644800	-5.31402600
H	-5.68426200	-1.67560600	-6.09576100
H	-4.84750300	-0.55153600	-4.97571900
H	-3.94714300	-1.89011800	-5.73365700
C	-2.70762500	-3.98236700	-4.07126700
C	5.99229100	-2.29588900	2.08328000
C	3.11682900	-4.67888000	-1.54182300
C	6.67378400	-3.91444800	-0.95092100
H	7.31691000	-3.17401300	-0.45118900
H	7.27235300	-4.80094900	-1.18785000
H	6.29662700	-3.46963500	-1.88387000
C	6.50130100	2.22355500	-1.60781200

C	2.57010300	5.43195200	-0.39385600
C	6.30180300	5.27772800	-0.07445400
H	6.25837200	6.35667400	0.11966600
H	6.11984600	4.74331800	0.86909000
H	7.31284100	5.03933900	-0.43475800
Cu	-0.19294600	0.49271500	-1.21392900
C	-2.03714000	2.82705200	-1.75573700
C	-2.12105000	4.23494100	-2.23130600
C	-3.31928900	4.95515900	-2.20474600
C	-0.95663400	4.89080200	-2.65132800
C	-3.35385000	6.29240700	-2.59080900
H	-4.23572600	4.47632000	-1.86197700
C	-0.99317900	6.21756100	-3.05011100
H	-0.02438900	4.32222500	-2.66639400
C	-2.19428000	6.92681100	-3.01935500
H	-4.29499400	6.83957300	-2.55463000
H	-0.08117000	6.70672800	-3.39090800
H	-2.22167300	7.97019600	-3.32959700
C	-3.32717300	2.08729700	-1.50181300
H	-3.71123800	2.31852800	-0.49188900
H	-4.10544700	2.33286300	-2.23247200
H	-3.14384600	1.00963200	-1.54529400
C	1.13289200	5.35187300	0.13660600
H	0.46337800	4.75010800	-0.49057000
H	1.10276800	4.93742900	1.15731000
H	0.70739700	6.36452200	0.17448800
C	3.32951000	6.34747600	0.57772800
H	3.56666500	5.82551800	1.51675900
H	4.25625700	6.73506700	0.14785700
H	2.70310500	7.21432700	0.83134600
C	2.54297600	6.07655700	-1.78438100
H	2.07049600	7.06921200	-1.73280300
H	3.55462400	6.19498400	-2.18922300
H	1.96454300	5.45856300	-2.48561500
C	6.92175300	3.22181600	-2.69493500
H	7.06032200	4.24090600	-2.32916500
H	7.86828600	2.89122400	-3.14508100
H	6.16630900	3.26212200	-3.49183400
C	6.50639000	0.84549900	-2.29481900
H	6.39576600	0.00808900	-1.59117700
H	5.71302900	0.76420700	-3.05017000
H	7.47112500	0.70457700	-2.80100400
C	7.55563800	2.15393800	-0.49521100
H	7.28745500	1.38194600	0.23981900

H	8.53407600	1.88517000	-0.92036500
H	7.67693700	3.09755000	0.04641700
C	5.40286000	-1.90573700	3.45137600
H	4.89791400	-0.93366700	3.45287600
H	4.67646400	-2.64888800	3.80451600
H	6.21211900	-1.84985400	4.19243900
C	6.74225400	-3.61197000	2.32039300
H	7.38904600	-3.90628700	1.48982100
H	7.38522200	-3.49237700	3.20389400
H	6.05349500	-4.44403600	2.51592800
C	6.99425200	-1.20623200	1.67853500
H	7.46941000	-1.42207200	0.71067900
H	6.49614700	-0.22933100	1.59105300
H	7.79049800	-1.11372200	2.43169500
C	3.08464000	-5.89413500	-0.60363700
H	2.35300100	-5.74837400	0.20360000
H	2.79188900	-6.79357300	-1.16518000
H	4.06444300	-6.07864100	-0.14990500
C	1.71784500	-4.54490600	-2.15816500
H	0.94385600	-4.36644700	-1.39529400
H	1.66107000	-3.73944500	-2.90645400
H	1.46489600	-5.48302500	-2.67196000
C	4.08853700	-4.95413200	-2.69611500
H	4.22762900	-4.06172300	-3.32335900
H	5.06637200	-5.29074000	-2.33849700
H	3.68442200	-5.75032300	-3.33772200
C	-2.11603100	-5.11512900	-3.21013400
H	-1.26163300	-4.79367100	-2.59951400
H	-2.87749400	-5.53195600	-2.53545200
H	-1.75859500	-5.92652200	-3.85973400
C	-3.76995700	-4.64919400	-4.95295000
H	-4.62101900	-5.00738200	-4.36028200
H	-4.16128500	-3.99702200	-5.73886600
H	-3.31435000	-5.51761900	-5.44952000
C	-1.59320300	-3.42292300	-4.96136300
H	-0.74787000	-3.04948200	-4.36697800
H	-1.20828200	-4.21103100	-5.62460700
H	-1.94214200	-2.59420000	-5.59284200
C	-7.41581600	-2.35629700	-2.03562700
H	-8.47017800	-2.05024000	-1.96825400
H	-7.28020300	-2.91185800	-2.96961600
H	-7.20616800	-3.03245500	-1.19479400
C	-6.88307700	-0.15559500	-3.10945800
H	-6.94128600	-0.65788300	-4.07949400

H	-7.87123600	0.28245400	-2.90746300
H	-6.16124700	0.67108400	-3.18436300
C	-6.79863500	-0.39612400	-0.66089200
H	-6.58582800	-1.02291000	0.21653700
H	-6.22369800	0.53724000	-0.56352000
H	-7.86457600	-0.13388200	-0.62679200
C	-4.18090500	-2.40152900	4.50923500
H	-3.88668200	-3.02961500	3.66070500
H	-3.26014000	-2.09817200	5.02463100
H	-4.76010000	-3.03792200	5.19217100
C	-5.50472600	-0.55324900	5.41824600
H	-6.28129800	0.20542000	5.29289200
H	-5.92566700	-1.34516500	6.05361600
H	-4.67509500	-0.08836600	5.96762800
C	-6.24416600	-1.70630500	3.32188400
H	-6.91029300	-0.89498800	2.99921700
H	-5.93065000	-2.25449300	2.42178600
H	-6.83246400	-2.39409700	3.94687800
C	-2.50433900	3.54766600	4.34035600
H	-1.62304300	2.93550800	4.58163100
H	-2.25680700	4.59687100	4.55895200
H	-3.32276900	3.24635800	5.00345300
C	-4.08880500	4.30420300	2.55317100
H	-4.91768500	4.14941400	3.25039900
H	-3.78257700	5.35673800	2.63719500
H	-4.45209900	4.15151100	1.52562800
C	-1.71669700	3.92321200	2.02344400
H	-0.80169500	3.33124500	2.17099100
H	-1.93423600	3.93900700	0.94522700
H	-1.49653600	4.95662100	2.32566600
C	0.18586200	0.66582600	-3.32221500
C	-1.17439000	0.75112900	-3.69691700
C	-1.84123300	1.93006300	-3.96104200
H	-1.74931500	-0.18846400	-3.68667200
H	-1.26469700	2.80990800	-4.24203500
H	-2.87707300	1.91373000	-4.30059100
C	0.95983400	-0.55397000	-3.44930500
C	2.30167800	-0.63261900	-3.52943300
H	0.37754900	-1.48553800	-3.48044900
H	2.82242300	-1.58467900	-3.61802300
H	2.91796000	0.26849800	-3.50972000
H	0.76415100	1.59744800	-3.39633500
O	-0.97542000	2.46122400	-1.18205400

**(Z)-(R)-C**

P	-1.62246500	-0.98523400	0.15327800
C	-0.78309700	-2.35013800	1.03387100
C	-2.81971200	-1.75401500	-0.98589000
C	-2.64360700	-0.16516400	1.41376800
C	0.26133000	-1.98452800	1.92841000
C	-1.03656900	-3.68861900	0.73774600
C	-2.36519300	-2.57033100	-2.01660600
C	-4.14105700	-1.31338200	-1.02328400
C	-3.52243800	-0.85376800	2.23793300
C	-2.52434900	1.21715600	1.52842400
C	0.47988600	-0.60655300	2.46167600
C	1.01257100	-3.03212100	2.42175100
C	-0.26737200	-4.73222700	1.27055700
H	-1.85860900	-3.93833700	0.06863600
C	-3.17297300	-2.93911500	-3.09601500
H	-1.33443700	-2.92848000	-1.98666200
C	-4.97000400	-1.55247200	-2.11676000
H	-4.50494700	-0.70737900	-0.19916500
C	-4.38685500	-0.18851900	3.11419000
H	-3.54829700	-1.94253800	2.17221500
C	-3.34038600	1.94438800	2.39122400
H	-1.79331800	1.72392100	0.89474800
C	1.27453600	0.42403000	1.88012600
C	-0.09695500	-0.30065000	3.67915600
C	0.76635000	-4.36343400	2.09502800
H	-0.47200500	-5.77556500	1.04181400
C	-4.43191000	-2.30846500	-3.18309600
C	-4.33893500	1.22439300	3.09071000
P	1.79035300	0.22900900	0.12189900
C	1.46952900	1.62795000	2.55638000
C	0.09732900	0.91234000	4.33292900
C	2.93486700	1.61354800	-0.20203500
C	2.86694600	-1.24443900	0.17705400
C	0.89429800	1.89664000	3.80577100
H	2.07723700	2.40327100	2.09411900
C	4.27274000	1.44996200	-0.53046400
C	2.38660000	2.89662700	-0.23036000
C	3.94460400	-1.32860300	1.04827900
C	2.59492300	-2.31632000	-0.66835300
H	1.05463100	2.84090100	4.32072600
C	5.11044500	2.52796200	-0.83742300
H	4.66849700	0.44109600	-0.59253900
C	3.18622100	4.02583200	-0.40133400

H	1.30750500	2.99609700	-0.10977800
C	4.84918300	-2.39612300	1.01719200
H	4.09684800	-0.51477700	1.75798500
C	3.43107200	-3.42782600	-0.73775900
H	1.68823300	-2.26420300	-1.26925200
C	4.56147400	3.82016000	-0.67778400
C	4.61905200	-3.38163800	0.03336200
C	2.65042100	-4.26735100	3.21661200
H	3.48798200	-4.24515400	2.49130300
H	2.98670400	-4.57606500	4.21144100
O	2.06513400	-2.97721100	3.28975900
O	1.65647800	-5.16179400	2.75047600
H	-1.51467100	-0.72168000	6.37698900
C	-1.45162600	-0.20862400	5.41199500
H	-2.44459900	0.14378200	5.07308100
O	-0.57715500	0.90010100	5.51803500
O	-0.91181900	-1.09019700	4.43893500
O	-5.17058700	-2.39545000	-4.34129800
O	-5.29021200	1.95274400	3.77037400
O	5.56315200	-4.35663700	-0.20068500
O	5.32981700	4.94830900	-0.86419100
C	-6.48966600	2.09486900	3.03755600
H	-7.14045500	2.75935800	3.61634800
H	-6.30539200	2.53634300	2.04639200
H	-6.99995900	1.12989200	2.89342900
C	-3.06726400	3.43900800	2.61974500
C	-5.29450900	-1.06412200	4.00218400
C	-6.41786200	-1.03762600	-2.10359800
C	-4.69165200	-1.52910900	-5.35164400
H	-5.43189600	-1.53601900	-6.15910600
H	-4.57250600	-0.50229200	-4.97247400
H	-3.72239300	-1.86197000	-5.75334100
C	-2.60501200	-4.00152800	-4.05526400
C	6.00251000	-2.37241200	2.04163600
C	3.03032800	-4.66387200	-1.55701400
C	6.60631300	-3.91688000	-1.04730400
H	7.26430300	-3.19123500	-0.54555800
H	7.19505900	-4.80062600	-1.31670900
H	6.21062100	-3.44910600	-1.96118000
C	6.53589000	2.21175000	-1.33708400
C	2.55026200	5.42236600	-0.31871500
C	6.25916700	5.29199400	0.13906700
H	6.18458500	6.37006500	0.32907600
H	6.05761000	4.75525600	1.07725600

H	7.28720200	5.07746700	-0.18662500
Cu	-0.22570200	0.48123100	-1.00721800
C	-1.75548000	2.56552200	-2.20741000
O	-0.80952500	2.36011100	-1.23432100
C	-1.86475700	4.06789900	-2.50505500
C	-3.05705900	4.79199100	-2.45587300
C	-0.69727300	4.76548200	-2.83391000
C	-3.08503700	6.15907300	-2.72819500
H	-3.98970000	4.29291000	-2.19743600
C	-0.71832000	6.12374300	-3.11855400
H	0.24843000	4.21898400	-2.83688000
C	-1.91811800	6.83076400	-3.06701300
H	-4.03086600	6.69801800	-2.67669200
H	0.20850500	6.63757900	-3.37500200
H	-1.93885000	7.89716600	-3.28778800
C	-3.12334600	1.98255800	-1.82395700
H	-3.49085600	2.42753800	-0.88699800
H	-3.88557500	2.12822200	-2.60630600
H	-3.02544700	0.90464200	-1.65518700
C	1.08208500	5.34081200	0.11515800
H	0.45503800	4.73255000	-0.54847200
H	0.99005300	4.93235800	1.13436800
H	0.65422800	6.35322100	0.12223500
C	3.25069300	6.30939800	0.72169700
H	3.42600000	5.76232700	1.66020600
H	4.20393500	6.70433600	0.36222700
H	2.61203800	7.17247000	0.95689800
C	2.61996600	6.09935300	-1.69227000
H	2.16335400	7.09954100	-1.64221900
H	3.65648100	6.20710300	-2.03180300
H	2.06776300	5.51494700	-2.44147000
C	6.98927500	3.17918900	-2.43799800
H	7.06795900	4.21585500	-2.10468000
H	7.97140700	2.86591900	-2.81939400
H	6.28098600	3.16127200	-3.27826400
C	6.59506300	0.80941900	-1.97016900
H	6.46792400	-0.00274000	-1.23923500
H	5.83679000	0.68299800	-2.75549500
H	7.58260300	0.66884700	-2.43045400
C	7.54302800	2.19668000	-0.17898400
H	7.22866000	1.48369600	0.59584800
H	8.53099200	1.87913000	-0.54432300
H	7.66687100	3.17197900	0.30111200
C	5.45120700	-2.00547900	3.43166400



H	4.95060100	-1.03178500	3.46426900
H	4.73343800	-2.75252600	3.79344800
H	6.28128200	-1.96547000	4.15012600
C	6.74355800	-3.70145100	2.23072500
H	7.36639100	-3.98441300	1.37816100
H	7.40973500	-3.60841300	3.10011600
H	6.05157800	-4.53084400	2.42575800
C	7.00776700	-1.28448600	1.64134900
H	7.46542500	-1.48196100	0.66141700
H	6.51928500	-0.30062000	1.58521900
H	7.81764600	-1.21681700	2.38234800
C	3.01616300	-5.89112000	-0.63445900
H	2.30363400	-5.75151900	0.19100600
H	2.70613700	-6.78193000	-1.20025600
H	4.00549600	-6.08540800	-0.20658700
C	1.61801700	-4.51726800	-2.13726700
H	0.86219800	-4.34014500	-1.35527200
H	1.55479900	-3.70640000	-2.87926400
H	1.34703900	-5.44833800	-2.65467900
C	3.96972300	-4.92208700	-2.74171500
H	4.09033900	-4.01833500	-3.35703300
H	4.95733500	-5.26370600	-2.41839100
H	3.54716900	-5.70734500	-3.38480200
C	-2.08198600	-5.17811200	-3.20869500
H	-1.26415800	-4.89788700	-2.53232100
H	-2.88951700	-5.61142900	-2.60186200
H	-1.69517900	-5.96632900	-3.87015900
C	-3.62376100	-4.61609900	-5.02146100
H	-4.51167800	-4.98188800	-4.49079900
H	-3.96152600	-3.93017000	-5.80323800
H	-3.15338800	-5.47288900	-5.52447300
C	-1.43184500	-3.42311600	-4.85554400
H	-0.62233600	-3.07836300	-4.19588000
H	-1.01209300	-4.18957000	-5.52347100
H	-1.73682700	-2.56811200	-5.47533100
C	-7.37230800	-2.23505500	-2.19518200
H	-8.41619900	-1.88913600	-2.17291000
H	-7.21822000	-2.79774300	-3.12274300
H	-7.22415900	-2.91719900	-1.34607800
C	-6.71283900	-0.06084400	-3.24968600
H	-6.74540300	-0.55951600	-4.22259000
H	-7.69540700	0.40585500	-3.08955900
H	-5.96536400	0.74519100	-3.28743100
C	-6.72999000	-0.28767500	-0.80277300

H	-6.58618300	-0.91644600	0.08752500
H	-6.11198700	0.61686300	-0.68941100
H	-7.78212800	0.02728500	-0.81564600
C	-4.45352300	-2.18386800	4.64224000
H	-3.93724900	-2.82111700	3.91627100
H	-3.69215600	-1.77103400	5.31809800
H	-5.10802800	-2.83466100	5.23866900
C	-5.96550000	-0.34147900	5.17629500
H	-6.76469000	0.34125800	4.87446300
H	-6.41837600	-1.09597700	5.83551100
H	-5.24169900	0.23279000	5.76880800
C	-6.37645900	-1.72143000	3.13496200
H	-7.02660400	-0.97387600	2.65893900
H	-5.93386000	-2.33327000	2.33574500
H	-7.01255100	-2.37641900	3.74834200
C	-2.76038400	3.64915500	4.11051800
H	-1.89778400	3.04133000	4.42601800
H	-2.51176300	4.70457100	4.29589500
H	-3.61569400	3.38595100	4.74307200
C	-4.23647400	4.33922600	2.20466400
H	-5.10670000	4.21940100	2.85768800
H	-3.92527800	5.39209800	2.26064500
H	-4.53779800	4.14283900	1.16476700
C	-1.84102800	3.90432000	1.82534000
H	-0.94092000	3.32665400	2.08437100
H	-1.96936700	3.83119400	0.73500200
H	-1.64230500	4.95798100	2.06741200
C	0.25761100	-0.10559400	-3.28912900
C	-0.98865500	0.42894700	-3.38671700
C	-1.31386200	1.87148300	-3.55639800
H	0.34203900	-1.19618500	-3.21596300
H	-1.82806300	-0.27561700	-3.34775000
H	-0.44235500	2.41460100	-3.94236700
H	-2.11781500	1.98596400	-4.30173200
C	1.52334300	0.61143900	-3.39318300
C	2.70805000	0.00038500	-3.51702600
H	1.48344900	1.70221900	-3.35034100
H	3.63537900	0.56449800	-3.59525500
H	2.79062900	-1.08882600	-3.53371700

**(E)-(R)-C**

P	-1.54837400	-0.97823200	0.04108700
C	-0.67906600	-2.30461900	0.95434300
C	-2.74887400	-1.80048700	-1.06065300

C	-2.57158700	-0.18630200	1.32366800
C	0.30868600	-1.89778800	1.89355900
C	-0.89084400	-3.65492200	0.67895700
C	-2.28805200	-2.57464600	-2.12180000
C	-4.09891200	-1.45751400	-1.02652900
C	-3.38859100	-0.92218600	2.17300000
C	-2.52501000	1.20068000	1.43731400
C	0.50509100	-0.50616300	2.39851800
C	1.04715400	-2.91940900	2.45691200
C	-0.14265400	-4.67083200	1.28994800
H	-1.66873500	-3.93580000	-0.03006800
C	-3.12232900	-2.98875700	-3.16517400
H	-1.23360700	-2.86388000	-2.14077300
C	-4.96170000	-1.74365200	-2.08138300
H	-4.46367900	-0.88502300	-0.17961400
C	-4.26491700	-0.30848700	3.07346400
H	-3.35541800	-2.01010900	2.10945000
C	-3.35678600	1.87849700	2.32751300
H	-1.85404200	1.75152600	0.77304300
C	1.28919300	0.51996900	1.79568500
C	-0.06250200	-0.18381200	3.61591700
C	0.83324200	-4.26345700	2.16561600
H	-0.31946700	-5.72323100	1.08049500
C	-4.42232300	-2.44127700	-3.18470100
C	-4.29399200	1.10533900	3.05379500
P	1.82833600	0.27322200	0.05220800
C	1.47912200	1.73700700	2.44783300
C	0.11740100	1.04557300	4.24198400
C	2.95236300	1.66005700	-0.32447700
C	2.93394800	-1.17286900	0.20006000
C	0.90263800	2.02690600	3.69195900
H	2.08690400	2.50362500	1.97219600
C	4.28292000	1.50316400	-0.68762600
C	2.38639800	2.93526200	-0.37264100
C	3.98087400	-1.17559900	1.11163700
C	2.72018100	-2.30068400	-0.58601100
H	1.05412700	2.98351400	4.18630700
C	5.08833400	2.58214100	-1.07143100
H	4.69659100	0.49872200	-0.71176800
C	3.16394300	4.06931600	-0.59703200
H	1.31069100	3.02644300	-0.21820300
C	4.91112500	-2.21808600	1.18119500
H	4.08799600	-0.31657300	1.77379400
C	3.59151500	-3.38600700	-0.56308900

H	1.84251000	-2.30928700	-1.22672200
C	4.52748000	3.87166500	-0.93169400
C	4.74508700	-3.26578400	0.25096700
C	2.64748800	-4.10435900	3.39263800
H	3.52986500	-4.10146300	2.72343600
H	2.92150300	-4.37015600	4.41848000
O	2.04985100	-2.81841000	3.37727500
O	1.69338700	-5.02727000	2.89898400
H	-1.46336000	-0.56465500	6.32999000
C	-1.41142100	-0.07496900	5.35229400
H	-2.41052500	0.25162800	5.00661800
O	-0.55722500	1.05306500	5.42689200
O	-0.85622500	-0.97031000	4.40102300
O	-5.20138300	-2.55606700	-4.31403100
O	-5.25357900	1.78817100	3.76847700
O	5.72067500	-4.22853200	0.11202300
O	5.26855400	5.00249600	-1.19125700
C	-6.49838700	1.87497800	3.10821500
H	-7.06878000	2.67056200	3.60064000
H	-6.37188400	2.12548300	2.04441400
H	-7.06794300	0.93586800	3.18052800
C	-3.19184600	3.39319700	2.52357700
C	-5.10645200	-1.22682800	3.98270200
C	-6.43947200	-1.33292800	-1.99499500
C	-4.82284800	-1.64035900	-5.32353500
H	-5.58386400	-1.69757600	-6.10942300
H	-4.77468600	-0.61154600	-4.93341200
H	-3.84231900	-1.88791700	-5.75825400
C	-2.54988900	-4.02268900	-4.15220600
C	6.01971000	-2.09539500	2.24585000
C	3.25877600	-4.66833100	-1.34162800
C	6.78975900	-3.81137300	-0.71312600
H	7.41102300	-3.04496300	-0.22556200
H	7.40691000	-4.69472300	-0.91034400
H	6.42351300	-3.40334800	-1.66723400
C	6.49128500	2.26835900	-1.63248500
C	2.50354800	5.45641000	-0.53367400
C	6.24381700	5.38049600	-0.24429200
H	6.17214700	6.46336200	-0.08396000
H	6.08891500	4.87292000	0.71849900
H	7.25610300	5.15757400	-0.61109800
Cu	-0.18056500	0.55335400	-1.09568200
C	-1.90339800	2.56990800	-2.14558700
O	-0.97209200	2.37902300	-1.15288800

C	0.62785700	0.57531600	-3.39030900
C	-0.70683200	0.77504900	-3.52573400
C	-1.30924200	2.13744300	-3.53877200
H	-1.35832600	-0.09836100	-3.66050500
H	-0.52489000	2.85723900	-3.80968400
H	-2.09447000	2.20404100	-4.30897700
C	1.30372300	-0.70670700	-3.49995700
C	2.63270500	-0.84044400	-3.58009300
H	0.66134900	-1.59425000	-3.53034600
H	3.11341300	-1.81262200	-3.67758200
H	3.28718000	0.03230600	-3.54509000
C	-2.23703500	4.06701300	-2.22301800
C	-3.50719700	4.59734700	-1.98913400
C	-1.19895800	4.96960400	-2.47488700
C	-3.72989400	5.97390400	-1.99884200
H	-4.34766800	3.93490800	-1.78640200
C	-1.41294800	6.34026300	-2.50007700
H	-0.19333000	4.57506200	-2.62654500
C	-2.68609300	6.85245500	-2.25800500
H	-4.73125400	6.35754900	-1.80418500
H	-0.57929900	7.01337800	-2.70372600
H	-2.85979600	7.92764500	-2.27078300
C	-3.18087500	1.74154900	-1.93923600
H	-3.62847300	1.94331700	-0.95365300
H	-3.93818800	1.93770600	-2.71522300
H	-2.94194600	0.67199200	-1.97894300
H	1.27357800	1.45751000	-3.30120400
C	1.10010200	5.37319500	0.08073400
H	0.40714700	4.72713900	-0.47221800
H	1.14235600	5.01305400	1.12089500
H	0.65353700	6.37713000	0.09680800
C	3.29067800	6.44489000	0.33931400
H	3.60032700	5.98451400	1.28927300
H	4.17658700	6.83259000	-0.16955500
H	2.65202200	7.30523400	0.58347000
C	2.39473600	6.02045900	-1.95473300
H	1.91613000	7.01145800	-1.93444800
H	3.38514700	6.12543600	-2.41459700
H	1.78645100	5.36328100	-2.59261700
C	6.88980400	3.21985100	-2.76861600
H	6.99657900	4.26044800	-2.45691200
H	7.84740400	2.89307600	-3.19771700
H	6.13723100	3.19609200	-3.56904900
C	6.52807000	0.85851300	-2.25050700

H	6.42982500	0.05425200	-1.50730500
H	5.74141500	0.72512100	-3.00596600
H	7.49775800	0.71248000	-2.74563800
C	7.54837800	2.27570400	-0.52024600
H	7.29069600	1.54540900	0.25969500
H	8.52929800	1.99400100	-0.93107600
H	7.66037800	3.25084500	-0.03584900
C	5.40195900	-1.65289000	3.58577700
H	4.89753600	-0.68158200	3.53897800
H	4.66940600	-2.38219900	3.95505400
H	6.19696400	-1.56574400	4.33913700
C	6.78392300	-3.38856100	2.55430300
H	7.44552900	-3.71442800	1.74730100
H	7.41296700	-3.21800800	3.43922600
H	6.10380700	-4.21998200	2.78133600
C	7.01248600	-1.00920500	1.81023800
H	7.51189000	-1.26105400	0.86376600
H	6.50123100	-0.04571900	1.66789500
H	7.79120400	-0.86945900	2.57428800
C	3.23908200	-5.85559500	-0.36794800
H	2.49649000	-5.69790400	0.42695300
H	2.96773300	-6.77649100	-0.90488700
H	4.21681700	-6.00907700	0.10084800
C	1.86721200	-4.58915400	-1.98363200
H	1.07732500	-4.39894800	-1.24098200
H	1.80341900	-3.81469200	-2.76412900
H	1.64429200	-5.55146100	-2.46509600
C	4.25535700	-4.95272000	-2.47186900
H	4.37685900	-4.07721600	-3.12728700
H	5.23792000	-5.24617600	-2.09009700
H	3.88553700	-5.78208800	-3.09182800
C	-1.96231700	-5.18371900	-3.32780800
H	-1.14351800	-4.87232200	-2.66633600
H	-2.73849400	-5.65122600	-2.70573500
H	-1.55988300	-5.95231800	-4.00273200
C	-3.57483300	-4.66629900	-5.09272800
H	-4.43025800	-5.07403400	-4.54019700
H	-3.96412800	-3.98335800	-5.85324500
H	-3.08612900	-5.49704500	-5.62147500
C	-1.42500200	-3.40279300	-4.98782500
H	-0.59605700	-3.05422100	-4.35555800
H	-1.01550900	-4.14584300	-5.68748900
H	-1.77584100	-2.54339300	-5.57650400
C	-7.31930600	-2.58603000	-2.08840800

H	-8.38033300	-2.30715900	-2.00875700
H	-7.17579200	-3.11042800	-3.03886700
H	-7.09166300	-3.28281700	-1.26938700
C	-6.83761100	-0.34053200	-3.09499200
H	-6.86274800	-0.80668000	-4.08415100
H	-7.84499600	0.05027300	-2.89117600
H	-6.14791100	0.51619300	-3.12197600
C	-6.75028600	-0.65031400	-0.65848400
H	-6.51983600	-1.29188900	0.20369000
H	-6.19909600	0.29505700	-0.54249200
H	-7.82269700	-0.41656500	-0.61800600
C	-4.23571600	-2.39498600	4.48258100
H	-3.91511600	-3.07041000	3.68109800
H	-3.33087000	-2.03920400	4.99236200
H	-4.81222700	-3.00040500	5.19527000
C	-5.65686900	-0.55029200	5.24482400
H	-6.44492400	0.18078300	5.04819300
H	-6.08428400	-1.32268100	5.89988900
H	-4.86412300	-0.03653500	5.80543400
C	-6.26512300	-1.83262400	3.17952600
H	-6.95396700	-1.06578400	2.80035700
H	-5.88966400	-2.39934300	2.31443600
H	-6.84627700	-2.52354000	3.80815400
C	-2.98706300	3.68365000	4.01686600
H	-2.11154700	3.13763800	4.39899400
H	-2.80578800	4.75786000	4.16777100
H	-3.85946900	3.39350300	4.61273000
C	-4.39464100	4.18442100	1.99567600
H	-5.29401100	4.03459900	2.60219900
H	-4.16287200	5.25924400	2.01005300
H	-4.61446000	3.91351700	0.95152000
C	-1.95786200	3.91614300	1.77751200
H	-1.03782400	3.39334300	2.08166700
H	-2.03723400	3.82187000	0.68525800
H	-1.83239200	4.98260600	2.01306800

**(Z)-(R)-TS3**

P	2.14831700	0.33295700	-0.06492400
C	1.78313700	-0.42513600	1.57339800
C	3.07926200	1.86555900	0.30613400
C	3.46189800	-0.82666600	-0.61241700
C	1.16744900	-1.70866400	1.57125000
C	2.09319300	0.20986300	2.77483500
C	2.43530100	2.89179100	0.98979000

C	4.39354300	2.06193900	-0.10972800
C	4.51121800	-1.10775700	0.25289600
C	3.41357300	-1.48430600	-1.83874700
C	0.89283600	-2.55899500	0.37573200
C	0.89645300	-2.23916300	2.81724200
C	1.81593000	-0.36329700	4.02426900
H	2.58477000	1.18046200	2.75229600
C	3.06948300	4.09639200	1.31201000
H	1.40756800	2.72832100	1.31868400
C	5.05814000	3.27035400	0.09025900
H	4.90309500	1.24787800	-0.61457300
C	5.57216200	-1.94607400	-0.09206400
H	4.50220700	-0.64863300	1.24106000
C	4.46288400	-2.29337100	-2.27778600
H	2.52382100	-1.36998600	-2.44991600
C	-0.22101700	-2.44265500	-0.50714200
C	1.72205500	-3.63846800	0.15091200
C	1.20562500	-1.59280300	4.00782800
H	2.06499500	0.14001200	4.95568900
C	4.35285700	4.29735500	0.75896600
C	5.58133200	-2.42221600	-1.41975500
P	-1.24971200	-0.93586500	-0.29874300
C	-0.41374800	-3.37000600	-1.52897900
C	1.51585800	-4.56263700	-0.86606600
C	-2.79358900	-1.11822600	-1.27405000
C	-1.90445500	-1.22599100	1.39419800
C	0.45226800	-4.45839600	-1.72909000
H	-1.27691800	-3.26442600	-2.18576300
C	-4.01857200	-0.88973900	-0.65812000
C	-2.77315500	-1.22267200	-2.66813600
C	-2.51051900	-2.44062900	1.69069800
C	-1.86451000	-0.23360600	2.37073000
H	0.28386800	-5.19026800	-2.51536000
C	-5.22645000	-0.83016500	-1.36031300
H	-4.04227000	-0.73305400	0.41693900
C	-3.94146800	-1.25859100	-3.42772700
H	-1.81049700	-1.27930400	-3.16823000
C	-3.19845900	-2.66607200	2.88664700
H	-2.47619300	-3.22901800	0.93894900
C	-2.51448600	-0.38894400	3.59628600
H	-1.31802500	0.68287500	2.15332700
C	-5.17105200	-1.12822900	-2.73400700
C	-3.27604200	-1.57085600	3.77199900
C	0.02713700	-3.39258400	4.48741300



H	-1.04135500	-3.14027800	4.63094900
H	0.27152300	-4.35646500	4.94616400
O	0.31618600	-3.44023800	3.09909000
O	0.83307800	-2.37596200	5.05956800
H	3.69643900	-5.86596000	0.83214400
C	3.42337300	-5.05578000	0.14674400
H	4.31187400	-4.67128800	-0.38834400
O	2.47385700	-5.53343200	-0.79369600
O	2.81797200	-4.00043200	0.87533300
O	4.98003100	5.51685900	0.87619200
O	6.70256100	-3.04926800	-1.91475500
O	-4.11587000	-1.62402900	4.86218200
O	-6.33231100	-1.28361600	-3.45898100
C	7.72038800	-2.13455800	-2.27033900
H	8.54306900	-2.72042300	-2.69388100
H	7.36340500	-1.41099800	-3.01878100
H	8.08950700	-1.57284600	-1.39877100
C	4.36248300	-3.04842500	-3.61338600
C	6.57661600	-2.28094200	1.02897600
C	6.53776000	3.40181500	-0.30608100
C	4.50181700	6.49327100	-0.02701700
H	3.50361300	6.85950500	0.25284900
H	5.20617000	7.33174800	0.00644600
H	4.45245500	6.10067000	-1.05300300
C	2.33094000	5.05043500	2.27449000
C	-3.79229200	-4.07261600	3.10919400
C	-2.33378900	0.63795500	4.72664100
C	-5.45333400	-1.31355400	4.52635400
H	-5.93094000	-2.12512800	3.95521400
H	-5.99685400	-1.17198100	5.46690200
H	-5.51129500	-0.38969100	3.92909600
C	-6.47396500	-0.42597800	-0.54815300
C	-3.87124600	-1.32789200	-4.96345000
C	-6.93929500	-2.54507700	-3.27721200
H	-7.73669200	-2.62863000	-4.02408900
H	-6.21727300	-3.36156600	-3.42579600
H	-7.38074100	-2.65202900	-2.27499900
Cu	0.21517300	0.78622700	-1.25458200
C	-1.69356800	3.35315300	-1.01086800
O	-1.33682300	2.07973700	-1.45349300
C	-3.06671000	3.71276700	-1.58908000
C	-3.57959900	5.00903800	-1.52399700
C	-3.86145200	2.71357800	-2.15850200
C	-4.83859300	5.30638100	-2.03756900

H	-2.99036700	5.80584400	-1.06750100
C	-5.11982600	3.00761200	-2.67419600
H	-3.47163100	1.69598900	-2.19720800
C	-5.61309600	4.30798900	-2.62049100
H	-5.21617800	6.32689100	-1.98276700
H	-5.71146400	2.21091300	-3.13048000
H	-6.59556300	4.54249400	-3.02786200
C	-0.61606100	4.35906200	-1.42915400
H	-0.56997200	4.43347900	-2.52397400
H	-0.78497400	5.36861800	-1.02884300
H	0.36040800	4.00141700	-1.06326000
C	-2.42583600	-1.43701700	-5.46140500
H	-1.81195000	-0.56936600	-5.18565500
H	-1.92890400	-2.34761900	-5.09308600
H	-2.42962500	-1.48609900	-6.55827200
C	-4.61658400	-2.53888200	-5.54296800
H	-4.30401400	-3.47310300	-5.05342200
H	-5.70178200	-2.44025900	-5.45704200
H	-4.38311300	-2.63318600	-6.61289500
C	-4.46725100	-0.03731300	-5.54421600
H	-4.38635800	-0.04638700	-6.64089500
H	-5.52554500	0.06993300	-5.28018300
H	-3.92780800	0.84710100	-5.17496400
C	-7.66903200	0.04274300	-1.38496200
H	-8.16508200	-0.75641200	-1.94190200
H	-8.41880400	0.47791800	-0.70933100
H	-7.37227700	0.82085400	-2.09997800
C	-6.11878100	0.76763900	0.35921000
H	-5.37794300	0.50987500	1.12886600
H	-5.72755900	1.61930100	-0.21675000
H	-7.02125900	1.10208900	0.89066500
C	-6.89356700	-1.58477500	0.36420000
H	-6.07734100	-1.84943500	1.05267800
H	-7.76696700	-1.29731800	0.96892300
H	-7.15724100	-2.49044600	-0.20026500
C	-2.74520200	-5.13221200	2.72039500
H	-2.43887100	-5.08396000	1.66923900
H	-1.83654600	-5.04223700	3.32930000
H	-3.16480300	-6.13384600	2.88811200
C	-4.18144900	-4.38848700	4.55840500
H	-5.05613000	-3.83316400	4.90832600
H	-4.42331100	-5.45841900	4.63064300
H	-3.35839400	-4.18176300	5.25550700
C	-5.01754200	-4.27522500	2.20879200

H	-5.84525400	-3.60804000	2.48652600
H	-4.77874000	-4.08553300	1.15208100
H	-5.38375900	-5.30895800	2.29376900
C	-1.73513100	-0.07358500	5.94977100
H	-0.75872900	-0.52138500	5.71423800
H	-1.58427400	0.65254000	6.76232300
H	-2.39504500	-0.86440500	6.32309600
C	-1.35354200	1.74552600	4.32330000
H	-0.37727500	1.33921700	4.02004300
H	-1.74756500	2.36808900	3.50687500
H	-1.18447100	2.40246000	5.18759100
C	-3.64461300	1.32250800	5.13597000
H	-4.18730200	1.69725300	4.25800600
H	-4.29864600	0.65258900	5.70310700
H	-3.42378800	2.19028600	5.77417800
C	1.69776000	4.22190400	3.40933200
H	0.93031700	3.51791000	3.06289400
H	2.46297400	3.65209100	3.95643100
H	1.20608700	4.89596600	4.12417300
C	3.23587400	6.07036300	2.97730000
H	4.10708300	5.58588300	3.43664700
H	3.60307800	6.86401600	2.32195800
H	2.65904800	6.55538700	3.77743200
C	1.19920000	5.78121600	1.54355200
H	0.45868100	5.07419000	1.14621900
H	0.67982500	6.46008800	2.23564800
H	1.56502900	6.37791400	0.69691900
C	7.36993500	3.58503900	0.97033400
H	8.43701900	3.66755100	0.71632000
H	7.07746400	4.48914300	1.51687300
H	7.24821700	2.71986800	1.63866800
C	6.80652400	4.56921400	-1.26438100
H	6.70241100	5.53971100	-0.77238200
H	7.83687800	4.50376000	-1.64220800
H	6.13375900	4.53602300	-2.13343400
C	7.04885300	2.13806900	-1.00848300
H	6.96552200	1.24134500	-0.37828800
H	6.51954300	1.94459600	-1.95287300
H	8.11320800	2.26993100	-1.24595300
C	5.77995200	-2.74334700	2.26445600
H	5.06038100	-1.99904500	2.62870300
H	5.21323300	-3.65905100	2.04789900
H	6.47496900	-2.96067600	3.08758700
C	7.55504500	-3.41989700	0.72014000

H	8.30647500	-3.16113200	-0.03181300
H	8.09567900	-3.67325600	1.64330800
H	7.03580800	-4.32374200	0.37693300
C	7.38196700	-1.03070400	1.40707800
H	8.02255500	-0.69572300	0.57833900
H	6.73054600	-0.18883500	1.68549700
H	8.03603900	-1.24589800	2.26443000
C	4.53922000	-4.55536100	-3.37890400
H	3.73512900	-4.95690800	-2.74468600
H	4.49531100	-5.08533300	-4.34171100
H	5.50441900	-4.78328300	-2.91242400
C	5.41102000	-2.56593300	-4.62439400
H	6.42462700	-2.86798500	-4.34258600
H	5.20071000	-3.00409400	-5.61054100
H	5.38347700	-1.47199800	-4.73412500
C	2.99049600	-2.85052100	-4.26491800
H	2.16657700	-3.16763000	-3.60785300
H	2.81350700	-1.80720500	-4.56282000
H	2.93909800	-3.46223200	-5.17565100
C	-1.05157500	2.02797400	-4.05551400
C	-1.23964600	3.29926500	-4.77162300
H	-1.26942900	2.17461500	-2.76314600
C	-2.39674600	3.83422000	-5.17376300
H	-0.32035800	3.87094600	-4.95284500
H	-2.43128000	4.79953500	-5.67442200
H	-3.35359000	3.33875000	-5.00202000
C	0.28377100	1.54165600	-3.87724600
H	1.05932000	2.31878400	-3.93242000
C	0.71083700	0.31137500	-3.44288600
H	0.09022700	-0.58581300	-3.52718500
H	1.78371500	0.14207800	-3.38021800
H	-1.81936600	1.26493200	-4.24775300
C	-3.91664100	3.02058400	1.88758200
C	-2.98482500	2.58020600	1.02606300
C	-1.79887300	3.33639600	0.53387100
H	-4.75162100	2.35432700	2.12807800
H	-3.10564800	1.57891800	0.60094100
H	-1.81123400	4.37083300	0.90981900
H	-0.86327800	2.86754300	0.89932600
C	-3.94724000	4.30517100	2.56228900
C	-4.89200800	4.65210200	3.44416400
H	-3.14945100	5.01700900	2.33982700
H	-4.89406700	5.62078600	3.93850200
H	-5.70622400	3.97127200	3.69673900

**(E)-(R)-TS3**

P	2.11227200	0.27684000	0.08880400
C	1.80621900	-0.46405600	1.74311900
C	3.14042300	1.75841800	0.38482000
C	3.31373300	-0.95156600	-0.55696600
C	1.08549100	-1.69026600	1.77828500
C	2.25531500	0.12964000	2.92189700
C	2.59608000	2.81598500	1.10574200
C	4.41208800	1.90626600	-0.16401400
C	4.41090100	-1.29361800	0.22240700
C	3.13594400	-1.59589500	-1.77878500
C	0.72686600	-2.53798000	0.60511700
C	0.84068700	-2.20011100	3.03743700
C	2.01538600	-0.43046800	4.18464100
H	2.82463400	1.05654400	2.86730200
C	3.28870000	4.01177800	1.32112500
H	1.60001600	2.69214400	1.53884800
C	5.12349600	3.10048600	-0.06825400
H	4.84783500	1.06682100	-0.69582500
C	5.40419200	-2.17084200	-0.21770600
H	4.49641400	-0.85211000	1.21550000
C	4.10444400	-2.45015300	-2.30603100
H	2.21159600	-1.42531300	-2.32083400
C	-0.37760600	-2.37557000	-0.27986800
C	1.49490400	-3.66868400	0.40449100
C	1.28879400	-1.59577500	4.20646600
H	2.37679100	0.03528700	5.09854500
C	4.50892200	4.16632400	0.62893300
C	5.28498300	-2.63211300	-1.54506600
P	-1.32257100	-0.79572200	-0.17353900
C	-0.62319700	-3.32490200	-1.27325400
C	1.23913000	-4.60493200	-0.58828700
C	-2.77972800	-1.00858800	-1.26665200
C	-2.00596700	-0.90503200	1.52910300
C	0.17694500	-4.46516400	-1.44713900
H	-1.47453300	-3.18958700	-1.93874900
C	-4.09574100	-0.93280800	-0.82913500
C	-2.54661000	-1.07185800	-2.64334300
C	-2.75235900	-2.00767800	1.92242100
C	-1.72649100	0.08253100	2.47369500
H	-0.03409500	-5.20248100	-2.21809100
C	-5.18943000	-0.95775900	-1.70758000
H	-4.27963400	-0.82853500	0.23712700

C	-3.57691700	-1.19479600	-3.57072800
H	-1.51748700	-1.04094400	-2.99151200
C	-3.32965200	-2.11322000	3.19143400
H	-2.89971700	-2.81165400	1.20047100
C	-2.26115400	0.05037700	3.76300200
H	-1.07110900	0.89987200	2.17884400
C	-4.90411300	-1.17372800	-3.07188400
C	-3.14773500	-1.01418600	4.05973500
C	-0.03302700	-3.26594400	4.75316500
H	-1.05323000	-2.87717500	4.93817500
H	0.10912200	-4.25032400	5.21011100
O	0.18492200	-3.35373500	3.35463700
O	0.91818700	-2.35477800	5.27738400
H	3.44315000	-5.94121300	1.06960800
C	3.14607800	-5.13595200	0.38938800
H	4.01367400	-4.75803300	-0.18594600
O	2.15467700	-5.61443200	-0.50563300
O	2.57662300	-4.07127100	1.13221700
O	5.14358600	5.38737900	0.62010900
O	6.33809500	-3.29228200	-2.13685600
O	-3.84210800	-0.97075000	5.24639000
O	-5.91264200	-1.30991100	-3.99955800
C	7.34055100	-2.40690100	-2.59434000
H	8.09460200	-3.01503500	-3.10533200
H	6.93104400	-1.66653400	-3.29813000
H	7.82019500	-1.86296600	-1.76554400
C	3.85297400	-3.19768000	-3.62525500
C	6.47891400	-2.56717300	0.81438800
C	6.56112800	3.17763600	-0.60787300
C	4.56228400	6.30175600	-0.28816600
H	3.52458700	6.54678900	-0.01697900
H	5.16656800	7.21473000	-0.25274700
H	4.56388600	5.90388300	-1.31382700
C	2.67683800	4.99800500	2.33649700
C	-4.07777000	-3.42760200	3.49430200
C	-1.84271300	1.09467000	4.81612200
C	-5.17339500	-0.51414100	5.09436800
H	-5.70877500	-1.07434700	4.31112700
H	-5.67501400	-0.66971700	6.05571700
H	-5.20563000	0.55242100	4.83076000
C	-6.59651900	-0.75714600	-1.10821700
C	-3.25576700	-1.30355600	-5.07039400
C	-6.59632300	-2.54344700	-4.03389500
H	-6.86423700	-2.74956200	-5.07728500

H	-5.96552600	-3.36337200	-3.65985000
H	-7.52516600	-2.50739600	-3.44700500
Cu	0.21436400	0.91533300	-1.07443100
C	-1.71048900	3.53243400	-0.94450400
O	-1.26137500	2.27775600	-1.35956500
C	-3.07188900	3.80986000	-1.58979100
C	-3.64107000	5.08444600	-1.58474300
C	-3.79411600	2.76406400	-2.17119900
C	-4.88303600	5.31597200	-2.16870400
H	-3.10810000	5.91789000	-1.12490300
C	-5.03009600	2.99499300	-2.76663000
H	-3.36432500	1.76210000	-2.16692800
C	-5.57997700	4.27338200	-2.77115100
H	-5.30425700	6.32084700	-2.16030100
H	-5.55257900	2.16761400	-3.25151200
H	-6.54528800	4.45671400	-3.24130900
C	-0.67535200	4.59995200	-1.31582700
H	-0.62545900	4.72422900	-2.40491100
H	-0.89090500	5.58209700	-0.87216500
H	0.31119300	4.26988600	-0.95334200
C	-1.74509200	-1.32310500	-5.33312300
H	-1.24645300	-0.39616600	-5.02166800
H	-1.24395800	-2.17180200	-4.84090500
H	-1.57650900	-1.42489800	-6.41327300
C	-3.80824600	-2.60205400	-5.67574300
H	-3.52823400	-3.47533400	-5.06778100
H	-4.89501700	-2.58502400	-5.78339300
H	-3.38635500	-2.74828700	-6.68017500
C	-3.83509200	-0.09360000	-5.81502900
H	-3.59526200	-0.16127500	-6.88628200
H	-4.92344200	-0.03708000	-5.70719000
H	-3.40031500	0.84291000	-5.43577200
C	-7.56121900	-0.01658000	-2.04492000
H	-7.74515200	-0.51676400	-2.99697800
H	-8.52624800	0.11167600	-1.53476000
H	-7.17291200	0.98666500	-2.27042900
C	-6.51986600	0.11907300	0.15217000
H	-6.04980500	-0.39557900	1.00373700
H	-5.97171400	1.05429800	-0.03343800
H	-7.53649200	0.38586200	0.47263200
C	-7.18066900	-2.10718700	-0.66970900
H	-6.52439900	-2.58097700	0.07405200
H	-8.16541300	-1.95847200	-0.20242900
H	-7.30476500	-2.81686000	-1.49496000

C	-3.13767200	-4.60728900	3.18463600
H	-2.73920400	-4.59702600	2.16391800
H	-2.27802100	-4.61249500	3.86826100
H	-3.67800100	-5.55475300	3.32005800
C	-4.53099500	-3.63741500	4.94375000
H	-5.36546900	-2.99359400	5.23753000
H	-4.87913400	-4.67535900	5.04611000
H	-3.71598400	-3.48244800	5.66055100
C	-5.30595300	-3.53165900	2.58031800
H	-6.00290000	-2.69572600	2.74091200
H	-5.02349000	-3.52796100	1.51780500
H	-5.85152200	-4.46599300	2.77761000
C	-1.20750900	0.37474000	6.01482000
H	-0.31336900	-0.18894500	5.71847500
H	-0.90208400	1.11434200	6.76973900
H	-1.91229300	-0.31838900	6.48725500
C	-0.79710900	2.06450200	4.25369300
H	0.10388600	1.54533600	3.89236500
H	-1.20692000	2.68119200	3.43866000
H	-0.48148700	2.74668400	5.05541100
C	-3.00576400	1.95592900	5.32828400
H	-3.58522200	2.39754400	4.50565100
H	-3.68111700	1.38596900	5.97285100
H	-2.60078300	2.77961900	5.93388900
C	2.33280000	4.21043500	3.61490300
H	1.58872800	3.42143300	3.45082200
H	3.23375200	3.74728900	4.04261500
H	1.91362300	4.89288600	4.36772200
C	3.60137400	6.13094600	2.79799500
H	4.57446400	5.75298000	3.13391700
H	3.78064100	6.89416500	2.03507700
H	3.12379900	6.63731100	3.64874600
C	1.38322300	5.60357500	1.78045100
H	0.63102600	4.83149700	1.56373700
H	0.94644000	6.29753500	2.51328600
H	1.55806900	6.16245900	0.85007800
C	7.51367300	3.39476400	0.57627300
H	8.55466500	3.43030500	0.22247000
H	7.30007100	4.33272200	1.10024700
H	7.43105900	2.56875600	1.29755200
C	6.76516200	4.29489100	-1.63850800
H	6.72514600	5.28831300	-1.18388700
H	7.75556400	4.18768100	-2.10348700
H	6.01524000	4.23847800	-2.44062800



C	6.97860600	1.87134600	-1.29477700
H	6.92348100	1.00256600	-0.62315000
H	6.36876900	1.65487000	-2.18405400
H	8.02245000	1.96224500	-1.62448100
C	5.76068100	-3.05884100	2.08607200
H	5.07296000	-2.32181300	2.51941700
H	5.17205500	-3.96334500	1.87935400
H	6.50576700	-3.30925100	2.85434000
C	7.40965500	-3.71202900	0.40006400
H	8.11069100	-3.44246600	-0.39588700
H	8.01085100	-4.00056600	1.27425400
H	6.85171500	-4.59732000	0.07036700
C	7.33601000	-1.34705500	1.17518700
H	7.90745300	-0.98555700	0.30810500
H	6.72765000	-0.50978900	1.54725800
H	8.05815400	-1.60974400	1.96165200
C	3.96382100	-4.70983500	-3.38534700
H	3.20752700	-5.05627300	-2.66579500
H	3.79683300	-5.24855600	-4.32964900
H	4.95478700	-4.98733400	-3.00923100
C	4.83782000	-2.78496400	-4.72734600
H	5.84826800	-3.16160800	-4.54187000
H	4.50583700	-3.19984800	-5.68985400
H	4.87872000	-1.69136600	-4.83525200
C	2.44556100	-2.92269800	-4.16765900
H	1.65952400	-3.17725600	-3.44103400
H	2.31196100	-1.87425300	-4.47103500
H	2.28264100	-3.54278000	-5.05950300
C	-0.83066000	2.25868800	-3.94298900
C	-1.04063900	3.52294600	-4.66032900
H	-1.11948000	2.38711600	-2.65898200
C	-2.18176100	3.95639900	-5.20515200
H	-0.16304700	4.18024900	-4.71042900
H	-2.24935300	4.92840700	-5.68898700
H	-3.09457800	3.35984100	-5.17747500
C	0.51204400	1.83306700	-3.68331000
H	1.25067700	2.64668200	-3.65833900
C	0.95823500	0.61028000	-3.25265000
H	0.37331200	-0.30153400	-3.41130100
H	2.02792800	0.47150000	-3.10231000
H	-1.54983100	1.46219200	-4.18459000
C	-3.98239700	3.03154000	1.85902100
C	-2.96884900	2.64115900	1.07310600
C	-1.87916000	3.52674400	0.58957700

H	-4.05744800	4.08027200	2.16643300
H	-2.93600600	1.60042700	0.73690700
H	-2.04900500	4.55394300	0.95310700
H	-0.90500000	3.18962900	0.99794100
C	-5.00568300	2.12266800	2.33571900
C	-6.11257800	2.48049100	2.99780900
H	-4.82166700	1.06209000	2.12913100
H	-6.84906500	1.74487600	3.31850300
H	-6.32983600	3.52488100	3.22372700

**(Z)-(R)-P<sub>l</sub>**

C	0.08094600	-0.74672200	0.43608500
O	0.18793900	-2.16562900	0.44873600
C	1.43827100	-0.10942200	0.16731600
C	1.70766900	1.21848000	0.50832700
C	2.42990500	-0.84120300	-0.48945900
C	2.93811900	1.79532600	0.21310200
H	0.94786400	1.81521400	1.01280600
C	3.66234900	-0.26736200	-0.78305500
H	2.22084600	-1.87217300	-0.77002400
C	3.92270100	1.05288000	-0.43132500
H	3.12901600	2.83089400	0.49124200
H	4.42405200	-0.85639900	-1.29222000
H	4.88782500	1.50267400	-0.65879600
C	-0.52503100	-0.28062000	1.75496700
H	0.18524800	-0.42727900	2.58127200
H	-0.80282300	0.78134300	1.73682400
H	-1.43320600	-0.85823700	1.96165800
C	-3.37194700	-0.42539500	-0.45650500
C	-2.20079100	-1.05826500	-0.63035700
C	-0.85201900	-0.42840600	-0.74665800
H	-4.28085800	-1.03040900	-0.39684600
H	-2.20496900	-2.14780500	-0.68091500
H	-0.34901700	-0.79989500	-1.65387400
H	-0.91446500	0.66402100	-0.84724000
C	-3.57816100	1.00622100	-0.33188700
C	-4.78176100	1.56465800	-0.16236300
H	-2.69840000	1.65262000	-0.37251900
H	-4.91174500	2.64012000	-0.06708500
H	-5.68530700	0.95587700	-0.11464200
H	0.76093100	-2.40655600	1.19134200

**(E)-(R)-P<sub>l</sub>**

C	-0.17189900	0.50606100	0.46426600
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O	-0.08073200	1.92528500	0.52413700
C	-1.59862000	0.07404600	0.15120100
C	-2.04203200	-1.22751700	0.40177200
C	-2.48314900	0.97511700	-0.44408100
C	-3.33936500	-1.61152100	0.08123500
H	-1.36834800	-1.95566000	0.85341900
C	-3.78290400	0.59421300	-0.76230600
H	-2.13603300	1.98472700	-0.65632600
C	-4.21717700	-0.70001200	-0.49756600
H	-3.66703100	-2.62916800	0.28919800
H	-4.45968300	1.31426200	-1.22038700
H	-5.23473800	-0.99926300	-0.74379800
C	0.33261800	-0.08023000	1.77813900
H	-0.37378600	0.12800100	2.59437500
H	0.47362000	-1.16733600	1.72421500
H	1.30219800	0.36696400	2.02483100
C	3.18133600	-0.38845800	-0.46958800
C	2.16471800	0.48263600	-0.52410400
C	0.73645200	0.10044700	-0.71007000
H	2.97587200	-1.45967700	-0.57395400
H	2.37004000	1.55052600	-0.41155900
H	0.32226500	0.58661100	-1.60867200
H	0.64666500	-0.98647000	-0.86132800
C	4.56827100	-0.00757200	-0.28354400
C	5.58696000	-0.87187700	-0.23142800
H	4.76288200	1.06369400	-0.18113200
H	6.61417600	-0.54483400	-0.08894200
H	5.42408800	-1.94544900	-0.33143200
H	-0.61756800	2.21879000	1.27484400

**(Z)-(S)-TS2**

P	-1.58136300	-0.79928100	0.28763400
C	-0.72782200	-1.94563300	1.43208400
C	-2.78148900	-1.81515200	-0.64974300
C	-2.58634000	0.27748700	1.35725500
C	0.29997200	-1.39828200	2.24970600
C	-0.95204900	-3.32123000	1.39229800
C	-2.26552700	-2.73228700	-1.56218300
C	-4.15769800	-1.58219200	-0.65221100
C	-3.51388100	-0.19339400	2.27812100
C	-2.40960800	1.65097500	1.20849200
C	0.52480900	0.05539200	2.50242800
C	1.05614200	-2.31729600	2.94814000
C	-0.17777600	-4.22833800	2.12928000

H	-1.74728500	-3.71232600	0.75925900
C	-3.05512200	-3.36681600	-2.52412000
H	-1.19544300	-2.94831600	-1.54001600
C	-4.99037500	-2.11529300	-1.63748400
H	-4.57858500	-0.93357500	0.11307300
C	-4.37922900	0.66957000	2.96107400
H	-3.57694200	-1.26969600	2.44954900
C	-3.22984600	2.56996100	1.85506200
H	-1.62230600	1.99388700	0.53800400
C	1.38309400	0.91969900	1.76277100
C	-0.08527300	0.61656600	3.60567600
C	0.83316000	-3.68988700	2.88629000
H	-0.36241500	-5.29961200	2.10150900
C	-4.38481800	-2.91501800	-2.63118300
C	-4.28974800	2.04016600	2.62801000
P	1.91514900	0.35133600	0.09238400
C	1.61103700	2.22381800	2.20110500
C	0.13070200	1.93020100	4.01158500
C	3.07796400	1.62568000	-0.51143400
C	2.99096300	-1.07732400	0.45711100
C	0.99718900	2.75741500	3.34359200
H	2.27466200	2.86830600	1.62783300
C	4.39210700	1.35134900	-0.86374300
C	2.56498100	2.89341400	-0.78023000
C	4.07578800	-0.97627400	1.31674900
C	2.72100100	-2.29978700	-0.15028100
H	1.18167600	3.77763400	3.67184300
C	5.23320100	2.30879800	-1.44133700
H	4.76143900	0.34012900	-0.72394300
C	3.37150500	3.92930700	-1.24664500
H	1.50408900	3.06058000	-0.60839100
C	4.98561100	-2.02362400	1.50211500
H	4.23098200	-0.03044200	1.83712100
C	3.57304200	-3.39223700	-0.00733900
H	1.81538200	-2.37875600	-0.74918300
C	4.72117100	3.62183600	-1.54818000
C	4.75968000	-3.18871700	0.73850200
C	2.67527800	-3.34222400	4.03676700
H	3.55484800	-3.46002800	3.37603300
H	2.95142100	-3.43364200	5.09226200
O	2.08633000	-2.07149400	3.80780500
O	1.71167500	-4.32833300	3.70907000
H	-1.66320400	0.80707100	6.24140700
C	-1.52205400	1.10560600	5.19789900

H	-2.47754100	1.40988700	4.72685900
O	-0.60462400	2.18398400	5.13195800
O	-0.96575200	0.02488900	4.46521400
O	-5.13295700	-3.22913700	-3.74232000
O	-5.26369800	2.91269800	3.05907900
O	5.70695900	-4.18802500	0.70368200
O	5.49439100	4.65479300	-2.03327200
C	-6.41870100	2.86760300	2.24539500
H	-7.10534600	3.63329600	2.62232400
H	-6.17623000	3.08073500	1.19262900
H	-6.91536900	1.88539200	2.29206500
C	-2.93120600	4.07294000	1.76176200
C	-5.32850200	0.04349900	4.00334400
C	-6.50744300	-1.87395300	-1.61152800
C	-4.77398400	-2.43954000	-4.86165400
H	-5.53623500	-2.60725700	-5.63033300
H	-4.74492200	-1.37034500	-4.59835100
H	-3.78920000	-2.72157800	-5.26432700
C	-2.41386600	-4.50672000	-3.33603800
C	6.14346400	-1.77849800	2.49026900
C	3.18279400	-4.76642000	-0.57310400
C	6.75074400	-3.92340000	-0.21196400
H	7.37122600	-3.07240200	0.10694500
H	7.37510400	-4.82257500	-0.25205200
H	6.35876600	-3.70547400	-1.21636300
C	6.62020000	1.84473300	-1.93140100
C	2.76863900	5.32917700	-1.43886500
C	6.49565500	5.19094700	-1.19831300
H	6.46827400	6.28466300	-1.28382500
H	6.33433900	4.91511000	-0.14607000
H	7.49386200	4.85455900	-1.51284500
Cu	-0.05598600	0.18980600	-1.21770100
C	1.31090700	5.37636400	-0.96722200
H	0.67362100	4.65915700	-1.49909300
H	1.21705000	5.17402700	0.11148500
H	0.90567000	6.38125800	-1.15068300
C	3.51783300	6.38522400	-0.61490800
H	3.65321800	6.05299900	0.42514300
H	4.49734100	6.62500200	-1.03554500
H	2.93629500	7.31804300	-0.59366100
C	2.79241700	5.71796300	-2.92180700
H	2.36525700	6.72337400	-3.05441300
H	3.81215700	5.72143200	-3.32147400
H	2.19053500	5.01758400	-3.51760800

C	7.01709100	2.51953500	-3.25084400
H	7.12231600	3.60391100	-3.17718400
H	7.97247200	2.10536300	-3.60319500
H	6.25953600	2.32018900	-4.02199100
C	6.62125400	0.33363700	-2.22411600
H	6.52832900	-0.27904600	-1.31542000
H	5.81363800	0.04778900	-2.91160800
H	7.57681600	0.06204000	-2.69315100
C	7.69310300	2.06503400	-0.85596100
H	7.43048300	1.52236000	0.06292800
H	8.66098700	1.67785900	-1.20766800
H	7.83530900	3.11622200	-0.58839200
C	5.59189900	-1.16531800	3.78969900
H	5.02203100	-0.24256900	3.63601300
H	4.93859000	-1.87295400	4.31701300
H	6.42840500	-0.92532200	4.46042900
C	6.91458800	-3.02944700	2.92865600
H	7.55039400	-3.45492800	2.14719100
H	7.57280400	-2.75596200	3.76567300
H	6.23898300	-3.82149300	3.27695100
C	7.11871900	-0.76795200	1.87243400
H	7.54644100	-1.13191600	0.92676900
H	6.61343600	0.18583100	1.66118600
H	7.95089100	-0.56430600	2.56200500
C	3.14021200	-5.78256400	0.57800300
H	2.39875300	-5.48810600	1.33604400
H	2.85206900	-6.77200100	0.19315500
H	4.11628500	-5.87802500	1.06729600
C	1.78495000	-4.73286000	-1.20061400
H	1.02366000	-4.39034200	-0.48452100
H	1.73726800	-4.09079400	-2.09405400
H	1.51110500	-5.74931400	-1.51571900
C	4.14180200	-5.26161500	-1.66281800
H	4.28500000	-4.49822500	-2.44173800
H	5.11868700	-5.54478200	-1.25958100
H	3.71770200	-6.15307900	-2.14668200
C	-1.33788400	-3.96953400	-4.28558100
H	-1.75120500	-3.27004300	-5.02507700
H	-0.54252100	-3.43472800	-3.74907200
H	-0.87156800	-4.80136400	-4.83310200
C	-1.74718600	-5.46684600	-2.33279900
H	-0.96161600	-4.98608700	-1.73669400
H	-2.49044800	-5.88398000	-1.63809500
H	-1.27955900	-6.30293800	-2.87230400

C	-3.40075900	-5.36633100	-4.13396300
H	-3.82604100	-4.85397300	-5.00202100
H	-2.86491900	-6.25024700	-4.50809900
H	-4.23253400	-5.71631700	-3.50948800
C	-7.24335900	-3.22110300	-1.67831900
H	-8.32966300	-3.05480700	-1.63536700
H	-7.01576000	-3.76485300	-2.60075900
H	-6.96779200	-3.85511900	-0.82353200
C	-6.96999500	-0.97675400	-2.76667300
H	-6.87509400	-1.47644000	-3.73600700
H	-8.03085600	-0.71950800	-2.63111800
H	-6.39657900	-0.03873100	-2.80077600
C	-6.94629100	-1.20966500	-0.30346400
H	-6.64957500	-1.80682800	0.56965100
H	-6.54626900	-0.19250400	-0.16986100
H	-8.04192600	-1.12853100	-0.29286400
C	-4.52118100	-0.87724200	4.93653300
H	-3.93204400	-1.63738700	4.41210200
H	-3.83359100	-0.29642000	5.56581200
H	-5.21075100	-1.40428500	5.61074200
C	-6.03580700	1.03839800	4.93093200
H	-6.82060100	1.61762200	4.43573900
H	-6.51402500	0.47428100	5.74450900
H	-5.32977700	1.74819400	5.38087700
C	-6.38221300	-0.81337200	3.29265900
H	-6.99762800	-0.21742600	2.60400700
H	-5.91517000	-1.61925000	2.70819200
H	-7.05621800	-1.27762500	4.02717700
C	-2.74732000	4.62299500	3.18389300
H	-1.92832700	4.10297800	3.70521000
H	-2.49362000	5.69252700	3.14310100
H	-3.66050600	4.51213200	3.77961900
C	-4.03544600	4.85401700	1.03910900
H	-4.96355100	4.88970100	1.61849500
H	-3.70685400	5.89182900	0.88357200
H	-4.24663600	4.42010000	0.04937200
C	-1.62779300	4.33535500	0.99569600
H	-0.76360500	3.82990100	1.45522500
H	-1.68457800	4.02302400	-0.05836000
H	-1.42429800	5.41550500	1.00897000
C	0.22984800	-0.63223300	-3.16352100
C	-0.99333200	-0.19390100	-3.72806000
C	-1.21244800	0.93031900	-4.49535400
H	-1.87662300	-0.77635400	-3.43193600

H	-0.38282000	1.40550700	-5.01765200
H	-2.20248500	1.11649500	-4.91015200
C	1.51620400	-0.05858700	-3.52514900
C	2.71762400	-0.65366700	-3.43025700
H	1.48881200	0.97927500	-3.87268700
H	3.63228800	-0.12611000	-3.69572600
H	2.82671600	-1.68041400	-3.07172100
C	-1.17358100	2.64721100	-2.79806000
C	-2.65799100	2.69993300	-2.68386100
C	-3.40984800	3.73297300	-3.25696500
C	-3.32154100	1.76243600	-1.88589400
C	-4.77894100	3.83165200	-3.02443400
H	-2.92155100	4.48191200	-3.87839900
C	-4.68047800	1.86883500	-1.63980500
H	-2.74569500	0.94201600	-1.46293200
C	-5.42075000	2.90625300	-2.20687400
H	-5.34373500	4.64575200	-3.47664900
H	-5.15943400	1.14194300	-0.98242100
H	-6.49028900	2.98741300	-2.01464300
C	-0.50825300	3.63806400	-3.72238000
H	-0.96889500	3.68289300	-4.71568900
H	-0.55971400	4.64798500	-3.28069200
H	0.55054700	3.37118700	-3.82421300
O	-0.49177000	2.15979400	-1.86145600
H	0.26083700	-1.67581600	-2.81907800

**(E)-(S)-TS2**

P	-1.58839100	-0.66411600	0.08748100
C	-0.76438800	-1.82081900	1.24934500
C	-2.81174100	-1.68521900	-0.81500100
C	-2.54792900	0.41382200	1.20130100
C	0.22327200	-1.29144900	2.12718600
C	-1.02434100	-3.19049600	1.21250500
C	-2.30786700	-2.54596700	-1.78685400
C	-4.19159400	-1.58518900	-0.66567000
C	-3.40244200	-0.08129000	2.18045800
C	-2.36386700	1.79007500	1.08502900
C	0.51965400	0.15396900	2.35457600
C	0.89588600	-2.22459400	2.89137100
C	-0.33468800	-4.10947900	2.01535800
H	-1.78687700	-3.56924800	0.53391800
C	-3.12761500	-3.29744500	-2.63224800
H	-1.22394500	-2.64163400	-1.86953000
C	-5.07441800	-2.24352600	-1.52501900



H	-4.58259500	-0.94969300	0.12463400
C	-4.19171700	0.76250700	2.96996700
H	-3.45637400	-1.16165300	2.32529900
C	-3.12302600	2.68948000	1.82795600
H	-1.62803400	2.15072100	0.36703800
C	1.37903900	0.96971600	1.56308400
C	0.00843100	0.75204600	3.48975800
C	0.63394500	-3.58999100	2.83765300
H	-0.54764900	-5.17544800	1.98427500
C	-4.51517400	-3.03923000	-2.55060900
C	-4.11593100	2.14235000	2.67383800
P	1.91024200	0.29863400	-0.06859200
C	1.67980200	2.27098100	1.96235300
C	0.30541000	2.05873700	3.86353300
C	3.13737800	1.48949500	-0.71295700
C	2.94299900	-1.12098500	0.44334000
C	1.15241900	2.84642900	3.12660100
H	2.34805800	2.87290100	1.35041300
C	4.43664000	1.12941900	-1.04507400
C	2.70555900	2.78203900	-1.01191700
C	3.96263300	-0.95690300	1.36949300
C	2.71328800	-2.38220700	-0.09515000
H	1.39682900	3.86232800	3.42788800
C	5.33893500	2.02171900	-1.63566500
H	4.74776500	0.10321700	-0.87134500
C	3.58551100	3.76117200	-1.46846300
H	1.65373400	3.01824700	-0.85824000
C	4.84812800	-1.98742300	1.69977800
H	4.08334800	0.02402800	1.82841600
C	3.54690800	-3.46229900	0.18924700
H	1.86096000	-2.49686800	-0.76015600
C	4.91366500	3.36396900	-1.75910700
C	4.67049100	-3.20859600	1.01391400
C	2.43124900	-3.28235000	4.06491100
H	3.32725200	-3.43558900	3.43134300
H	2.66941700	-3.37008700	5.12963400
O	1.88477400	-1.99865900	3.80459500
O	1.44779900	-4.24236100	3.71505500
H	-1.32463800	1.01755000	6.25156900
C	-1.26734800	1.30457000	5.19675100
H	-2.24976100	1.63940000	4.81198800
O	-0.32567800	2.34948700	5.03719400
O	-0.81749900	0.20065700	4.42719000
O	-5.38770900	-3.59422200	-3.45698900

O	-5.03314000	3.01425200	3.21609900
O	5.60113500	-4.21675500	1.14300700
O	5.75514700	4.34092900	-2.24351700
C	-6.26302400	3.00556400	2.51882000
H	-6.83917800	3.86730000	2.87338800
H	-6.10859000	3.09286000	1.43142000
H	-6.83732600	2.08720600	2.71550700
C	-2.84418100	4.19757900	1.75114500
C	-5.03449900	0.12069600	4.09196100
C	-6.59270500	-2.11534900	-1.31946200
C	-5.42332800	-2.99827000	-4.73791500
H	-6.45546000	-3.05540300	-5.10421200
H	-5.11396600	-1.94323600	-4.69892700
H	-4.78038100	-3.53538900	-5.44964700
C	-2.46496700	-4.34300100	-3.55036900
C	5.92976200	-1.66303000	2.75016200
C	3.20522900	-4.86528900	-0.33569700
C	6.73083300	-4.04120300	0.31228800
H	7.38683200	-3.23615800	0.67550000
H	7.28901400	-4.98385500	0.32488900
H	6.43697700	-3.80536000	-0.72099700
C	6.68965100	1.45791500	-2.12033100
C	3.07428000	5.19326400	-1.69518800
C	6.79294600	4.79396200	-1.40233600
H	6.83720100	5.88860300	-1.46339800
H	6.61581100	4.50812000	-0.35567400
H	7.76492100	4.39667100	-1.72794300
Cu	-0.07589000	0.33114200	-1.41359200
C	1.66931600	5.38090100	-1.11053000
H	0.92970100	4.69089400	-1.53074100
H	1.66295700	5.25290500	-0.01668600
H	1.32473200	6.40209800	-1.32613100
C	3.95707800	6.25153400	-1.01724100
H	4.20456000	5.96610700	0.01603300
H	4.88552800	6.43169200	-1.56406800
H	3.41485000	7.20674700	-0.97462600
C	3.01662200	5.47202300	-3.20164600
H	2.64664100	6.49161000	-3.38684600
H	4.00807500	5.37572100	-3.66031300
H	2.33727700	4.76933400	-3.70375300
C	7.14555100	2.10181500	-3.43646900
H	7.32492700	3.17644500	-3.36388300
H	8.07380300	1.62096900	-3.77568600
H	6.38556000	1.95316600	-4.21633700

C	6.57583300	-0.04843100	-2.41687300
H	6.45386100	-0.65449600	-1.50728700
H	5.74050900	-0.27227000	-3.09470900
H	7.50258200	-0.38794500	-2.89925800
C	7.77010100	1.59585000	-1.03926000
H	7.46319100	1.07193600	-0.12297900
H	8.70891700	1.13959900	-1.38673700
H	7.98660500	2.63406600	-0.76991200
C	5.29702000	-0.88179500	3.91709900
H	4.88508600	0.08934000	3.62132600
H	4.48561700	-1.44947900	4.39117800
H	6.06252900	-0.68490100	4.68008800
C	6.60943100	-2.87787800	3.39247600
H	7.26692600	-3.43031200	2.71707500
H	7.22920000	-2.52805000	4.23017900
H	5.87511600	-3.58838700	3.79454800
C	6.99017200	-0.75947700	2.10565400
H	7.50906900	-1.25721300	1.27383400
H	6.53113000	0.15726300	1.70590000
H	7.74868300	-0.46469300	2.84563000
C	3.06303100	-5.82629700	0.85310200
H	2.26112400	-5.49852100	1.52987400
H	2.80820800	-6.83420300	0.49322000
H	3.99279000	-5.89500200	1.42887000
C	1.87115000	-4.86231700	-1.08841600
H	1.04696300	-4.47282600	-0.47424100
H	1.91966000	-4.26791700	-2.01408200
H	1.61473900	-5.89178700	-1.37500400
C	4.25428200	-5.40924600	-1.31352800
H	4.45847900	-4.68582100	-2.11691900
H	5.19559900	-5.66324900	-0.81746200
H	3.87506700	-6.32827200	-1.78301800
C	-1.98383700	-3.70111800	-4.85849900
H	-2.79828100	-3.23682800	-5.42717000
H	-1.23341500	-2.92132200	-4.66906900
H	-1.51747100	-4.46237700	-5.50088300
C	-1.22823700	-4.93359600	-2.84978200
H	-0.41107200	-4.21056500	-2.73122400
H	-1.47801600	-5.32831400	-1.85357500
H	-0.82792600	-5.76039200	-3.45208200
C	-3.37528300	-5.54109000	-3.85079800
H	-4.22741600	-5.30240300	-4.49051800
H	-2.78652500	-6.31714900	-4.35909500
H	-3.77227200	-5.97441800	-2.92230200

C	-7.22230000	-3.50510900	-1.14962100
H	-8.30578900	-3.40649100	-0.98842300
H	-7.06074100	-4.13627200	-2.02721600
H	-6.79818000	-4.01516400	-0.27315200
C	-7.26203100	-1.37440300	-2.48446000
H	-7.26869600	-1.96602900	-3.40437800
H	-8.30977800	-1.15667800	-2.23079400
H	-6.76090700	-0.41742500	-2.69195500
C	-6.92161200	-1.33853500	-0.04154100
H	-6.48431100	-1.81851500	0.84398600
H	-6.58116000	-0.29186100	-0.06214100
H	-8.01115100	-1.32211400	0.09716900
C	-4.17296100	-0.90455400	4.85157100
H	-3.79241800	-1.71271700	4.21697800
H	-3.30661400	-0.43063400	5.33059200
H	-4.77838200	-1.37080000	5.64118600
C	-5.54480700	1.10010100	5.15619200
H	-6.33098600	1.77013200	4.79694700
H	-5.96337400	0.52024400	5.99108000
H	-4.73539800	1.72639300	5.55428900
C	-6.22697200	-0.63632400	3.49685500
H	-6.88917000	0.01991100	2.91532800
H	-5.89101000	-1.44347700	2.83138600
H	-6.82605900	-1.09301500	4.29814100
C	-2.56804400	4.72525100	3.16604800
H	-1.69457800	4.22205300	3.60710900
H	-2.35105100	5.80296000	3.12851300
H	-3.42637500	4.57131900	3.83013000
C	-4.00895400	4.97326900	1.12244600
H	-4.89125900	4.99321000	1.77037200
H	-3.70452300	6.01623700	0.95151000
H	-4.29041900	4.54440100	0.14811100
C	-1.60441900	4.49514500	0.89848400
H	-0.70269000	3.97800200	1.26356100
H	-1.75170500	4.21981200	-0.15585100
H	-1.40328300	5.57514000	0.93484200
C	-1.35892100	2.92506500	-2.64147300
C	-2.84353900	2.90910700	-2.49780000
C	-3.62363600	4.01860300	-2.84604900
C	-3.48161500	1.81322900	-1.90770900
C	-4.99461500	4.03316300	-2.60023000
H	-3.15840200	4.89309400	-3.29832900
C	-4.84314400	1.82906300	-1.65393500
H	-2.88655700	0.93118400	-1.67754000

C	-5.61117100	2.94252500	-1.99696700
H	-5.58055600	4.90942200	-2.87495800
H	-5.30900500	0.96091500	-1.18599000
H	-6.68259300	2.95321400	-1.79991700
C	-0.75435300	4.04344200	-3.45555800
H	-1.27733500	4.22620300	-4.40131800
H	-0.77108600	4.97870000	-2.87057500
H	0.29414700	3.79733200	-3.66354300
O	-0.63662300	2.38108600	-1.76469400
C	0.45707600	0.07447900	-3.46767700
C	1.08728900	-1.22605000	-3.32888800
C	2.41344900	-1.45550000	-3.28274400
H	2.82485100	-2.45859100	-3.17566600
H	3.13012100	-0.63329600	-3.34926400
C	-0.86571700	0.24780100	-3.93451400
H	-1.56388800	-0.58338400	-3.76109800
C	-1.35358400	1.41699900	-4.48521500
H	-0.64357400	2.09367600	-4.95816900
H	-2.37666800	1.46459900	-4.85558400
H	1.14836000	0.90583500	-3.66625400
H	0.40956100	-2.08919500	-3.26698300

**(Z)-(S)-C**

P	-1.58914600	-0.80384500	0.29698000
C	-0.74590200	-1.93076300	1.46658400
C	-2.78078900	-1.84105400	-0.62746200
C	-2.58831400	0.30850400	1.33106000
C	0.29658500	-1.36896900	2.25448700
C	-0.99015500	-3.30342000	1.47789400
C	-2.26576300	-2.79029000	-1.50873100
C	-4.15568800	-1.60348100	-0.64327600
C	-3.52484100	-0.13168500	2.25851500
C	-2.39680000	1.67614800	1.14218200
C	0.53163500	0.08982800	2.46004900
C	1.04972200	-2.27246100	2.97531300
C	-0.21881500	-4.19424900	2.23786700
H	-1.79796700	-3.70535200	0.86764600
C	-3.05577200	-3.45263600	-2.45145100
H	-1.20013800	-3.02572200	-1.46278200
C	-4.98971500	-2.16961400	-1.60917500
H	-4.57454400	-0.92422000	0.09603100
C	-4.39108700	0.75658500	2.90613900
H	-3.59491400	-1.20225200	2.46014500
C	-3.21907100	2.61650900	1.75520500

H	-1.61445600	1.99722300	0.45223100
C	1.39430200	0.92758000	1.69561600
C	-0.07488200	0.68583400	3.54743100
C	0.80875300	-3.64335300	2.96295700
H	-0.41660000	-5.26353000	2.24960100
C	-4.38535200	-3.00300000	-2.57445000
C	-4.29069500	2.11541000	2.53001600
P	1.91143500	0.32230000	0.03153800
C	1.63669500	2.23854500	2.10323400
C	0.15238200	2.00779700	3.91860400
C	3.06444300	1.59036200	-0.60781800
C	2.99359100	-1.09789200	0.42172000
C	1.02972300	2.80733000	3.23180400
H	2.30237200	2.86362000	1.51213100
C	4.38030100	1.32928200	-0.96930800
C	2.53811000	2.85999700	-0.85330300
C	4.08952400	-0.96591700	1.26346000
C	2.70975900	-2.34661400	-0.12523000
H	1.22410300	3.83462500	3.53088600
C	5.21046800	2.30698700	-1.53213000
H	4.76472900	0.32151900	-0.83413400
C	3.34819800	3.91738700	-1.26439300
H	1.46832300	3.00592400	-0.71041400
C	4.99913900	-2.00779700	1.47969000
H	4.25359000	-0.00020900	1.74357900
C	3.55801100	-3.43585500	0.05723300
H	1.79195900	-2.45366500	-0.70048200
C	4.69817300	3.62317600	-1.57519800
C	4.76075700	-3.20112500	0.76745600
C	2.67718100	-3.28031700	4.06183700
H	3.53259700	-3.42832100	3.37553000
H	2.98587400	-3.34413300	5.11002100
O	2.09403800	-2.01131200	3.81340500
O	1.69357100	-4.26534200	3.79292900
H	-1.65364000	0.96086100	6.17559600
C	-1.50873300	1.22979500	5.12457700
H	-2.46064400	1.52993700	4.64447700
O	-0.58114500	2.29749500	5.03069100
O	-0.96043400	0.12458400	4.42211200
O	-5.13359700	-3.35712100	-3.67370800
O	-5.27611900	3.00238300	2.90183000
O	5.71419000	-4.19538100	0.74654800
O	5.48070600	4.67774200	-1.99304000
C	-6.39963300	2.92813200	2.04542800

H	-7.06231000	3.75778800	2.31428900
H	-6.10407000	3.02155800	0.98831700
H	-6.94427900	1.97790800	2.16778900
C	-2.91776200	4.11504800	1.61246900
C	-5.35264800	0.17234500	3.96000200
C	-6.50589700	-1.92146600	-1.59121600
C	-4.78142700	-2.60676500	-4.81999600
H	-5.54146900	-2.80861300	-5.58256600
H	-4.76260400	-1.52853800	-4.59722400
H	-3.79441100	-2.89681500	-5.21288300
C	-2.42050100	-4.62510000	-3.22077500
C	6.16442600	-1.73087100	2.44988700
C	3.15039600	-4.83802100	-0.42035900
C	6.72885400	-3.95117300	-0.20667700
H	7.32980100	-3.06534400	0.05075400
H	7.37884700	-4.83285300	-0.21400100
H	6.30608000	-3.80097200	-1.21154900
C	6.58761600	1.86715500	-2.07194800
C	2.75057900	5.32838700	-1.38365900
C	6.47947800	5.14114400	-1.11193900
H	6.46885700	6.23810200	-1.12121400
H	6.30147100	4.79579000	-0.08327100
H	7.47718100	4.81200100	-1.43560700
Cu	-0.12793100	0.34220100	-1.14405700
C	1.31133500	5.36549800	-0.85844800
H	0.64309700	4.66017000	-1.36588900
H	1.27009300	5.14314100	0.21991500
H	0.90252400	6.37564800	-1.00208200
C	3.53148000	6.35084900	-0.54544100
H	3.71196500	5.97657100	0.47365000
H	4.48968800	6.61744300	-0.99761200
H	2.94448900	7.27632600	-0.45901000
C	2.74346400	5.77537900	-2.85042500
H	2.33460500	6.79366600	-2.93143100
H	3.75452800	5.77653300	-3.27437600
H	2.11167600	5.11430300	-3.45901500
C	6.99607500	2.64386200	-3.33086100
H	7.14987000	3.71154800	-3.16470100
H	7.93006500	2.22431900	-3.73103500
H	6.22405800	2.54616100	-4.10689900
C	6.55194800	0.39025200	-2.50373900
H	6.42940600	-0.30794700	-1.66359400
H	5.74475500	0.20344200	-3.22562600
H	7.50333400	0.13549700	-2.99041300

C	7.66911500	1.97397300	-0.98916000
H	7.40621700	1.35035400	-0.12357900
H	8.63298600	1.61561100	-1.38022600
H	7.81811300	2.99532900	-0.62490700
C	5.61311300	-1.10243300	3.74177400
H	5.02615600	-0.19271900	3.57479000
H	4.97539600	-1.81154000	4.28601300
H	6.45003300	-0.83646300	4.40213000
C	6.95954800	-2.96146700	2.90181400
H	7.58800700	-3.39265600	2.11727300
H	7.62839100	-2.66035700	3.72085000
H	6.30337800	-3.75636300	3.27870700
C	7.12264500	-0.72263500	1.80375000
H	7.55600500	-1.10978600	0.86982500
H	6.60443700	0.21739100	1.56473100
H	7.95225100	-0.48730000	2.48613800
C	3.16134400	-5.79419500	0.78192900
H	2.46741300	-5.45124500	1.56435800
H	2.84277200	-6.79817400	0.46516600
H	4.16163300	-5.87681300	1.22156400
C	1.72575800	-4.84519300	-0.98624800
H	0.98744900	-4.48511600	-0.25359900
H	1.63203900	-4.24154200	-1.90318100
H	1.45327300	-5.87637000	-1.25125100
C	4.06802100	-5.38107700	-1.52244800
H	4.16817900	-4.65824900	-2.34616200
H	5.06562900	-5.62713800	-1.14646300
H	3.63976400	-6.30358700	-1.94023500
C	-1.33345400	-4.12723800	-4.17943000
H	-1.72450700	-3.40027700	-4.90523500
H	-0.50672500	-3.64225000	-3.64292100
H	-0.91024100	-4.97171200	-4.74216100
C	-1.76876100	-5.56146600	-2.18616400
H	-0.99673100	-5.06633700	-1.58343700
H	-2.52366700	-5.96698800	-1.49754800
H	-1.28858000	-6.40669800	-2.70011800
C	-3.40732000	-5.50031200	-4.00236300
H	-3.81619500	-5.01295300	-4.89262400
H	-2.87587600	-6.40142400	-4.34017900
H	-4.25013600	-5.82118500	-3.37777400
C	-7.25113800	-3.26476500	-1.62577900
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H	-7.03189900	-3.83151700	-2.53581200
H	-6.97850200	-3.88136700	-0.75733500



C	-6.96013800	-1.04748800	-2.76702000
H	-6.87051900	-1.57073700	-3.72454700
H	-8.01891800	-0.77889100	-2.63802200
H	-6.37959900	-0.11453300	-2.82049400
C	-6.94084100	-1.22395400	-0.29972800
H	-6.64576500	-1.80109900	0.58722500
H	-6.53534500	-0.20633900	-0.19332600
H	-8.03595100	-1.13739500	-0.29020100
C	-4.55902700	-0.72594300	4.92593900
H	-3.98589500	-1.51491200	4.42645300
H	-3.85844700	-0.13448300	5.53062800
H	-5.25504800	-1.21582700	5.62137300
C	-6.05398100	1.20601700	4.84759900
H	-6.82559000	1.77897300	4.32522300
H	-6.54618300	0.67707700	5.67655700
H	-5.34134000	1.92175400	5.27788600
C	-6.41070600	-0.69785400	3.27258700
H	-7.01752400	-0.11949600	2.56190200
H	-5.94719700	-1.52581000	2.71662600
H	-7.09222600	-1.13319200	4.01795200
C	-2.75983600	4.71369400	3.01802200
H	-1.95270700	4.20854200	3.57258700
H	-2.49895900	5.77976400	2.94450900
H	-3.68460200	4.62834400	3.60059200
C	-4.00880800	4.86914900	0.84229800
H	-4.94825800	4.92675500	1.40164100
H	-3.67540000	5.90028200	0.65584500
H	-4.20013100	4.40024800	-0.13520200
C	-1.60206300	4.34727500	0.85863400
H	-0.74581100	3.86836200	1.35998700
H	-1.62419600	3.97790600	-0.17819300
H	-1.40279700	5.42838000	0.82880900
C	0.31048300	-0.80019900	-3.17536100
C	-0.81238000	-0.07370200	-3.42576600
C	-0.83222900	1.30512900	-3.98822500
H	-1.77610200	-0.55915600	-3.23277700
H	0.14517800	1.52490800	-4.44067500
H	-1.57489300	1.36311800	-4.80032600
C	1.68940300	-0.38928700	-3.41624500
C	2.72105100	-1.24134300	-3.39178100
H	1.87474400	0.67039200	-3.60802600
H	3.74330000	-0.91123600	-3.56433500
H	2.57871800	-2.30608600	-3.19360200
C	-1.12537400	2.44769100	-2.93692500

C	-2.65133300	2.59235900	-2.77778700
C	-3.40622700	3.59056600	-3.40362900
C	-3.33299000	1.71043400	-1.93707800
C	-4.77568800	3.71640500	-3.17763300
H	-2.92310900	4.30019100	-4.07345300
C	-4.69506800	1.83487000	-1.69539900
H	-2.76343300	0.92882600	-1.44100700
C	-5.42946100	2.84379000	-2.31382800
H	-5.33090200	4.51155000	-3.67456900
H	-5.17978700	1.14503900	-1.00189800
H	-6.49819000	2.94564600	-2.12493400
C	-0.53447500	3.71818200	-3.56103500
H	-0.84514800	3.87763800	-4.60481000
H	-0.80380600	4.60905400	-2.97674800
H	0.55895700	3.60883200	-3.54172000
O	-0.51513100	2.20368400	-1.73361700
H	0.18911400	-1.83322800	-2.83229300

**(E)-(S)-C**

P	-1.59481100	-0.66713000	0.07644600
C	-0.77465400	-1.84200500	1.22049600
C	-2.83232200	-1.67356400	-0.82941300
C	-2.53384200	0.41546100	1.19999100
C	0.22544100	-1.33119900	2.09517800
C	-1.05237400	-3.20774700	1.17505300
C	-2.35771500	-2.49004500	-1.85332200
C	-4.20876000	-1.58666900	-0.63547800
C	-3.37131000	-0.06966300	2.19918500
C	-2.35177100	1.79150500	1.05906700
C	0.54400100	0.10940300	2.32172600
C	0.88444600	-2.27713900	2.85553800
C	-0.37323000	-4.14028300	1.97123600
H	-1.82151700	-3.57185000	0.49517900
C	-3.20495700	-3.18024200	-2.72620500
H	-1.27574300	-2.60165100	-1.95585900
C	-5.11653200	-2.18318700	-1.51316600
H	-4.57615400	-0.99686500	0.19998000
C	-4.16686000	0.78351500	2.97280700
H	-3.41745100	-1.14769400	2.36858300
C	-3.09604200	2.69624700	1.81104300
H	-1.64033000	2.15045000	0.31128900
C	1.40228900	0.92211700	1.52571200
C	0.04965300	0.70778500	3.46400200
C	0.60076000	-3.63783100	2.79746100

H	-0.59924000	-5.20351500	1.93463200
C	-4.58411600	-2.90374900	-2.60496600
C	-4.09421700	2.15721300	2.65556800
P	1.91447500	0.27196100	-0.12172400
C	1.71856400	2.21837500	1.92863400
C	0.35932800	2.01063400	3.84046800
C	3.16464300	1.45442800	-0.74003500
C	2.91949400	-1.18032600	0.36535800
C	1.20845400	2.79291700	3.10064800
H	2.37981500	2.82063700	1.31014700
C	4.48098700	1.11347400	-1.02726700
C	2.72322700	2.74414100	-1.03848500
C	3.94584000	-1.03624500	1.28916300
C	2.65659500	-2.44284200	-0.15747100
H	1.46209800	3.80669200	3.40110400
C	5.39300500	2.03202400	-1.56070200
H	4.79901300	0.08806900	-0.85990400
C	3.60671700	3.74385000	-1.44278500
H	1.65800400	2.95693400	-0.94014600
C	4.81022900	-2.08323600	1.62259100
H	4.08965400	-0.05655700	1.74447900
C	3.46463100	-3.54047400	0.13575100
H	1.78988000	-2.55273500	-0.80484600
C	4.95204700	3.37067300	-1.67553700
C	4.60499000	-3.30181100	0.94134700
C	2.40576200	-3.36340600	4.02130400
H	3.29956000	-3.52860400	3.38620200
H	2.64468600	-3.45902600	5.08521100
O	1.87957000	-2.07075000	3.76675500
O	1.40750400	-4.30701900	3.66972600
H	-1.25295700	0.96848300	6.23963600
C	-1.20547100	1.25930400	5.18531800
H	-2.19069700	1.59942700	4.81252800
O	-0.25965200	2.30026100	5.02040600
O	-0.76809800	0.15648000	4.40766500
O	-5.47008200	-3.34758200	-3.55973300
O	-5.03781600	3.02574600	3.15769800
O	5.52812400	-4.31921800	1.05154600
O	5.81322300	4.35766500	-2.09880400
C	-6.22443400	2.99815500	2.38830900
H	-6.85357400	3.82443500	2.73701200
H	-6.00903300	3.12594200	1.31543000
H	-6.77165800	2.05032300	2.51870500
C	-2.78765900	4.19908500	1.75390000

C	-5.01655900	0.15023600	4.09394800
C	-6.62992400	-2.08925000	-1.25423000
C	-5.47919200	-2.55860700	-4.73256800
H	-6.38753300	-2.81810000	-5.28758000
H	-5.49340400	-1.48545200	-4.49085100
H	-4.60644400	-2.76235000	-5.36919700
C	-2.57125700	-4.19297000	-3.70072800
C	5.89720600	-1.78084900	2.67459600
C	3.08264200	-4.94707100	-0.35276000
C	6.64269200	-4.14061400	0.20113900
H	7.28261200	-3.30793600	0.53026600
H	7.22390700	-5.06862700	0.23399500
H	6.32916400	-3.94253700	-0.83464500
C	6.77566600	1.51116500	-2.00477700
C	3.05647500	5.15342300	-1.71573200
C	6.75879100	4.84073200	-1.16894900
H	6.68110300	5.93410600	-1.11152100
H	6.58388000	4.42665100	-0.16596400
H	7.77824200	4.58541800	-1.49226500
Cu	-0.12080700	0.54460000	-1.30302100
C	1.67614700	5.34273600	-1.07123800
H	0.92014400	4.62562200	-1.40979600
H	1.73787000	5.26894800	0.02612000
H	1.30277300	6.34739200	-1.31588800
C	3.93851200	6.28163100	-1.16291000
H	4.26358500	6.07526400	-0.13232900
H	4.81988800	6.45868700	-1.78434600
H	3.35984800	7.21567600	-1.14307500
C	2.93438600	5.32247700	-3.23486400
H	2.49905700	6.30300300	-3.47952600
H	3.91796400	5.25090400	-3.71738500
H	2.28634200	4.54614100	-3.66460300
C	7.26341400	2.19021800	-3.29194500
H	7.43742000	3.26251800	-3.18081500
H	8.20218600	1.72122200	-3.61891500
H	6.52514800	2.06248400	-4.09608900
C	6.71158600	0.00879200	-2.32991200
H	6.54555300	-0.61892500	-1.44273100
H	5.92362100	-0.21597400	-3.06178300
H	7.67127300	-0.30485600	-2.76271200
C	7.81941400	1.66378000	-0.89065500
H	7.49376100	1.14114800	0.01965800
H	8.77377000	1.21843500	-1.20875200
H	8.01652600	2.70648500	-0.62389400

C	5.26694200	-1.03605900	3.86576700
H	4.79145500	-0.08799200	3.59139100
H	4.50679000	-1.64891800	4.36707100
H	6.04856800	-0.80380800	4.60213400
C	6.59046500	-3.00724700	3.27934500
H	7.25882700	-3.52503500	2.58659000
H	7.20311200	-2.67591800	4.12977600
H	5.86634800	-3.74213300	3.65415300
C	6.95092200	-0.85680400	2.04927900
H	7.45618500	-1.32641000	1.19278800
H	6.49138600	0.07650400	1.69131900
H	7.72055200	-0.59382000	2.78952700
C	2.99058900	-5.89434700	0.85194000
H	2.24919100	-5.53444000	1.57843500
H	2.67969600	-6.89557500	0.51905900
H	3.95460200	-5.98818500	1.36422800
C	1.71030800	-4.94676200	-1.03707000
H	0.90898400	-4.57928500	-0.37649000
H	1.70693500	-4.34469700	-1.95950300
H	1.45411200	-5.97636000	-1.32416200
C	4.08482300	-5.51153800	-1.36774500
H	4.25915200	-4.80535500	-2.19307000
H	5.04700700	-5.75475500	-0.90699400
H	3.68708500	-6.43982500	-1.80240600
C	-1.90867900	-3.47943600	-4.88588400
H	-2.63318200	-2.92680200	-5.49767000
H	-1.14547800	-2.76061200	-4.55817700
H	-1.41451200	-4.21355200	-5.53870200
C	-1.47993300	-4.97812800	-2.95003700
H	-0.62765700	-4.35708500	-2.64852200
H	-1.88338200	-5.45554000	-2.04516900
H	-1.07979600	-5.76785000	-3.60066500
C	-3.54767400	-5.25051500	-4.23062900
H	-4.28291600	-4.85658900	-4.93690500
H	-2.97278200	-6.02683100	-4.75493500
H	-4.09726000	-5.73377200	-3.41212000
C	-7.21871400	-3.50344200	-1.14707600
H	-8.29509600	-3.44436600	-0.92918800
H	-7.08757700	-4.06892200	-2.07401800
H	-6.74083900	-4.06038800	-0.32872200
C	-7.37035500	-1.30486700	-2.34584100
H	-7.41487700	-1.85257500	-3.29161900
H	-8.40697800	-1.12489900	-2.02616000
H	-6.90368300	-0.32538600	-2.52785800

C	-6.92425900	-1.39392400	0.07709400
H	-6.44615900	-1.91382600	0.91741100
H	-6.60362800	-0.34019200	0.10155500
H	-8.00795700	-1.40753300	0.25601900
C	-4.11608000	-0.74136400	4.96695300
H	-3.53050100	-1.46943600	4.39439000
H	-3.41101000	-0.13699600	5.55270800
H	-4.73872500	-1.29972700	5.68023100
C	-5.67943200	1.13853400	5.06044800
H	-6.49983300	1.70430600	4.60841700
H	-6.09920400	0.56882100	5.90222900
H	-4.96068500	1.86156300	5.46651300
C	-6.10576100	-0.73924300	3.48484400
H	-6.77639700	-0.17022600	2.82601000
H	-5.67025600	-1.55831300	2.89535500
H	-6.71769300	-1.19040400	4.27956600
C	-2.53023000	4.70359700	3.18094000
H	-1.68219100	4.17183300	3.63805700
H	-2.28005100	5.77454100	3.15845600
H	-3.40887100	4.57117500	3.82329500
C	-3.92170200	5.00931600	1.11661800
H	-4.81719200	5.03775700	1.74685500
H	-3.59068700	6.04764800	0.96791700
H	-4.18721500	4.59842400	0.13156800
C	-1.52205800	4.47048400	0.93164700
H	-0.64517200	3.93426100	1.32799800
H	-1.62385600	4.18191700	-0.12401800
H	-1.29972800	5.54683100	0.97086000
C	0.64244300	0.01699200	-3.51214000
C	-0.64930800	0.40549200	-3.67199700
C	-0.99318600	1.81673400	-4.01413700
H	-1.44198900	-0.34997700	-3.61518400
H	-0.12549400	2.23509700	-4.54651600
H	-1.84108800	1.84483700	-4.71494600
C	1.12231700	-1.34737700	-3.36826200
C	2.41874900	-1.67767800	-3.39544200
H	0.36632000	-2.13130600	-3.25602900
H	2.75505100	-2.70990800	-3.31222000
H	3.19047700	-0.91205600	-3.49436800
C	-1.28041900	2.79745100	-2.79867600
C	-2.79632100	2.80567000	-2.51316900
C	-3.60752500	3.93393200	-2.67613300
C	-3.41343000	1.64815900	-2.03093800
C	-4.96452100	3.91349400	-2.35574900

H	-3.18616400	4.86165300	-3.05748800
C	-4.75968000	1.62278600	-1.69191700
H	-2.81293900	0.74748500	-1.90704900
C	-5.54959600	2.75847900	-1.85070900
H	-5.56159000	4.81436900	-2.49640000
H	-5.18961700	0.70329100	-1.29629300
H	-6.60845900	2.73584700	-1.59140100
C	-0.83721100	4.17590400	-3.30356300
H	-1.32261900	4.46159900	-4.24932300
H	-1.03263500	4.95521300	-2.55440300
H	0.24599800	4.14128900	-3.47358500
O	-0.55958400	2.46028600	-1.68149200
H	1.42015700	0.78363700	-3.61689500

**(Z)-(S)-TS3**

P	1.95146500	0.00807400	0.10347300
C	1.47928900	-0.08468800	1.88703100
C	3.16839900	1.36836700	0.00296800
C	2.97321600	-1.50576300	-0.02110200
C	0.60266800	-1.13127400	2.28563600
C	1.89652800	0.86677100	2.81804100
C	2.76392800	2.65305300	0.35219400
C	4.46270300	1.18239300	-0.47183600
C	4.02227200	-1.69950400	0.86857000
C	2.65865700	-2.51781200	-0.92299200
C	0.20890600	-2.34404700	1.51395800
C	0.16027800	-1.08059400	3.59289200
C	1.45313100	0.87471300	4.14897300
H	2.59612100	1.63893700	2.50693600
C	3.63072000	3.74863200	0.33144200
H	1.73889100	2.79399100	0.69591000
C	5.35243300	2.24553000	-0.62239600
H	4.77624800	0.17767400	-0.73677800
C	4.83924400	-2.83020800	0.83244700
H	4.20505500	-0.93296600	1.62114300
C	3.44441000	-3.66505800	-1.03938300
H	1.76570600	-2.40124000	-1.53006400
C	-0.90245300	-2.44380400	0.63310600
C	0.84478600	-3.52924400	1.82643000
C	0.55792900	-0.10538000	4.49946600
H	1.78884800	1.62658100	4.85972100
C	4.90673100	3.53253400	-0.23904900
C	4.59159300	-3.74536800	-0.21480500
P	-1.60156400	-0.84775400	0.03109300

C	-1.32881800	-3.69587000	0.18764600
C	0.42939200	-4.76432900	1.34416900
C	-2.99077600	-1.27671400	-1.08114000
C	-2.48022800	-0.23150800	1.52063900
C	-0.67374000	-4.88668300	0.53602900
H	-2.20935600	-3.76550600	-0.44651300
C	-4.13308000	-0.48679000	-1.07433200
C	-2.83120000	-2.18597100	-2.13057600
C	-3.44304000	-1.03442500	2.11633400
C	-2.17710500	1.00220400	2.09622300
H	-1.02203700	-5.85562400	0.18670200
C	-5.15554400	-0.63157500	-2.01945900
H	-4.22623700	0.28877100	-0.31359800
C	-3.83092800	-2.43254900	-3.06584700
H	-1.88714800	-2.71103100	-2.22676500
C	-4.19008200	-0.61909100	3.21950500
H	-3.62268300	-2.02122000	1.69022800
C	-2.89302900	1.49508600	3.19143600
H	-1.36548700	1.58772200	1.66550800
C	-5.03213800	-1.69729800	-2.93067400
C	-3.96471700	0.70080900	3.66428900
C	-1.06625400	-1.27538500	5.40424500
H	-2.01888300	-0.73845000	5.22223300
H	-1.15658500	-1.99264100	6.22499200
O	-0.68389900	-1.95267700	4.21924500
O	-0.04434000	-0.33582500	5.70197900
H	2.61381100	-5.51661100	3.36562000
C	2.33245600	-5.04714700	2.41737200
H	3.17654200	-5.04663100	1.70025900
O	1.23468600	-5.74263300	1.84951200
O	1.91694600	-3.71070400	2.65261200
O	5.79463100	4.57062400	-0.39939200
O	5.47738700	-4.77153400	-0.45519300
O	-4.80622600	1.25792300	4.60077600
O	-6.09278400	-2.04083700	-3.73850500
C	6.62199400	-4.34881400	-1.16932400
H	7.18792900	-5.24979300	-1.42959600
H	6.34477300	-3.81334200	-2.08962900
H	7.26157800	-3.68652200	-0.56649500
C	3.03121400	-4.79987300	-1.99137200
C	5.88671800	-2.96609600	1.95607500
C	6.78438900	1.97185700	-1.11014000
C	5.53919500	5.47860800	-1.45346600
H	5.13001200	6.42443900	-1.07027900



H	6.48983200	5.69801200	-1.95554800
H	4.83347000	5.05567800	-2.18317500
C	3.13468500	5.07342300	0.94494800
C	-5.15473500	-1.64952800	3.83433300
C	-2.46970200	2.79221300	3.90742900
C	-6.00383000	1.74510600	4.03069100
H	-6.62531000	0.93359000	3.62180800
H	-6.55632400	2.24970500	4.83076900
H	-5.79935700	2.46320400	3.22176900
C	-6.26109500	0.44088000	-2.00202000
C	-3.56439200	-3.37568700	-4.24916500
C	-7.06320900	-2.81279300	-3.06474100
H	-7.87030200	-3.00628200	-3.77970700
H	-6.64606300	-3.77096600	-2.71818900
H	-7.47493900	-2.28416100	-2.19119300
Cu	0.10282600	0.32946900	-1.24849900
C	-1.01994000	3.23198700	-2.10424700
O	-1.04751700	1.84373500	-1.99350300
C	-2.14479500	-3.95221300	-4.19833500
H	-1.37328200	-3.16896600	-4.22896800
H	-1.97744400	-4.57559700	-3.30576100
H	-1.99002900	-4.59269800	-5.07686600
C	-4.52715100	-4.56889800	-4.28172300
H	-4.53984500	-5.09825200	-3.31715700
H	-5.54845100	-4.26892200	-4.53371700
H	-4.19824400	-5.28521600	-5.04821500
C	-3.68547400	-2.58029200	-5.55697200
H	-3.47081200	-3.23750400	-6.41266500
H	-4.69294600	-2.16942700	-5.68832100
H	-2.97015400	-1.74496400	-5.58296900
C	-7.24596600	0.40745900	-3.17552600
H	-7.92619700	-0.44974000	-3.15764200
H	-7.86874500	1.31217000	-3.12591800
H	-6.72616300	0.41054000	-4.14121800
C	-5.56558300	1.81139800	-2.09562500
H	-4.88731900	2.01463600	-1.25811400
H	-4.97494300	1.87732300	-3.02163500
H	-6.31648800	2.61430100	-2.11083400
C	-7.05276500	0.36294500	-0.69030900
H	-6.40533500	0.47058600	0.19288900
H	-7.80384600	1.16551400	-0.65448500
H	-7.58318200	-0.59616600	-0.59593300
C	-4.40366600	-2.98339000	4.00724800
H	-4.04240300	-3.40984200	3.06446600

H	-3.53264000	-2.86298900	4.66670500
H	-5.07317700	-3.72581600	4.46320100
C	-5.68562900	-1.29634900	5.22847900
H	-6.40541300	-0.47308200	5.23017900
H	-6.20081800	-2.17641200	5.63908200
H	-4.87147300	-1.02986500	5.91535000
C	-6.33751700	-1.87611400	2.88377200
H	-6.93282800	-0.96140700	2.75274100
H	-5.99902700	-2.19343800	1.88706600
H	-7.00496900	-2.65496700	3.28087900
C	-2.11744600	2.45914700	5.36446400
H	-1.28378300	1.74627000	5.42051000
H	-1.80898900	3.37528300	5.88947600
H	-2.97430500	2.03518600	5.90163000
C	-1.22483300	3.40531400	3.25989000
H	-0.37389200	2.70860300	3.23952000
H	-1.43081500	3.74617600	2.23507400
H	-0.91463000	4.28305100	3.84404100
C	-3.54939600	3.88306200	3.90022100
H	-3.90849100	4.08742300	2.88316800
H	-4.39874200	3.62792700	4.54089000
H	-3.11917300	4.81963300	4.28313800
C	2.09528200	4.79804100	2.04788500
H	1.14778000	4.40299000	1.65849000
H	2.47554800	4.09951400	2.80814200
H	1.85152300	5.74127100	2.55517700
C	4.25538700	5.86168600	1.63507000
H	4.76123200	5.23800000	2.38562900
H	5.02226900	6.23565600	0.95530900
H	3.81873000	6.72528300	2.15568700
C	2.42652200	5.92593700	-0.11456900
H	1.58412800	5.37180200	-0.55324400
H	2.03179600	6.84520500	0.34335800
H	3.07998700	6.21572400	-0.94434000
C	7.77422800	2.31334300	0.01133000
H	8.80494200	2.12310400	-0.32303400
H	7.69596400	3.36511800	0.30767700
H	7.58671300	1.68860400	0.89680100
C	7.13296200	2.77542000	-2.37013800
H	7.28520800	3.83594500	-2.15667500
H	8.06820400	2.39434000	-2.80468300
H	6.34772300	2.68006800	-3.13464600
C	6.99019700	0.49583600	-1.47217600
H	6.80376600	-0.18244200	-0.62731900

H	6.35028400	0.18385000	-2.31034200
H	8.03404100	0.34975400	-1.78115500
C	5.20899100	-2.64004100	3.30132400
H	4.88081700	-1.59671100	3.38026000
H	4.32489600	-3.26946400	3.46737400
H	5.91855700	-2.81531200	4.12150300
C	6.48506600	-4.36798300	2.12096900
H	7.13792300	-4.66959500	1.29776200
H	7.09083400	-4.38321800	3.03793000
H	5.70521000	-5.13427600	2.22348200
C	7.02086700	-1.95586300	1.74065400
H	7.58191400	-2.15496600	0.81661400
H	6.63337000	-0.92748400	1.68144200
H	7.73279700	-1.99794200	2.57786600
C	2.89540500	-6.11406500	-1.20934900
H	2.10624700	-6.04302600	-0.44669000
H	2.61878400	-6.92630200	-1.89744200
H	3.83291100	-6.39301500	-0.71511400
C	4.03477700	-4.98884400	-3.13612600
H	4.98293400	-5.41127700	-2.79011000
H	3.61853700	-5.68496500	-3.87836000
H	4.23500300	-4.03692500	-3.64915600
C	1.67150200	-4.51627500	-2.63907400
H	0.87951500	-4.35420000	-1.89229900
H	1.69774100	-3.64370800	-3.30794500
H	1.37843400	-5.38370100	-3.24611000
C	-1.48815800	0.39658900	-4.12173700
C	-1.95512400	1.08103200	-5.32890400
H	-1.35327200	1.27114700	-3.12679100
C	-3.22522200	1.14555300	-5.74764300
H	-1.18492000	1.61688600	-5.89853000
H	-3.51584100	1.71456600	-6.62802600
H	-4.02130500	0.61707200	-5.21542000
C	-0.12263400	-0.03853300	-4.03916100
H	0.58411000	0.56564800	-4.62441000
C	0.42686300	-0.94704100	-3.17357600
H	-0.18618200	-1.72043200	-2.70292900
H	1.50011000	-1.13562200	-3.20463200
H	-2.22727600	-0.28582000	-3.67795000
C	-3.55238900	4.20949800	0.30499000
C	-2.57539400	3.41097100	-0.15492500
C	-1.24058600	3.80859200	-0.68415400
H	-4.48880600	3.73905600	0.62807200
H	-2.76524400	2.33530000	-0.20099600

H	-1.10397300	4.90092000	-0.68340900
H	-0.43881200	3.38177700	-0.05069200
C	-3.50225200	5.65364400	0.43877400
C	-4.50042200	6.38666000	0.94530900
H	-2.59081700	6.15785500	0.10940000
H	-4.43541400	7.46837400	1.03566700
H	-5.42545900	5.92092600	1.28897700
C	0.30048700	3.76991000	-2.66680200
C	1.42538400	2.95688200	-2.80967900
C	0.40850000	5.10747300	-3.07100300
C	2.60899900	3.45094900	-3.35515800
H	1.37258900	1.91071700	-2.50574300
C	1.58248900	5.60463700	-3.62366000
H	-0.44726200	5.77474300	-2.96583900
C	2.68915900	4.77326200	-3.77808300
H	3.47023700	2.78893900	-3.45550900
H	1.62927400	6.64452900	-3.94534100
H	3.60381800	5.15307900	-4.23397800
C	-2.17430500	3.68015800	-3.01427000
H	-3.08599300	3.14240400	-2.72601100
H	-2.37783200	4.75687700	-2.92911000
H	-1.96375700	3.44797900	-4.06546800

**(E)-(S)-TS3**

P	1.95088000	0.07620700	0.10433500
C	1.53566000	0.11326200	1.89946800
C	3.13307600	1.45135400	-0.14502200
C	3.01638000	-1.41525100	0.08076900
C	0.67027500	-0.90122800	2.39377000
C	2.00700400	1.10994300	2.75394700
C	2.71474600	2.75305800	0.10631800
C	4.41897100	1.24868400	-0.64219300
C	4.08036800	-1.50627100	0.96924000
C	2.73488300	-2.49919800	-0.74498200
C	0.26941100	-2.16665300	1.71265500
C	0.28977300	-0.77057500	3.71460400
C	1.63141900	1.19422400	4.10233800
H	2.69729000	1.85676700	2.36681300
C	3.55106400	3.86040500	-0.06789900
H	1.70269200	2.91176100	0.48566400
C	5.27938700	2.30856300	-0.92421200
H	4.74817300	0.23001200	-0.81796300
C	4.93972600	-2.60530500	1.00128200
H	4.23878600	-0.68755200	1.67062700

C	3.56681700	-3.61787200	-0.79657600
H	1.83319200	-2.45971700	-1.34868100
C	-0.85656600	-2.36135600	0.86316700
C	0.95324500	-3.30951300	2.08015000
C	0.74319300	0.24663300	4.54658100
H	2.00615800	1.98100000	4.75307600
C	4.80165100	3.61756900	-0.67493100
C	4.72505300	-3.59406500	0.01644100
P	-1.60490100	-0.84677900	0.12499900
C	-1.24098400	-3.65398900	0.50311800
C	0.57889200	-4.58632100	1.68011900
C	-2.97751100	-1.41276000	-0.94562900
C	-2.44249100	-0.06839100	1.55920100
C	-0.53441000	-4.79743200	0.90497800
H	-2.12559400	-3.79421700	-0.11411600
C	-4.19302100	-0.73644900	-0.96121600
C	-2.73323100	-2.34517200	-1.95267800
C	-3.41400200	-0.76408300	2.26446900
C	-2.05149600	1.19188900	2.01318600
H	-0.85089800	-5.79758600	0.61928300
C	-5.17631500	-0.98136800	-1.92431800
H	-4.36288100	0.02449400	-0.20460200
C	-3.67226500	-2.66999500	-2.93081500
H	-1.75566000	-2.81365100	-2.00028900
C	-4.07268700	-0.21886400	3.36874200
H	-3.66485800	-1.77297600	1.93683400
C	-2.67869900	1.81641200	3.09482200
H	-1.23558500	1.68496100	1.48585700
C	-4.91217700	-1.98988400	-2.88105200
C	-3.75383800	1.11668600	3.69692800
C	-0.85595700	-0.84283300	5.58550000
H	-1.80770000	-0.29937900	5.41404800
H	-0.92225500	-1.50906700	6.45017700
O	-0.53490900	-1.59343100	4.42762700
O	0.19229300	0.09284200	5.78560000
H	2.82626500	-5.13117200	3.69829300
C	2.51282500	-4.73170400	2.72788500
H	3.34702200	-4.74331700	1.99902800
O	1.43362000	-5.50094300	2.22238200
O	2.05014000	-3.39978100	2.88851200
O	5.61525900	4.67341700	-1.01506800
O	5.65382100	-4.59407800	-0.16374100
O	-4.49297800	1.77334800	4.65242500
O	-5.83946600	-2.23200200	-3.86650100

C	6.78068500	-4.16561000	-0.90234100
H	7.41986400	-5.04303500	-1.04685400
H	6.48603800	-3.76331600	-1.88338100
H	7.35099500	-3.38904200	-0.37025200
C	3.19378100	-4.82973300	-1.66501000
C	5.98834100	-2.63364200	2.13215100
C	6.72450000	2.01893700	-1.36527100
C	5.22076300	5.34626000	-2.19476200
H	4.14607900	5.57671900	-2.19681000
H	5.79693000	6.27698200	-2.23970500
H	5.43967000	4.74416300	-3.09013700
C	3.02521500	5.20638200	0.47481600
C	-5.04658000	-1.15015400	4.11670500
C	-2.15871300	3.15307700	3.65792300
C	-5.71708800	2.28270000	4.15703700
H	-6.33754400	1.49072100	3.70970200
H	-6.24880000	2.71567900	5.01135200
H	-5.55247400	3.06228200	3.39812300
C	-6.47533500	-0.15589300	-1.88560600
C	-3.30377100	-3.71830600	-3.99718500
C	-6.84131500	-3.20299000	-3.68333500
H	-6.76167200	-3.96436000	-4.47285300
H	-6.76170000	-3.69435500	-2.70295300
H	-7.83117500	-2.73113200	-3.76937100
Cu	0.06269300	0.25966100	-1.24127800
C	-1.33981000	2.97839500	-2.34226900
O	-1.24575800	1.61134100	-2.07931400
C	-0.07036400	3.56080800	-2.97615600
C	1.15267800	2.89412200	-2.89778800
C	-0.09125200	4.80780800	-3.61331400
C	2.31341000	3.44128800	-3.43826400
H	1.20159400	1.92006400	-2.40990200
C	1.06020500	5.35548200	-4.16749400
H	-1.02768900	5.36075000	-3.68589000
C	2.27112000	4.67182700	-4.08505200
H	3.25649000	2.90035400	-3.33588300
H	1.00952200	6.31992700	-4.67188000
H	3.17232500	5.09547300	-4.52852200
C	-2.55205200	3.22516500	-3.25259900
H	-2.34310400	2.93571000	-4.28939500
H	-3.38824400	2.60896400	-2.89629900
H	-2.87820100	4.27465600	-3.23951500
C	-1.80698000	-4.05837800	-3.97177800
H	-1.17406600	-3.17683200	-4.14561500

H	-1.49586700	-4.53646300	-3.03013100
H	-1.59680500	-4.77708700	-4.77525800
C	-4.04044500	-5.03321300	-3.70909700
H	-3.80358800	-5.39364300	-2.69697200
H	-5.12744500	-4.94210700	-3.78833200
H	-3.72119400	-5.80514200	-4.42454400
C	-3.60599700	-3.22575900	-5.41871900
H	-3.27769300	-3.98402100	-6.14422900
H	-4.66917000	-3.02998300	-5.58148700
H	-3.05794500	-2.29674500	-5.63628500
C	-6.85398900	0.38720300	-3.27029400
H	-7.08424600	-0.40139400	-3.99082000
H	-7.73083400	1.04400400	-3.17962700
H	-6.02851200	0.98357800	-3.68480200
C	-6.32814100	1.06815200	-0.97457000
H	-6.19246700	0.78996900	0.08245900
H	-5.48835300	1.71067900	-1.27393900
H	-7.24180700	1.67593300	-1.02826100
C	-7.62064000	-0.98567100	-1.29062700
H	-7.35415400	-1.34219600	-0.28477700
H	-8.52213500	-0.36240700	-1.19760100
H	-7.88771400	-1.85777700	-1.89440200
C	-4.34220600	-2.50005600	4.35514300
H	-4.08513900	-3.03032600	3.43100600
H	-3.41130600	-2.36403500	4.92383100
H	-4.99997100	-3.16212500	4.93503600
C	-5.48861700	-0.67025100	5.50356000
H	-6.15856800	0.19346300	5.47813600
H	-6.03294600	-1.48768800	5.99752200
H	-4.62874200	-0.40786500	6.13364100
C	-6.28676500	-1.39570100	3.24734200
H	-6.87090900	-0.47544500	3.10628900
H	-6.01173700	-1.76811500	2.24990100
H	-6.94579700	-2.13900900	3.71939500
C	-1.69593900	2.92856900	5.10406200
H	-0.89814600	2.17848100	5.15726600
H	-1.30195600	3.86820100	5.51890000
H	-2.52375400	2.59831100	5.74252700
C	-0.95879700	3.66716100	2.85468200
H	-0.14003100	2.93446200	2.81158000
H	-1.24192300	3.94410100	1.82701400
H	-0.56493500	4.57031300	3.34162300
C	-3.19787900	4.28208200	3.65822700
H	-3.67044700	4.40344900	2.67573900

H	-3.97618800	4.12798400	4.41151500
H	-2.69458900	5.22853300	3.90341700
C	2.54931600	4.98090000	1.92353300
H	1.73845200	4.24732500	2.00618000
H	3.38054000	4.64240100	2.55970500
H	2.16933000	5.92504900	2.33870900
C	4.05429700	6.33954700	0.56921100
H	4.96847400	6.02170500	1.08481500
H	4.33853600	6.75931800	-0.39980600
H	3.60703900	7.15995400	1.14805200
C	1.83062100	5.68036100	-0.36263200
H	1.00414200	4.95575200	-0.34136700
H	1.44981100	6.63340800	0.03330200
H	2.09472500	5.83034300	-1.41966400
C	7.67524700	2.48941100	-0.25618500
H	8.71851100	2.28692800	-0.54039100
H	7.57315900	3.56434000	-0.06975200
H	7.47122700	1.95391800	0.68232300
C	7.10256400	2.70522300	-2.68415200
H	7.22385900	3.78514700	-2.56613300
H	8.06142000	2.30760600	-3.04656200
H	6.35061600	2.51415800	-3.46418900
C	6.96379800	0.51880200	-1.57359700
H	6.77727800	-0.07278600	-0.66606800
H	6.34125400	0.11087100	-2.38301600
H	8.01458800	0.36168700	-1.85201900
C	5.28822900	-2.26462100	3.45518300
H	4.89626500	-1.24040000	3.46887900
H	4.44306800	-2.93381500	3.66355400
H	6.00512700	-2.34571000	4.28381900
C	6.64566700	-3.99708500	2.37533200
H	7.32558400	-4.30788700	1.57739100
H	7.23664800	-3.93930800	3.30028200
H	5.89873200	-4.79173600	2.50385600
C	7.07891600	-1.58750300	1.86897200
H	7.65978000	-1.81253800	0.96323200
H	6.64694800	-0.58284700	1.74885200
H	7.78192700	-1.55137700	2.71381500
C	3.12653200	-6.09395600	-0.79647400
H	2.34028200	-6.01032200	-0.03181800
H	2.88478400	-6.96287900	-1.42588300
H	4.08048600	-6.29332800	-0.29524100
C	4.19597600	-5.04683800	-2.80577800
H	5.16030900	-5.41432000	-2.44126500



H	3.80251100	-5.79741800	-3.50620300
H	4.35911800	-4.11795100	-3.37139000
C	1.81536100	-4.64816400	-2.30800400
H	1.03026300	-4.47302900	-1.55674200
H	1.79401500	-3.82068400	-3.03195800
H	1.55082900	-5.56437300	-2.85364600
C	-1.39610700	0.05255400	-4.17889400
C	-1.83934400	0.64037700	-5.44514700
H	-1.41183400	0.95711500	-3.20335100
C	-3.08594600	0.59221600	-5.93111100
H	-1.07591600	1.19806000	-6.00287900
H	-3.36359400	1.08883000	-6.85846600
H	-3.87727900	0.05209700	-5.40401100
C	-0.00736900	-0.26191100	-4.00045500
H	0.68348500	0.36784500	-4.57695500
C	0.55856300	-1.08294300	-3.06136400
H	-0.02258600	-1.87880400	-2.58601700
H	1.64287000	-1.19043700	-3.02917500
H	-2.10092700	-0.67729200	-3.75529300
C	-3.83805300	4.15560300	-0.01312800
C	-2.84895900	3.31387200	-0.34805200
C	-1.56752500	3.70157300	-0.99373700
H	-3.73376100	5.22754200	-0.21393000
H	-2.98711100	2.24380800	-0.16385500
H	-1.52429000	4.79504900	-1.13126000
H	-0.71600100	3.41802000	-0.34491600
C	-5.06642600	3.71419400	0.61926200
C	-6.11954400	4.49317000	0.89393500
H	-5.09960900	2.65170000	0.88738100
H	-7.01798800	4.09705900	1.36395500
H	-6.12302100	5.55433700	0.64351400

**(Z)-(S)-P<sub>t</sub>**

C	-1.75095900	-0.10253200	0.08006800
O	-2.36115900	-0.32959200	-1.18381400
C	0.93937500	-2.27531100	-0.40792400
C	-0.40028400	-2.19889400	-0.43149900
C	-1.27232000	-1.49005000	0.55397700
H	1.43732100	-2.83145500	-1.20708400
H	-0.92593600	-2.67145100	-1.26179300
H	-2.17487400	-2.09362300	0.74016300
H	-0.76918000	-1.36077500	1.52286200
C	1.82807500	-1.67492300	0.57017700
C	3.15990700	-1.78453300	0.51659200

H	1.37796100	-1.08651200	1.37259300
H	3.80762500	-1.31495100	1.25323000
H	3.65018100	-2.34775800	-0.27838400
H	-2.67086600	0.52700500	-1.51305200
C	-0.56062800	0.83693400	-0.04438200
C	0.07890700	1.00205600	-1.27375000
C	-0.03250900	1.49125500	1.07264600
C	1.21544600	1.79672300	-1.38489500
H	-0.31422600	0.48086700	-2.14439500
C	1.10422800	2.28481400	0.96446600
H	-0.50510900	1.37403100	2.04821100
C	1.73397800	2.43952700	-0.26655100
H	1.70184500	1.90771000	-2.35309700
H	1.49933300	2.78470800	1.84779900
H	2.62576200	3.05829700	-0.35179800
C	-2.80810800	0.42943400	1.04274600
H	-3.11603100	1.44672700	0.76187400
H	-3.68732100	-0.22526900	1.00154000
H	-2.45785600	0.46218900	2.08181700

**(E)-(S)-P<sub>l</sub>**

C	1.04110500	-1.42601000	0.04001900
O	0.98086400	-1.94516800	1.36224000
C	-2.35028200	-0.41948400	-0.43674200
C	-1.49066900	-1.29664600	0.09723700
C	-0.29309600	-1.83496500	-0.60744200
H	-2.18442200	-0.06156900	-1.45890500
H	-1.64284000	-1.63923500	1.12409100
H	-0.31731300	-2.93738400	-0.61025900
H	-0.29019900	-1.50398300	-1.65708800
C	-3.51121100	0.10472600	0.25571800
C	-4.37338700	0.97885900	-0.27346400
H	-3.66721000	-0.25833400	1.27540400
H	-5.23390200	1.34748200	0.27986700
H	-4.24308600	1.35915100	-1.28707700
H	1.82044500	-1.73276600	1.79597700
C	1.18365000	0.08975400	0.04657500
C	0.97352000	0.82037600	1.21606300
C	1.48841600	0.78708600	-1.12586500
C	1.09073900	2.20689400	1.22246900
H	0.69903000	0.29010700	2.12605100
C	1.60165600	2.17232500	-1.12386500
H	1.63950300	0.24412000	-2.05939100
C	1.40937200	2.88870200	0.05394700

H	0.92373100	2.75671800	2.14772300
H	1.84348900	2.69510300	-2.04827400
H	1.50125500	3.97354500	0.05740500
C	2.19930800	-2.09656500	-0.69274200
H	3.16089000	-1.79637800	-0.25220000
H	2.09895900	-3.18562500	-0.60381700
H	2.23002000	-1.83992900	-1.75887900

**(Z)-(S)-TS2'**

C	-3.09735600	-1.38362400	1.75423900
C	-0.63789100	-0.91590700	2.88378400
C	-1.71529700	-1.53881100	3.77107500
C	-2.62441100	-2.34601200	2.85365700
H	-3.76015500	-0.63944000	2.22914900
H	0.05128900	-1.71628800	2.57276000
H	-1.27155400	-2.14530000	4.57336200
H	-2.31791400	-0.75550000	4.25745000
H	-2.06288600	-3.17931300	2.39823400
H	-3.48116400	-2.78853300	3.38104800
C	0.18872200	0.21710700	3.42408000
C	1.41257700	0.51206300	2.80563900
C	-0.23524200	1.02657400	4.48045900
C	2.17963900	1.59185000	3.22595600
H	1.74921900	-0.10416000	1.96807700
C	0.53401500	2.11010600	4.90064000
H	-1.17407600	0.81475800	4.99264500
C	1.74054600	2.40017000	4.27334700
H	3.12422400	1.80065200	2.72398800
H	0.18671900	2.72686800	5.72860300
H	2.34136900	3.24609700	4.60464200
C	-3.84210500	-2.02369700	0.61760400
C	-5.23414100	-1.93048200	0.56154900
C	-3.18109100	-2.73108900	-0.39071300
C	-5.95076500	-2.52352700	-0.47318700
H	-5.76078800	-1.37422400	1.33896400
C	-3.89118200	-3.31861700	-1.43144100
H	-2.09112000	-2.79069700	-0.37381300
C	-5.28023900	-3.21680000	-1.47668300
H	-7.03617900	-2.43698000	-0.49963200
H	-3.35505500	-3.85301800	-2.21530200
H	-5.83621800	-3.67621300	-2.29226200
P	-1.52787100	-0.46430700	1.27451500
C	-1.24918100	2.67410400	-1.83811600
C	1.10021100	3.30559300	-0.57055200

C	0.68682100	4.14444600	-1.79329500
C	-0.83213500	4.14110300	-1.86587600
H	-0.89021000	2.19887500	-2.76793400
H	0.91517300	3.90322700	0.33806200
H	1.11081900	5.15608100	-1.72781500
H	1.09862500	3.68239500	-2.70476000
H	-1.23525900	4.67926500	-0.99248400
H	-1.21285700	4.65282800	-2.76184300
C	2.54115400	2.88546300	-0.58580800
C	3.03369000	2.04833400	-1.59151300
C	3.43081800	3.36828100	0.37502300
C	4.38315600	1.72063400	-1.64428200
H	2.34421000	1.64065900	-2.33418700
C	4.78104900	3.03061200	0.33360900
H	3.05690500	4.02306500	1.16474800
C	5.26255100	2.20956600	-0.68032100
H	4.74728700	1.06721400	-2.43772000
H	5.46034400	3.41912200	1.09132900
H	6.32018200	1.95206800	-0.72051600
C	-2.69544900	2.32804100	-1.64662500
C	-3.11771200	1.02407700	-1.93814500
C	-3.63360800	3.22583500	-1.13192600
C	-4.42277500	0.61935200	-1.69382200
H	-2.39785800	0.31420800	-2.34928100
C	-4.94588600	2.82347100	-0.88725700
H	-3.34496500	4.25419300	-0.91582900
C	-5.34223700	1.51789500	-1.15592700
H	-4.72219000	-0.40398100	-1.91948500
H	-5.66044200	3.53972800	-0.48340900
H	-6.36523700	1.19951800	-0.95827100
P	-0.15525500	1.89150200	-0.51228400
C	-2.08262600	1.29557400	1.50588500
C	-1.05224200	2.33233800	1.06378800
H	-2.37236400	1.46656900	2.55464700
H	-2.99802200	1.38084700	0.89821300
H	-1.52567500	3.32224500	0.96888500
H	-0.26330600	2.43005700	1.82444800
Cu	-0.08967200	-0.51111600	-0.59579900
C	2.13376500	-2.46131800	0.07144300
O	1.70576700	-1.27739100	0.08379900
C	3.59182400	-2.66874700	-0.15969500
C	4.23024100	-3.90587700	-0.02100700
C	4.36010200	-1.55258800	-0.50885400
C	5.59897900	-4.02204800	-0.23640300

H	3.65883800	-4.79312600	0.24950500
C	5.72481300	-1.67004000	-0.72624900
H	3.85831000	-0.58953800	-0.59557000
C	6.35226500	-2.90677100	-0.59160900
H	6.08051500	-4.99274500	-0.12515600
H	6.30363500	-0.78571600	-0.99473100
H	7.42404100	-3.00183400	-0.75967200
C	1.35837100	-3.51013200	0.83375100
H	1.57358100	-4.54004000	0.53244800
H	1.59931400	-3.41615700	1.90611700
H	0.28416300	-3.32499000	0.70730600
C	-0.06242800	-1.42060200	-2.53506800
C	0.31981500	-2.73481300	-2.16725900
C	1.59178300	-3.25190200	-2.04164200
H	-0.50785600	-3.38597900	-1.85999100
H	2.44088600	-2.75489200	-2.50924500
H	1.72145100	-4.31912900	-1.86490800
C	0.85988100	-0.51353900	-3.20487800
C	0.53185300	0.45583800	-4.07864700
H	1.91681200	-0.64031600	-2.94246800
H	1.28356400	1.09951000	-4.53390800
H	-0.50261700	0.61013300	-4.39497200
H	-1.12010200	-1.30742900	-2.80750600

**(E)-(S)-TS2'**

C	-2.68692400	-2.01623300	1.50291600
C	-0.17056400	-1.54754000	2.51298000
C	-1.07770500	-2.51293400	3.27987200
C	-2.00664500	-3.16332300	2.26356000
H	-3.34149000	-1.48912300	2.21890000
H	0.58019800	-2.13528000	1.96420400
H	-0.48726700	-3.24536100	3.84827600
H	-1.69657700	-1.96742500	4.00931200
H	-1.42984600	-3.78523200	1.55834400
H	-2.75437100	-3.82084400	2.72932900
C	0.55767100	-0.48164600	3.28664000
C	1.75597600	0.03179500	2.76948200
C	0.06580500	0.06722800	4.47518800
C	2.42309400	1.07205100	3.40508400
H	2.15288800	-0.38473400	1.84253400
C	0.73612900	1.10816200	5.11397800
H	-0.85259700	-0.31517600	4.92152900
C	1.91358700	1.62053500	4.58007500
H	3.35206900	1.44800500	2.97604100

H	0.33328900	1.51676000	6.03995200
H	2.43590300	2.43315100	5.08288700
C	-3.51705700	-2.44191000	0.32553400
C	-4.90709900	-2.50402300	0.44927900
C	-2.94169700	-2.81662200	-0.89268600
C	-5.70431800	-2.93050000	-0.60835600
H	-5.36931800	-2.20262500	1.39104800
C	-3.73485000	-3.23659200	-1.95481300
H	-1.85930400	-2.75069500	-1.02173700
C	-5.11962000	-3.29686500	-1.81676700
H	-6.78616000	-2.97122900	-0.48915600
H	-3.26576200	-3.51498200	-2.89814800
H	-5.73909300	-3.62501100	-2.64974500
P	-1.26337700	-0.85008000	1.12281600
C	-1.74357400	2.97301200	-1.10003000
C	0.78392900	3.43904400	-0.12988800
C	0.12344100	4.53937800	-0.98147900
C	-1.38505600	4.42656300	-0.80463900
H	-1.54248300	2.76838500	-2.16506800
H	0.80262400	3.76909100	0.92184500
H	0.50952000	5.52984300	-0.70480500
H	0.37933600	4.38562400	-2.04175200
H	-1.64532000	4.68838100	0.23416300
H	-1.93721900	5.11944700	-1.45632100
C	2.17504500	3.05746600	-0.54810600
C	2.42261500	2.56138400	-1.83282400
C	3.24664100	3.16979600	0.33743300
C	3.70589100	2.20850400	-2.22765600
H	1.59275500	2.43944600	-2.53278500
C	4.53798800	2.82428000	-0.05505300
H	3.06402100	3.54120500	1.34737200
C	4.77207700	2.35091700	-1.34165300
H	3.87341300	1.81498100	-3.22955500
H	5.36305800	2.92817700	0.64911800
H	5.77982100	2.08030400	-1.65353100
C	-3.12259500	2.47508500	-0.77622700
C	-3.53417600	1.24748900	-1.31363300
C	-3.99008400	3.14280500	0.09082900
C	-4.75923600	0.69046600	-0.97265400
H	-2.86828300	0.72819900	-2.00481700
C	-5.21954700	2.58352500	0.43645900
H	-3.70941400	4.10950600	0.50807500
C	-5.60401600	1.35193200	-0.08272000
H	-5.05061500	-0.27145000	-1.39427100

H	-5.87942500	3.11909200	1.11791900
H	-6.56067000	0.91071200	0.19481600
P	-0.41143300	1.98247900	-0.20391300
C	-1.93295800	0.73601000	1.82784600
C	-1.04073400	1.94275400	1.54801600
H	-2.09970400	0.62288200	2.91009400
H	-2.92070000	0.86686200	1.35995400
H	-1.56577200	2.87796900	1.79720300
H	-0.13888200	1.90291100	2.17879500
Cu	0.01620300	-0.28043400	-0.82810700
C	2.38202800	-2.18537500	-0.42040900
O	1.81767700	-1.09849400	-0.15058600
C	3.86842900	-2.21494700	-0.43722300
C	4.60675500	-3.40202200	-0.48623700
C	4.55429800	-0.99777800	-0.33496800
C	5.99558900	-3.37351000	-0.43767500
H	4.09644600	-4.36143400	-0.56280100
C	5.94034400	-0.97178300	-0.28843400
H	3.97033000	-0.07786300	-0.29213400
C	6.66838000	-2.15908200	-0.33817400
H	6.55630100	-4.30649600	-0.47453300
H	6.45770600	-0.01592300	-0.20236700
H	7.75632000	-2.13797200	-0.29662000
C	1.62839800	-3.47460800	-0.19938500
H	1.98829000	-4.31232300	-0.80465300
H	1.71286200	-3.76752400	0.86146500
H	0.56817100	-3.30891100	-0.42297700
C	0.44622200	-0.53622200	-2.90479600
C	0.92221000	-1.87163200	-2.94803200
C	2.23240600	-2.25076300	-2.79655500
H	0.15860600	-2.65665000	-3.04132900
H	3.01659800	-1.49320400	-2.85654500
H	2.54267500	-3.28143400	-2.96220600
C	-0.84129200	-0.18447300	-3.47869400
C	-1.16838200	0.99714100	-4.03553200
H	-1.60528600	-0.97350900	-3.45364300
H	-2.15928700	1.19066300	-4.44205600
H	-0.43471400	1.80335700	-4.11786700
H	1.22629300	0.23035400	-3.01474800
<b>(Z)-(S)-C'</b>			
C	-2.89984000	-1.58388400	1.93782700
C	-0.32622100	-1.10473400	2.78228800
C	-1.28738700	-1.75327200	3.77706600

C	-2.28868300	-2.55820000	2.95666200
H	-3.52476300	-0.86692200	2.49696600
H	0.31847900	-1.89279000	2.36087300
H	-0.74871500	-2.36990900	4.51038400
H	-1.83841500	-0.98671300	4.34593100
H	-1.77099400	-3.37571100	2.42736600
H	-3.07185800	-3.02088600	3.57319100
C	0.55617400	0.02667400	3.23063000
C	1.69064800	0.32278700	2.46039600
C	0.25465400	0.84470200	4.32215200
C	2.47879600	1.42940800	2.75597800
H	1.92634000	-0.31041600	1.59583800
C	1.05230800	1.94796100	4.62251200
H	-0.60830500	0.62894800	4.95277300
C	2.15932200	2.25073400	3.83626500
H	3.34302600	1.65185400	2.12840300
H	0.80228200	2.57340800	5.47885500
H	2.77586700	3.11788500	4.06898700
C	-3.73397200	-2.19713500	0.85262200
C	-5.11533900	-1.99962600	0.82352500
C	-3.15295100	-2.97619100	-0.15357700
C	-5.89849000	-2.56183100	-0.18129500
H	-5.58126700	-1.38640000	1.59675600
C	-3.92745300	-3.52946200	-1.16564900
H	-2.07350700	-3.14113400	-0.13901600
C	-5.30591300	-3.32310100	-1.18360200
H	-6.97507500	-2.39624300	-0.18455400
H	-3.45351900	-4.12768200	-1.94347300
H	-5.91403500	-3.75772500	-1.97507500
P	-1.41165300	-0.60846500	1.31478600
C	-1.43715800	2.69302300	-1.67516600
C	0.96722800	3.30769500	-0.51739500
C	0.54616800	4.09268700	-1.77154500
C	-0.97563700	4.14336100	-1.77547700
H	-1.17687300	2.19660300	-2.62514500
H	0.72477900	3.94023300	0.35574200
H	1.00831300	5.08986100	-1.78052100
H	0.91017700	3.56121800	-2.66715200
H	-1.31649400	4.72414800	-0.90226500
H	-1.38391300	4.63558200	-2.67007900
C	2.44331000	2.99947500	-0.46846800
C	2.99610300	1.74718900	-0.74707400
C	3.30474100	4.05575900	-0.14859000
C	4.38007700	1.57279400	-0.72414800



H	2.37281700	0.86744600	-0.92675800
C	4.68215700	3.87905800	-0.11977000
H	2.87936700	5.03408300	0.08573300
C	5.22639400	2.63154300	-0.41498100
H	4.78859100	0.58473300	-0.93679900
H	5.33087000	4.71559500	0.13701900
H	6.30529100	2.48471000	-0.39409200
C	-2.87286500	2.38927400	-1.36601600
C	-3.34384100	1.08727400	-1.58265400
C	-3.75506000	3.32838100	-0.82925600
C	-4.64496100	0.72730400	-1.26212300
H	-2.66096200	0.33681700	-1.98540300
C	-5.06287700	2.97101700	-0.50381400
H	-3.42470000	4.35389400	-0.66466600
C	-5.51084500	1.67090600	-0.71229500
H	-4.97983300	-0.29503000	-1.43529900
H	-5.73577200	3.71884000	-0.08619800
H	-6.53222000	1.39230700	-0.45559900
P	-0.25879500	1.88527600	-0.44525100
C	-1.97505800	1.11979000	1.71065900
C	-1.03034100	2.21256800	1.21814300
H	-2.13440500	1.21799000	2.79617600
H	-2.96003400	1.21212900	1.22778100
H	-1.54151000	3.18778800	1.20641900
H	-0.17726800	2.30653200	1.90738900
Cu	-0.00926200	-0.43967600	-0.58573000
C	2.03725600	-2.46101500	-0.68788300
O	1.79828800	-1.17594700	-0.29080500
C	3.53871300	-2.76921500	-0.65461700
C	4.09274600	-3.90789300	-1.24617600
C	4.39029200	-1.90769100	0.03754200
C	5.45777600	-4.16641500	-1.16716000
H	3.45278700	-4.61323600	-1.77892400
C	5.75570300	-2.16358700	0.12278700
H	3.95437300	-1.02483400	0.50299900
C	6.29753100	-3.29257600	-0.48322500
H	5.86701000	-5.05785500	-1.64190800
H	6.39973600	-1.47396200	0.66922300
H	7.36629900	-3.49335600	-0.42089300
C	1.34796400	-3.47449500	0.24630700
H	1.49839400	-4.52102500	-0.05844200
H	1.76109300	-3.35335600	1.25833500
H	0.26551000	-3.27374000	0.29517500
C	-0.42313200	-1.15426000	-2.88483800

C	0.08157800	-2.25665300	-2.27284000
C	1.51409500	-2.64089600	-2.14938700
H	-0.64760800	-2.96253100	-1.86671200
H	2.14673100	-2.01764400	-2.79570000
H	1.62668300	-3.68384200	-2.48631300
C	0.33937500	-0.13333000	-3.59222600
C	-0.22625700	0.76368900	-4.41026800
H	1.42054200	-0.12089100	-3.44109100
H	0.36124100	1.50730500	-4.94452200
H	-1.30428000	0.76993300	-4.58513500
H	-1.51224300	-1.07756300	-2.96807400

**(E)-(S)-C'**

C	-2.68039600	-2.11410500	1.45031600
C	-0.17281500	-1.65863200	2.49171200
C	-1.08426600	-2.63754500	3.23344900
C	-1.99891700	-3.27176200	2.19504300
H	-3.35941700	-1.61228200	2.16162200
H	0.57975300	-2.22869900	1.92613600
H	-0.49788200	-3.37974200	3.79319800
H	-1.71119100	-2.10573700	3.96665600
H	-1.40604200	-3.87009700	1.48270100
H	-2.74580300	-3.94730800	2.63599200
C	0.55529900	-0.61172900	3.29049400
C	1.74566000	-0.08395300	2.76847600
C	0.07515600	-0.10536100	4.50196500
C	2.42292100	0.92812500	3.43896100
H	2.11217300	-0.46978700	1.80971200
C	0.75481200	0.91216900	5.16851200
H	-0.83735900	-0.50514800	4.94633100
C	1.92952100	1.43619000	4.63939900
H	3.35137100	1.31476100	3.01628200
H	0.36432500	1.29052900	6.11264300
H	2.46200900	2.22755500	5.16551800
C	-3.46882500	-2.52688200	0.24086700
C	-4.86078100	-2.61545400	0.30893500
C	-2.84171000	-2.86795300	-0.96185000
C	-5.60857200	-3.02911800	-0.79001700
H	-5.36457200	-2.34474700	1.23860500
C	-3.58398700	-3.27338000	-2.06512600
H	-1.75418700	-2.79726400	-1.03331800
C	-4.97263700	-3.35477800	-1.98391100
H	-6.69324900	-3.09201900	-0.71363500
H	-3.07356600	-3.53107400	-2.99332800

H	-5.55462400	-3.67234500	-2.84745800
P	-1.25625800	-0.92846300	1.11737100
C	-1.83834800	2.95404300	-1.04771200
C	0.70746200	3.42250800	-0.12594300
C	0.03429900	4.52266900	-0.96358900
C	-1.47009400	4.40738000	-0.75788600
H	-1.67985300	2.76333300	-2.12393600
H	0.72390700	3.74508200	0.92805600
H	0.42297600	5.51271500	-0.68982000
H	0.27014000	4.37550600	-2.02926000
H	-1.70912600	4.66592000	0.28658400
H	-2.03747900	5.10149000	-1.39497200
C	2.09808600	3.04061800	-0.54080000
C	2.37019000	2.62835900	-1.84878500
C	3.14249100	3.05322500	0.38308500
C	3.65313700	2.25482100	-2.22661000
H	1.55765400	2.59058600	-2.57973300
C	4.43042200	2.68010800	0.00945600
H	2.93765700	3.35613400	1.41152300
C	4.69030600	2.28296100	-1.29743800
H	3.84582400	1.93332900	-3.24957100
H	5.23314300	2.69416300	0.74673900
H	5.69398600	1.97821300	-1.58885600
C	-3.20734700	2.46177600	-0.67735400
C	-3.64131000	1.23873000	-1.20419900
C	-4.04566900	3.12957700	0.21765600
C	-4.86049300	0.68683700	-0.83686900
H	-2.99283400	0.71341400	-1.90515000
C	-5.26890600	2.57610100	0.59264200
H	-3.74839200	4.09173300	0.63325800
C	-5.67780900	1.35127100	0.07585200
H	-5.16689300	-0.27035500	-1.25803000
H	-5.90594200	3.11181100	1.29518100
H	-6.63153600	0.91860700	0.37485000
P	-0.47382500	1.95934500	-0.20189400
C	-1.92751700	0.64457500	1.85186200
C	-1.04504500	1.85815100	1.56577000
H	-2.06672100	0.52599300	2.93733800
H	-2.92509200	0.78039500	1.40717600
H	-1.55703600	2.78755000	1.86000600
H	-0.11680500	1.79961000	2.15742000
Cu	0.20697300	-0.19402100	-0.69603900
C	2.44777600	-2.01502100	-0.81133400
O	1.93238500	-0.94438100	-0.14076400

C	3.97360300	-2.05979000	-0.66029200
C	4.74974200	-3.13714000	-1.09736500
C	4.62568200	-0.96026300	-0.10198200
C	6.13523100	-3.12082300	-0.96991500
H	4.27219300	-4.00848300	-1.54832100
C	6.01101500	-0.93834700	0.02402400
H	4.01200700	-0.11917000	0.21854300
C	6.77358100	-2.01994800	-0.40580900
H	6.71979500	-3.97452100	-1.31232900
H	6.49656900	-0.06536200	0.46345300
H	7.85820500	-2.00671400	-0.30410800
C	1.83556700	-3.33026600	-0.29642500
H	2.17704100	-4.22561100	-0.83612700
H	2.09241100	-3.45593200	0.76497700
H	0.73837400	-3.28317000	-0.37741500
C	0.26966100	-0.40168700	-3.09557600
C	0.72398400	-1.59300400	-2.63127500
C	2.15731500	-1.86925400	-2.34221000
H	0.00172000	-2.40866700	-2.50663600
H	2.76807900	-1.02755400	-2.70268400
H	2.48306400	-2.77236500	-2.88408000
C	-1.09676400	-0.13743000	-3.51472800
C	-1.47204400	0.97142600	-4.16401400
H	-1.83623400	-0.91381900	-3.28629400
H	-2.49992400	1.13780500	-4.47956200
H	-0.74935400	1.75299100	-4.40778200
H	1.00469700	0.38919800	-3.28575400

**(Z)-(S)-TS3'**

C	-0.49683300	-2.85690400	-2.19416700
C	2.04783500	-1.97580300	-2.67126000
C	1.72990500	-3.38610800	-3.16233500
C	0.23794300	-3.41126400	-3.43337600
H	-0.62290000	-3.66698100	-1.45669400
H	1.83128500	-1.27412900	-3.49663800
H	2.32581300	-3.64575400	-4.04973000
H	1.97178400	-4.12905300	-2.38596500
H	0.01156700	-2.76065600	-4.29288400
H	-0.13682900	-4.41194200	-3.68912900
C	3.44249100	-1.71226000	-2.18514000
C	3.93267200	-0.40055800	-2.18353200
C	4.27659900	-2.72896300	-1.70949100
C	5.20491800	-0.11205500	-1.70699700
H	3.30079800	0.40541300	-2.56005900

C	5.54945600	-2.44009300	-1.22496800
H	3.93927500	-3.76452500	-1.71806600
C	6.01784100	-1.13102300	-1.21600900
H	5.55655300	0.91874200	-1.71539300
H	6.18130000	-3.24875500	-0.86030000
H	7.01609500	-0.90730800	-0.84282700
C	-1.84740800	-2.30870000	-2.56789100
C	-2.99324600	-3.08484600	-2.38841000
C	-1.97591500	-1.05581300	-3.17373800
C	-4.23975500	-2.62204200	-2.80120700
H	-2.90335000	-4.06588000	-1.91725800
C	-3.21637200	-0.58973500	-3.58636400
H	-1.09618800	-0.41959400	-3.29953100
C	-4.35324300	-1.37412600	-3.40495100
H	-5.12453700	-3.23749300	-2.64549600
H	-3.29930800	0.40508500	-4.02437000
H	-5.32743300	-1.00450800	-3.72097000
P	0.68326500	-1.60550700	-1.40832100
C	0.62600600	-0.44891100	3.20859300
C	2.73475600	0.98239500	2.17123700
C	2.23677300	1.37978000	3.56511900
C	1.65319700	0.12570100	4.19020200
H	-0.28942400	0.16269000	3.27420900
H	3.57883500	0.28276100	2.29999000
H	3.05106000	1.81355800	4.16162500
H	1.45597000	2.15390000	3.48001100
H	2.46792100	-0.59527500	4.35792200
H	1.19084600	0.31357500	5.16917200
C	3.17946400	2.12265300	1.30494600
C	2.33206700	3.20375200	1.04517700
C	4.45810100	2.13459100	0.74752400
C	2.75341600	4.27344300	0.26650700
H	1.31841700	3.20246800	1.44502100
C	4.88369000	3.20251600	-0.03987700
H	5.12956900	1.29497700	0.93702600
C	4.03466100	4.27688900	-0.28110500
H	2.07161800	5.10329800	0.08131300
H	5.89011700	3.19771700	-0.45817500
H	4.36654600	5.11330200	-0.89346000
C	0.24193900	-1.88866800	3.40294200
C	-1.07060000	-2.29066800	3.13706700
C	1.15626500	-2.86972800	3.80638700
C	-1.45670700	-3.62203300	3.24214700
H	-1.80677900	-1.54812000	2.83162900

C	0.77512700	-4.20354400	3.91268900
H	2.18379100	-2.59888200	4.04913300
C	-0.53108900	-4.58727700	3.62604800
H	-2.49275900	-3.89002300	3.03445000
H	1.50565300	-4.94623200	4.23053500
H	-0.82780000	-5.63122700	3.71267800
P	1.31411500	-0.04166100	1.47095900
C	1.29270500	-2.50166000	0.10465200
C	2.19238600	-1.59164500	0.94480700
H	1.81478700	-3.43560500	-0.15274700
H	0.39518800	-2.78235900	0.68204300
H	2.57484100	-2.13055600	1.82312000
H	3.06856400	-1.25735500	0.36506800
Cu	0.14965000	0.54837000	-0.48590300
C	-2.89582100	1.33296500	0.11116900
O	-1.82442200	0.97797200	-0.71830100
C	-3.94587400	-2.11319900	1.12118300
C	-3.20076500	-1.10424700	0.64191100
C	-3.03051700	0.26244000	1.21618400
H	-2.64134100	-1.26544400	-0.28230900
H	-2.10117600	0.30061100	1.81410100
H	-3.85222700	0.53683400	1.89674200
C	-4.72941200	-2.10520900	2.34271600
C	-5.40657500	-3.16778700	2.79592000
H	-4.74632300	-1.17912800	2.92327500
H	-5.98092100	-3.13959700	3.71890400
H	-5.41194400	-4.10872500	2.24313800
H	-3.95862500	-3.05344600	0.55989900
C	-1.11340100	2.82505200	-2.41778500
C	-1.93406700	4.03744400	-2.33952400
H	-1.63358000	1.93718700	-1.58640500
C	-2.93973100	4.36993400	-3.15734600
H	-1.72205800	4.68753800	-1.48138300
H	-3.53987900	5.26272000	-2.99471700
H	-3.19346300	3.75818100	-4.02542300
C	0.18665700	2.82416000	-1.79977200
H	0.32342800	3.55540200	-0.99122800
C	1.18606700	1.90193900	-1.97427400
H	1.16810800	1.24502500	-2.84976600
H	2.14805000	2.03027100	-1.47588700
H	-1.16690500	2.29626700	-3.38188200
C	-2.65260000	2.69299400	0.78120700
C	-3.58118100	3.73486600	0.75004900
C	-1.44639200	2.92252800	1.45475800

C	-3.31650900	4.96032000	1.35851100
H	-4.52322500	3.60744000	0.22131500
C	-1.17470600	4.14292800	2.06221800
H	-0.69467300	2.12954300	1.47298300
C	-2.11178700	5.17254500	2.01621500
H	-4.05932700	5.75546900	1.30784700
H	-0.22674000	4.29662400	2.58117000
H	-1.90266500	6.12999000	2.49110300
C	-4.16979700	1.33702100	-0.73365200
H	-4.28568000	0.35312100	-1.20220000
H	-5.06975000	1.53465800	-0.13397100
H	-4.10095600	2.09127700	-1.53200600

**(E)-(S)-TS3'**

C	-0.73729400	-2.85979800	-2.06844300
C	1.83051900	-2.11425400	-2.68048000
C	1.37268600	-3.47184200	-3.20901300
C	-0.12970100	-3.37410700	-3.38760200
H	-0.81233300	-3.70160500	-1.36001600
H	1.65734500	-1.36760500	-3.47505500
H	1.89634700	-3.73365700	-4.14013100
H	1.59844100	-4.26734300	-2.48131600
H	-0.36050300	-2.65151900	-4.18660200
H	-0.59279000	-4.32658200	-3.68027500
C	3.25721900	-1.99742500	-2.22865700
C	3.87013400	-0.73891200	-2.19884400
C	4.00346000	-3.10336900	-1.80986500
C	5.17882200	-0.59007200	-1.75735900
H	3.30664700	0.13687900	-2.52271500
C	5.31142000	-2.95453000	-1.35694600
H	3.56787300	-4.10112500	-1.84229200
C	5.90444700	-1.69736700	-1.32489200
H	5.62831100	0.40189500	-1.74854700
H	5.87225600	-3.83177500	-1.03755400
H	6.93017000	-1.58208500	-0.97819800
C	-2.10089400	-2.26457900	-2.28788400
C	-3.24789400	-3.00891100	-2.00734800
C	-2.24950100	-0.99724800	-2.85695600
C	-4.51452800	-2.49888600	-2.28091000
H	-3.14291000	-4.00423100	-1.56955800
C	-3.50924200	-0.48815700	-3.13944400
H	-1.36701000	-0.38466400	-3.05765900
C	-4.64722000	-1.23780300	-2.85155400
H	-5.39879200	-3.08655300	-2.03707900

H	-3.60230300	0.51435800	-3.55745700
H	-5.63591000	-0.83105200	-3.05812200
P	0.54383700	-1.66742800	-1.35456400
C	0.72712700	-0.41212300	3.20804800
C	2.88660000	0.85777600	2.06921900
C	2.46043700	1.31521500	3.46835900
C	1.82515700	0.10923100	4.13987400
H	-0.14219600	0.26022700	3.29545300
H	3.68710300	0.10722000	2.18967700
H	3.31852600	1.71059800	4.02902100
H	1.72433300	2.13340400	3.39053100
H	2.60114500	-0.65806100	4.28716100
H	1.41598500	0.34148200	5.13281300
C	3.37429900	1.94107200	1.15462400
C	2.58347200	3.06026300	0.88144800
C	4.63132800	1.85627700	0.55614200
C	3.03799800	4.07388200	0.04843200
H	1.58538200	3.12858700	1.31101100
C	5.08907600	2.86525300	-0.28882300
H	5.25994000	0.98783800	0.76095900
C	4.29559100	3.97844700	-0.54393800
H	2.40022400	4.93652900	-0.14501000
H	6.07715700	2.78372500	-0.74170100
H	4.65326600	4.76819300	-1.20205300
C	0.24975600	-1.82065600	3.42074200
C	-1.07980900	-2.13953100	3.12543800
C	1.08987900	-2.85324700	3.85079700
C	-1.55367000	-3.44259200	3.22420900
H	-1.76211800	-1.35159700	2.80988900
C	0.62062900	-4.15972300	3.95339500
H	2.12661700	-2.64493300	4.11534300
C	-0.69913000	-4.46253900	3.63439900
H	-2.59759700	-3.65058200	2.98721100
H	1.29446800	-4.94560700	4.29213500
H	-1.06279000	-5.48536600	3.71765100
P	1.37901900	-0.08753000	1.44101200
C	1.18600000	-2.58132000	0.13364400
C	2.14925700	-1.70053300	0.93169500
H	1.67365300	-3.52580900	-0.15210600
H	0.30864500	-2.84092300	0.74935100
H	2.52613700	-2.23857000	1.81355600
H	3.02439300	-1.43076400	0.31918600
Cu	0.14220900	0.53602500	-0.46760100
C	-2.77914800	1.66294700	0.26349800



O	-1.79983000	1.14372800	-0.59420400
C	-4.36484500	-1.35009800	1.68689100
C	-3.38369200	-0.67234600	1.07184000
C	-2.94578200	0.69896600	1.45615200
H	-2.83834700	-1.14712500	0.24564100
H	-1.95797100	0.64177200	1.94985800
H	-3.64419100	1.12995400	2.19280900
C	-4.73539700	-2.71452600	1.36413000
C	-5.67728100	-3.41684900	2.00552200
H	-4.17756900	-3.17620500	0.54390100
H	-5.91759900	-4.44286400	1.73603500
H	-6.24822100	-2.97957000	2.82535900
H	-4.91579500	-0.87145000	2.50427100
C	-1.04097600	2.80726900	-2.45917900
C	-1.76329300	4.08291700	-2.44241600
H	-1.57960700	2.02517300	-1.53565800
C	-2.78724200	4.42682700	-3.23260600
H	-1.45126000	4.78437300	-1.65846800
H	-3.30598800	5.37635400	-3.11837300
H	-3.13690600	3.76844000	-4.03034900
C	0.28826100	2.75641800	-1.90784800
H	0.51397000	3.52435800	-1.15591700
C	1.21811200	1.76400900	-2.07085700
H	1.12084000	1.06484200	-2.90686700
H	2.20609500	1.85740900	-1.61686000
H	-1.18447300	2.21100900	-3.37399500
C	-2.36610000	3.03435200	0.81775600
C	-3.19079300	4.15995400	0.76345600
C	-1.10750000	3.18509400	1.41123200
C	-2.77362900	5.38955600	1.26902300
H	-4.17217400	4.09427000	0.29821300
C	-0.68511500	4.40793800	1.92001100
H	-0.43692300	2.32276900	1.44365400
C	-1.51869800	5.52172800	1.84891600
H	-3.43787400	6.25032800	1.20228200
H	0.30031600	4.49874200	2.38099800
H	-1.18960900	6.48147800	2.24440800
C	-4.10023000	1.73761400	-0.50056400
H	-4.33080800	0.74429900	-0.90110200
H	-4.93721300	2.04317700	0.14371900
H	-4.02257700	2.44140800	-1.34250400
<b>(Z)-(R)-TS2'</b>			
C	3.08284800	0.58680700	1.53695700

C	0.64904300	1.25523700	2.61716200
C	1.88731800	1.54027500	3.46338600
C	3.01917700	1.79994800	2.47863700
H	3.47388200	-0.26570000	2.11844800
H	0.35212000	2.19850200	2.13118200
H	1.71782200	2.38318800	4.14854800
H	2.14992100	0.66813700	4.08438000
H	2.80188900	2.70765300	1.89018700
H	3.98954400	1.96216100	2.96873500
C	-0.57129300	0.66846300	3.26404900
C	-1.79248600	0.76139800	2.58206100
C	-0.53405500	-0.01742200	4.47948200
C	-2.93802000	0.16691400	3.09593700
H	-1.83035400	1.28456400	1.62292500
C	-1.68398200	-0.61314200	4.99479600
H	0.39872500	-0.08902100	5.03908700
C	-2.88741300	-0.52975200	4.30274900
H	-3.87394900	0.24703400	2.54389400
H	-1.63555400	-1.14218700	5.94574800
H	-3.78610200	-0.99369000	4.70748800
C	3.95830400	0.77665400	0.33122500
C	5.23291400	0.20590500	0.30158300
C	3.54572000	1.53774300	-0.76625600
C	6.07262000	0.38194700	-0.79395600
H	5.56365900	-0.39651400	1.14965900
C	4.37678100	1.70838400	-1.86757000
H	2.54902800	1.98394900	-0.77066200
C	5.64389500	1.13019800	-1.88620400
H	7.06205300	-0.07341500	-0.79684900
H	4.03022600	2.29433500	-2.71805000
H	6.29371000	1.26297000	-2.74945000
P	1.27258200	0.18050200	1.18781600
C	-0.03564700	-3.49737700	-1.01077700
C	-2.47152900	-2.87397500	0.07355100
C	-2.35074300	-4.18305700	-0.73204700
C	-0.91526000	-4.68041700	-0.62445400
H	-0.22387400	-3.25614300	-2.07195600
H	-2.57554500	-3.12304700	1.14253700
H	-3.08450400	-4.92206700	-0.38230600
H	-2.58362800	-3.97978500	-1.78936200
H	-0.71331000	-4.99507200	0.41250800
H	-0.72704900	-5.55412200	-1.26563400
C	-3.61648700	-1.99208700	-0.33239500
C	-3.70312700	-1.49185900	-1.63488400

C	-4.61579300	-1.65170400	0.57841800
C	-4.76108800	-0.67701800	-2.01442600
H	-2.91650500	-1.73096500	-2.35365000
C	-5.67483100	-0.82801700	0.20453000
H	-4.55962100	-2.03809300	1.59805100
C	-5.75061400	-0.33728400	-1.09408300
H	-4.80989100	-0.29806400	-3.03546900
H	-6.44530700	-0.57429000	0.93183000
H	-6.57775800	0.30588800	-1.39046800
C	1.44486200	-3.56546600	-0.79164000
C	2.24399900	-2.57256300	-1.37412100
C	2.05860000	-4.51406300	0.02783200
C	3.60603800	-2.50213700	-1.11826900
H	1.76932500	-1.83215700	-2.01965700
C	3.42841200	-4.45105600	0.28194600
H	1.46687600	-5.30946900	0.48070200
C	4.20342800	-3.44026700	-0.27697000
H	4.19995200	-1.70533900	-1.56647500
H	3.88915200	-5.19838600	0.92680400
H	5.27156500	-3.38631600	-0.06930400
P	-0.78790900	-2.03142200	-0.09742800
C	1.19931500	-1.54689300	1.87861000
C	-0.12833700	-2.25776500	1.63340400
H	1.42874200	-1.52666200	2.95562000
H	2.02142900	-2.08714700	1.38453400
H	-0.03644300	-3.32798800	1.87646800
H	-0.90309200	-1.84471500	2.29702400
Cu	-0.07687800	0.17170200	-0.77437700
C	-1.92540400	2.61364400	-1.12188000
O	-1.66936400	1.48026300	-0.63373100
C	-1.18560300	3.81612100	-0.62533900
C	-1.71678700	5.10814600	-0.68574100
C	0.07685900	3.65016100	-0.04485500
C	-1.00504000	6.19537500	-0.18587300
H	-2.70013600	5.27412000	-1.12326400
C	0.79316400	4.73255100	0.44412000
H	0.49471300	2.64370800	-0.01287800
C	0.25264300	6.01595700	0.37925000
H	-1.44076900	7.19219700	-0.24031900
H	1.78314300	4.57812100	0.87696600
H	0.80932600	6.86849300	0.76472000
C	0.33290700	0.48304200	-2.86839200
C	0.22869400	1.89172400	-2.91115700
C	-0.89730600	2.65098500	-3.16728700

H	1.12989500	2.43532700	-2.60295400
H	-1.74388600	2.20146500	-3.68642100
H	-0.79588300	3.72897800	-3.28606000
C	-0.69819500	-0.37149300	-3.44289800
C	-0.51915000	-1.58252200	-3.99983800
H	-1.71845600	0.02609700	-3.38564400
H	-1.35237700	-2.15969700	-4.39980300
H	0.47487300	-2.02494300	-4.09879100
H	1.35614500	0.08673800	-2.89627400
C	-3.31064100	2.81643900	-1.68983000
H	-4.01111400	3.03599100	-0.86784700
H	-3.37405500	3.62833200	-2.42342000
H	-3.63652100	1.87929200	-2.15535600

**(E)-(R)-TS2'**

C	2.12473800	2.25615200	1.58293700
C	-0.26141000	1.30161100	2.56241400
C	0.48700500	2.32630500	3.41218200
C	1.27088500	3.19911300	2.44471700
H	2.93201800	1.84918700	2.21708900
H	-1.06217500	1.81716900	2.00906200
H	-0.20388500	2.90308500	4.04387300
H	1.20001500	1.82678100	4.08770600
H	0.57673800	3.75465600	1.79164900
H	1.90183900	3.94481400	2.94917500
C	-0.86300600	0.11225900	3.25552100
C	-1.93076200	-0.55944600	2.64528400
C	-0.37864000	-0.38648800	4.46849700
C	-2.48899500	-1.69247100	3.22316500
H	-2.30340000	-0.17844200	1.69418600
C	-0.93222200	-1.52770200	5.04487200
H	0.43741400	0.12011800	4.98405400
C	-1.98731900	-2.18794600	4.42502700
H	-3.32405600	-2.18844800	2.72765000
H	-0.53785800	-1.89713100	5.99070900
H	-2.42395600	-3.07523000	4.88126800
C	2.74425900	2.93272900	0.39061900
C	4.04148100	3.44178800	0.48699400
C	2.04614500	3.11122100	-0.80722700
C	4.63665800	4.09694300	-0.58650500
H	4.59524000	3.30628700	1.41837100
C	2.64279100	3.75255400	-1.88801400
H	1.02823400	2.72470700	-0.90064400
C	3.94109600	4.24479400	-1.78320800

H	5.64990800	4.48502100	-0.49076200
H	2.08669700	3.86708600	-2.81823600
H	4.40771400	4.74497600	-2.63025000
P	0.95944900	0.82877700	1.19076200
C	2.34425900	-2.56765400	-1.18380500
C	0.01582400	-3.78607300	-0.37219400
C	0.89814300	-4.53029200	-1.38278100
C	2.33312500	-4.09399900	-1.12752400
H	2.17020800	-2.25136300	-2.22578400
H	0.18583000	-4.23021500	0.62281000
H	0.76119200	-5.61684700	-1.29559800
H	0.61377200	-4.25519300	-2.41075200
H	2.63860300	-4.44740600	-0.12953400
H	3.04165000	-4.52538300	-1.84920400
C	-1.45914100	-3.77171500	-0.64721900
C	-2.36410800	-3.95730800	0.40036000
C	-1.96788600	-3.53795200	-1.92907900
C	-3.73698600	-3.93630400	0.17363600
H	-1.98023600	-4.12055300	1.40977100
C	-3.33859800	-3.52096400	-2.16002500
H	-1.28472500	-3.36295500	-2.76159500
C	-4.22983400	-3.72577900	-1.11004700
H	-4.42494500	-4.09331400	1.00399800
H	-3.71310000	-3.33910500	-3.16670500
H	-5.30327500	-3.71412900	-1.29154500
C	3.55910500	-1.84334700	-0.67661600
C	3.74921200	-0.50757900	-1.05384100
C	4.48142500	-2.42322600	0.19775600
C	4.81846900	0.22989500	-0.56276200
H	3.03922000	-0.04819200	-1.74494200
C	5.54976500	-1.68193100	0.69883700
H	4.37434100	-3.46543500	0.49749900
C	5.71916600	-0.35221400	0.32727400
H	4.94298500	1.26549800	-0.87794600
H	6.25580400	-2.15194700	1.38231800
H	6.55659900	0.22454700	0.71746800
P	0.75606200	-2.05045200	-0.29262900
C	1.87996900	-0.62243100	1.90512500
C	1.27328900	-1.96714200	1.49800900
H	1.93674500	-0.54712300	3.00198000
H	2.90635400	-0.53828600	1.52058900
H	1.97164700	-2.78764400	1.72764100
H	0.35068800	-2.16291800	2.06863300
Cu	-0.16275100	0.03176100	-0.84957500

C	-3.01809900	1.04701000	-0.63370300
C	-3.81857000	2.29319100	-0.50527300
C	-5.20364900	2.32533900	-0.69378400
C	-3.16032100	3.47726500	-0.14775500
C	-5.91163000	3.51163000	-0.53397500
H	-5.73629300	1.41552100	-0.96807100
C	-3.86612000	4.66077700	0.00622600
H	-2.07937900	3.43981500	-0.00827400
C	-5.24686100	4.68309800	-0.18526200
H	-6.99056600	3.52017400	-0.68242900
H	-3.33913900	5.57453600	0.27822400
H	-5.80156800	5.61207700	-0.06271400
C	-3.72094000	-0.27576000	-0.79612800
H	-4.21084400	-0.54945900	0.15480500
H	-4.48658100	-0.28769400	-1.57998900
H	-2.97837600	-1.05217400	-1.01647400
O	-1.85068100	1.04848200	-0.16439100
C	-0.28073200	0.72093500	-2.88851400
C	-1.66329000	0.52869300	-3.13593900
C	-2.66197700	1.44560800	-2.92473100
H	-1.95759100	-0.48484400	-3.44414000
H	-2.40098600	2.49048200	-2.74871000
H	-3.67735700	1.25694700	-3.26973400
C	0.68266900	-0.17331900	-3.51311900
C	1.94240900	0.12291200	-3.87878400
H	0.30796900	-1.18710500	-3.71565000
H	2.59549500	-0.61146800	-4.34733600
H	2.35955100	1.11892300	-3.71270400
H	0.04363500	1.76712500	-2.79983300

**(Z)-(R)-C'**

C	-2.58465500	1.35152000	1.74003500
C	-1.08918800	-0.73393800	2.69028800
C	-2.08411100	-0.11673100	3.66812900
C	-3.21293000	0.44319900	2.81215000
H	-2.34497600	2.32606500	2.19652200
H	-1.59518000	-1.56931800	2.18299700
H	-2.44250700	-0.85563100	4.40057200
H	-1.61628300	0.70231700	4.23932000
H	-3.74141100	-0.39167500	2.32480800
H	-3.95956300	0.99508600	3.39933900
C	0.23932400	-1.21734600	3.19460800
C	1.03116900	-2.01934700	2.35676300
C	0.73187200	-0.86887800	4.45436200

C	2.28145800	-2.45319400	2.78164700
H	0.67504900	-2.29020700	1.35395600
C	1.99137300	-1.29682300	4.86975900
H	0.12776900	-0.26111200	5.12828200
C	2.77179100	-2.08844500	4.03489600
H	2.87227800	-3.08674900	2.12167000
H	2.35759800	-1.01385600	5.85599000
H	3.75153600	-2.43218100	4.36473400
C	-3.41996100	1.57894400	0.51303100
C	-3.70385800	2.87529300	0.08112700
C	-3.89491800	0.50425400	-0.24837500
C	-4.43752500	3.10145800	-1.08096600
H	-3.34425100	3.72029200	0.67151300
C	-4.63133400	0.72725900	-1.40600600
H	-3.67549100	-0.52508600	0.04939000
C	-4.90332300	2.02643200	-1.83032000
H	-4.64986600	4.12268600	-1.39644100
H	-4.98543600	-0.12860600	-1.98132100
H	-5.47746400	2.19857000	-2.73921100
P	-0.93061700	0.54106600	1.31810000
C	2.46822000	2.62527000	-0.88110100
C	3.74371800	0.31333500	-0.13329000
C	4.55868000	1.37686900	-0.89143300
C	3.95955700	2.74020200	-0.58008600
H	2.34964700	2.45966500	-1.96643400
H	4.07061200	0.29221900	0.91979500
H	5.62363700	1.31076500	-0.63077700
H	4.48384600	1.18305400	-1.97345100
H	4.12381200	2.97131100	0.48535000
H	4.42924700	3.54930000	-1.15893300
C	3.84470400	-1.07185800	-0.70593800
C	3.36227200	-1.35112400	-1.98769000
C	4.41070400	-2.11047600	0.03161500
C	3.42764100	-2.63527000	-2.50948100
H	2.91091600	-0.55004700	-2.57745300
C	4.47763200	-3.40108500	-0.48640800
H	4.79565800	-1.90332600	1.03193900
C	3.98114700	-3.66817700	-1.75705200
H	3.03672900	-2.83493700	-3.50716800
H	4.91884600	-4.20047200	0.10782600
H	4.02404800	-4.67789700	-2.16202600
C	1.55807800	3.74374500	-0.46771800
C	0.24388200	3.76044600	-0.95366500
C	1.94438800	4.75089400	0.41902100

C	-0.65746900	4.74016400	-0.55975900
H	-0.07277400	2.97206900	-1.63839600
C	1.04113600	5.73343800	0.82006800
H	2.96351800	4.77776100	0.80332800
C	-0.26258500	5.73122300	0.33725700
H	-1.67292700	4.72365800	-0.95415500
H	1.36506200	6.50828300	1.51350300
H	-0.96522100	6.50175700	0.65032700
P	1.97296400	0.97075100	-0.12134400
C	0.29244100	1.75524500	2.03314800
C	1.73820800	1.40604300	1.67634800
H	0.17897100	1.82226400	3.12640700
H	0.02245000	2.73877800	1.62097800
H	2.41727800	2.22192600	1.96824300
H	2.05160500	0.51134500	2.23387500
Cu	0.09888700	-0.31265600	-0.65300100
C	-0.79166700	-2.87537400	-1.54845600
O	0.10402800	-2.28383500	-0.69325000
C	-2.18592400	-3.02055200	-0.90313400
C	-3.39711800	-2.96861200	-1.59911900
C	-2.24504400	-3.24004800	0.47583900
C	-4.61956900	-3.07907000	-0.93674700
H	-3.40203500	-2.82575100	-2.68043800
C	-3.45924000	-3.35463300	1.14515300
H	-1.30089100	-3.31230800	1.01508800
C	-4.65850300	-3.25985400	0.44170400
H	-5.54767600	-3.02034200	-1.50580600
H	-3.46907500	-3.51862200	2.22408100
H	-5.61285300	-3.33974400	0.96025900
C	-0.64004800	0.51020600	-2.88988600
C	-1.28166400	-0.63642700	-2.54811800
C	-0.87539600	-2.03963000	-2.85182700
H	-2.23194700	-0.52164900	-2.02031800
H	0.12333600	-2.08093600	-3.30810800
H	-1.57558600	-2.47922800	-3.58237300
C	0.57565600	0.60409000	-3.68308800
C	1.09709700	1.75268600	-4.13390700
H	1.06996700	-0.33676100	-3.93616900
H	1.99754000	1.77191000	-4.74469200
H	0.62862700	2.71569700	-3.92191500
H	-1.12582000	1.45662300	-2.62586100
C	-0.30240500	-4.28475400	-1.91042700
H	-0.22186400	-4.88951600	-0.99767100
H	-0.97657100	-4.80039100	-2.61176200



H	0.70062300	-4.21000700	-2.35523200
<b>(E)-(R)-C'</b>			
C	2.90903000	0.67666100	1.67628900
C	0.38429100	0.99566000	2.72666900
C	1.56200600	1.55100000	3.53162700
C	2.65878500	1.91867000	2.54537900
H	3.36317700	-0.10009800	2.31669500
H	-0.15409000	1.81801300	2.22794000
H	1.24791200	2.40408600	4.14947600
H	1.95898100	0.78788200	4.21979200
H	2.32972200	2.75482200	1.90576100
H	3.58696500	2.24137800	3.03839300
C	-0.63907700	0.18790600	3.47598500
C	-1.98077500	0.24682600	3.06888200
C	-0.30769000	-0.64646000	4.54940700
C	-2.94998900	-0.50681500	3.72404900
H	-2.23556400	0.88307800	2.21283300
C	-1.27910500	-1.40706400	5.19491500
H	0.72267300	-0.70565400	4.90103600
C	-2.60602600	-1.34151100	4.78494700
H	-3.99120200	-0.43762100	3.40632500
H	-0.99522700	-2.04689500	6.02963800
H	-3.36912700	-1.92735400	5.29529100
C	3.81161000	0.92782400	0.50224400
C	5.13962200	0.49797800	0.54317200
C	3.37553700	1.63408700	-0.62523400
C	6.01274200	0.75951900	-0.50849500
H	5.48946500	-0.05771000	1.41506700
C	4.24400700	1.89478400	-1.67905100
H	2.33988100	1.97736100	-0.68279300
C	5.56622600	1.45760300	-1.62636600
H	7.04450900	0.41425400	-0.45482900
H	3.88639800	2.44906700	-2.54598200
H	6.24531000	1.66435100	-2.45195400
P	1.16813200	0.09934700	1.24784500
C	0.31151100	-3.26963600	-1.46012200
C	-2.24935000	-3.06311500	-0.50858900
C	-1.95004100	-4.14218200	-1.55416100
C	-0.49635000	-4.56137600	-1.37631300
H	0.18216500	-2.85765800	-2.47389400
H	-2.38817100	-3.54996400	0.47166400
H	-2.65433200	-4.98160600	-1.47704800
H	-2.05784400	-3.72321300	-2.56762200

H	-0.36966900	-5.04422000	-0.39351700
H	-0.17198000	-5.28775900	-2.13559300
C	-3.40909500	-2.13555000	-0.75767600
C	-4.03674200	-1.99615300	-1.99633900
C	-3.82780200	-1.31214200	0.29267400
C	-5.04733900	-1.05249200	-2.17996900
H	-3.74877100	-2.62672700	-2.83723800
C	-4.83197900	-0.37217600	0.11380700
H	-3.34026200	-1.40341100	1.26616200
C	-5.44679700	-0.23521000	-1.12921200
H	-5.52404200	-0.96037700	-3.15496000
H	-5.13240500	0.26180600	0.94783900
H	-6.23080900	0.50612100	-1.27541400
C	1.77747000	-3.29191500	-1.15181600
C	2.56102800	-2.20683400	-1.56555800
C	2.38861800	-4.31664800	-0.42741400
C	3.90927800	-2.13464600	-1.24570200
H	2.09230200	-1.40436100	-2.13856200
C	3.74252100	-4.24536100	-0.10288200
H	1.80769600	-5.18225000	-0.10911300
C	4.50384300	-3.15179400	-0.50101900
H	4.49612200	-1.27458600	-1.56632600
H	4.20219600	-5.05306400	0.46523500
H	5.55987900	-3.09095700	-0.24053700
P	-0.64810000	-2.06739300	-0.36957300
C	1.22818800	-1.69729000	1.73484500
C	-0.03581500	-2.47029700	1.34334800
H	1.40943700	-1.80283400	2.81554100
H	2.10508000	-2.11432600	1.21683800
H	0.12732500	-3.55402100	1.45100100
H	-0.86348700	-2.19928200	2.01863800
Cu	-0.61941100	0.22902600	-0.46094900
C	-2.08070700	2.74430100	-0.38977300
O	-1.54052100	1.74480800	0.37889500
C	-1.10642000	0.39203500	-2.99261300
C	0.06474900	-0.10420700	-3.69400200
C	0.08833300	-1.24018700	-4.40171900
H	0.96397100	0.51885400	-3.63289300
H	-0.80295600	-1.86677300	-4.48525200
H	0.97774600	-1.57791300	-4.92924600
C	-1.18852100	1.62688700	-2.45030000
C	-2.40358900	2.20298400	-1.80969000
H	-0.30789400	2.27837900	-2.51030100
H	-2.80888700	3.00503400	-2.45056600

H	-3.18138900	1.42641700	-1.71132800
H	-1.98995600	-0.25818000	-2.97067100
C	-1.11476400	3.93245800	-0.55295800
C	-1.46708000	5.09330700	-1.24915100
C	0.17852500	3.85261900	-0.03752400
C	-0.55838400	6.13178800	-1.42585400
H	-2.46946000	5.19251000	-1.66925500
C	1.09682200	4.88417600	-0.21555000
H	0.44461000	2.94458800	0.50223000
C	0.73189800	6.03118800	-0.91197900
H	-0.85876300	7.02487100	-1.97340000
H	2.10554300	4.78708600	0.18934900
H	1.44615500	6.84104800	-1.05428000
C	-3.38075400	3.23052900	0.26295000
H	-3.16214600	3.58190800	1.28012900
H	-3.87561000	4.04408500	-0.28684700
H	-4.07924300	2.38392100	0.33389100

**(Z)-(R)-TS3'**

C	0.09093500	1.38178300	3.12902500
C	2.23545200	-0.33769600	3.11283100
C	1.85275600	0.32476000	4.44218300
C	0.35260700	0.58983700	4.41249100
H	0.62024500	2.34614800	3.22171100
H	1.93831000	-1.39700200	3.16772000
H	2.15695200	-0.30068600	5.29285100
H	2.37004400	1.29006500	4.55708500
H	-0.20163900	-0.36297500	4.39029900
H	0.00516800	1.14233800	5.29613700
C	3.67391500	-0.27833700	2.68144800
C	4.21618000	-1.33581500	1.93978100
C	4.49176500	0.83045500	2.92694100
C	5.51070100	-1.27681500	1.43712900
H	3.60951000	-2.22014600	1.74770900
C	5.78830800	0.89283000	2.42506400
H	4.11785000	1.66563300	3.51909100
C	6.30264400	-0.15623100	1.67017300
H	5.89979400	-2.11775500	0.86428700
H	6.40113200	1.76894600	2.63215600
H	7.31715100	-0.10574000	1.27843800
C	-1.33881300	1.65288800	2.76368400
C	-1.74545300	2.95905100	2.47786000
C	-2.28276300	0.62459100	2.67198200
C	-3.06430900	3.23841300	2.12866200

H	-1.01357300	3.76788900	2.53419400
C	-3.60287800	0.90221000	2.33663500
H	-1.98087200	-0.41291500	2.82812600
C	-3.99846000	2.20953500	2.06501200
H	-3.36011900	4.26468500	1.90928200
H	-4.31959800	0.08624300	2.25378900
H	-5.02994200	2.41589000	1.78256400
P	1.02695600	0.39927100	1.83080800
C	0.61998600	1.97871400	-2.44662200
C	2.43955600	-0.02329600	-2.89224700
C	1.57258500	0.36753000	-4.08916800
C	1.18753800	1.82553900	-3.86902500
H	-0.45652200	1.74856000	-2.46867300
H	3.32989000	0.63032200	-2.89125500
H	2.10383300	0.21212700	-5.03829900
H	0.66454800	-0.25719400	-4.12290100
H	2.08828600	2.44505100	-3.98995300
H	0.46134800	2.18234700	-4.61149400
C	2.88751500	-1.44714100	-2.76792800
C	2.05215900	-2.51830400	-3.09797900
C	4.15606900	-1.72717400	-2.25150100
C	2.48114200	-3.83031400	-2.93143000
H	1.04810100	-2.32813400	-3.47998600
C	4.58367700	-3.03933300	-2.07499200
H	4.81773400	-0.89970000	-1.98636900
C	3.74760400	-4.09698300	-2.41770000
H	1.81843800	-4.65213900	-3.20004800
H	5.57860800	-3.23467500	-1.67631000
H	4.07946500	-5.12504200	-2.28512500
C	0.78806600	3.32014300	-1.78887700
C	-0.22281100	3.80172800	-0.94907700
C	1.95318100	4.08351400	-1.91664000
C	-0.07486500	4.99975500	-0.25915300
H	-1.13428200	3.21463700	-0.83470100
C	2.10604800	5.28063000	-1.22395400
H	2.76356400	3.73948100	-2.56057000
C	1.09336600	5.74482500	-0.39026300
H	-0.88280100	5.35068900	0.38304400
H	3.02412700	5.85485700	-1.33997800
H	1.21260100	6.68394100	0.14743300
P	1.37893200	0.53300600	-1.45081900
C	1.98336200	1.75338600	0.99253700
C	2.63095700	1.28081000	-0.30438400
H	2.73407100	2.18363500	1.67042600

H	1.24767800	2.54669100	0.78208400
H	3.17114600	2.10457500	-0.79322800
H	3.36398600	0.48036300	-0.10332800
Cu	0.21504800	-0.91579200	-0.02891600
C	-2.74148700	-1.45464800	-0.95209200
O	-1.73164600	-1.49333000	0.01961800
C	-3.38228800	2.18073300	-1.51140300
C	-2.74577000	1.08000200	-1.07382100
C	-2.55709600	-0.19571300	-1.81933400
H	-2.33233200	1.08363300	-0.06089500
H	-1.52032600	-0.26684600	-2.20069400
H	-3.20914100	-0.24638900	-2.70392100
C	-3.98677400	2.37388700	-2.81675500
C	-4.59714500	3.50469200	-3.19023200
H	-3.93069500	1.54702900	-3.52939800
H	-5.04214600	3.62395900	-4.17544900
H	-4.66898600	4.35698500	-2.51362500
H	-3.46701300	3.03042600	-0.82592500
C	-0.84469400	-3.82573600	0.79551200
C	-1.64727400	-5.01059300	0.47690300
H	-1.46388000	-2.70557800	0.37451900
C	-2.52455200	-5.61915200	1.28302200
H	-1.52662600	-5.39860600	-0.54232400
H	-3.11549100	-6.47069900	0.95378200
H	-2.67982000	-5.28187300	2.30976500
C	0.35668200	-3.57834300	0.04347100
H	0.34837800	-3.93157500	-0.99709700
C	1.41663000	-2.80322400	0.42667900
H	1.55198200	-2.59254400	1.48940100
H	2.28467200	-2.68118300	-0.22204800
H	-0.75369800	-3.61546500	1.87416600
C	-4.10865700	-1.49180200	-0.26181400
C	-4.25447800	-2.23312400	0.91475500
C	-5.24024200	-0.86246800	-0.78482800
C	-5.48600400	-2.33637900	1.55164800
H	-3.38510200	-2.73568200	1.33609800
C	-6.47200500	-0.94772200	-0.14025100
H	-5.17083500	-0.28253000	-1.70460500
C	-6.60145000	-1.68427400	1.03174100
H	-5.57225200	-2.92774700	2.46278400
H	-7.33553100	-0.43488800	-0.56252800
H	-7.56572500	-1.75562600	1.53320000
C	-2.65114100	-2.66897900	-1.88635800
H	-1.65358800	-2.70709400	-2.35427400

H	-2.81670700	-3.60137400	-1.33263500
H	-3.41078400	-2.61276500	-2.67876000

**(E)-(R)-TS3'**

C	-0.49441600	1.80551700	2.79125200
C	1.74944800	0.28587200	3.20947300
C	1.21316200	1.09956900	4.39332000
C	-0.28602600	1.24511100	4.20326700
H	-0.03974500	2.81210400	2.76909800
H	1.51551700	-0.77331100	3.40118300
H	1.47926000	0.61916900	5.34511700
H	1.66498200	2.10355200	4.40787900
H	-0.78575300	0.26482300	4.28225900
H	-0.75052000	1.90266400	4.95176900
C	3.22315600	0.39074200	2.93688400
C	3.94508800	-0.74999700	2.56797400
C	3.91377900	1.60675900	3.01167400
C	5.29947400	-0.67718800	2.26308900
H	3.43362100	-1.71175400	2.52225800
C	5.26683400	1.68411000	2.69942700
H	3.39159600	2.51167700	3.32250400
C	5.96570700	0.54322300	2.31734900
H	5.83847100	-1.58448700	1.99462400
H	5.77918200	2.64294900	2.76433900
H	7.02668900	0.60265700	2.08043700
C	-1.94483500	1.92600500	2.41478300
C	-2.58361300	3.15506000	2.61654000
C	-2.70418400	0.83948800	1.96938500
C	-3.94802300	3.29848700	2.39136200
H	-1.99758900	4.00739900	2.96619300
C	-4.06993600	0.98615100	1.73575400
H	-2.22782400	-0.12125100	1.74989600
C	-4.69482400	2.20999500	1.95105900
H	-4.42601900	4.26432200	2.55195000
H	-4.64108500	0.13610900	1.36298600
H	-5.76029400	2.31981400	1.75597400
P	0.61935500	0.72107800	1.72990600
C	0.91556800	1.46648200	-2.85893500
C	2.90116400	-0.39128000	-2.55236700
C	2.22197900	-0.37951900	-3.92138300
C	1.69611900	1.03632900	-4.11750700
H	-0.14058000	1.18255200	-2.97847900
H	3.70890400	0.36246900	-2.56826700
H	2.91570700	-0.68415800	-4.71715500

H	1.38110900	-1.09318200	-3.93627200
H	2.54945600	1.71154900	-4.27677500
H	1.06089900	1.12290600	-5.00887400
C	3.46546700	-1.68751700	-2.05628500
C	2.84376600	-2.91433400	-2.30867900
C	4.62942600	-1.68054900	-1.28253000
C	3.37334300	-4.09722500	-1.80519100
H	1.93020900	-2.94933900	-2.90323000
C	5.16101500	-2.86322900	-0.77803200
H	5.12765600	-0.73073400	-1.07618600
C	4.53382500	-4.07728700	-1.03634900
H	2.87459100	-5.04278600	-2.01443100
H	6.07772800	-2.83638200	-0.19011300
H	4.94708100	-5.00475500	-0.64425300
C	0.96263500	2.93254600	-2.53213100
C	-0.20500500	3.58778100	-2.12925100
C	2.15108500	3.67098400	-2.56943300
C	-0.18576400	4.92647600	-1.75324200
H	-1.14314700	3.03372700	-2.11604700
C	2.17515900	5.00921100	-2.19088900
H	3.07802300	3.19559100	-2.89512100
C	1.00726300	5.64193300	-1.77478100
H	-1.11437100	5.40843800	-1.44919100
H	3.11311900	5.56167900	-2.22535100
H	1.02650500	6.68977000	-1.47992600
P	1.54856400	0.31592200	-1.46288400
C	1.55542200	2.00586000	0.76624700
C	2.48407200	1.37954000	-0.27110400
H	2.11586800	2.67404900	1.43586200
H	0.78448300	2.62066500	0.26878000
H	3.05559400	2.15549500	-0.79852500
H	3.20934900	0.70296400	0.21179400
Cu	0.28017100	-0.98512300	0.00992900
C	-2.51995900	-1.74920800	-1.19608200
O	-1.63680900	-1.65979500	-0.11242700
C	-3.37115200	1.73048600	-1.87572300
C	-2.51856200	0.78277200	-1.45744400
C	-2.29962700	-0.53076100	-2.11613800
H	-1.94061000	0.96839700	-0.54502100
H	-1.24841200	-0.61595900	-2.44952300
H	-2.91866000	-0.60832600	-3.02317400
C	-3.55232500	2.99302300	-1.18453100
C	-4.36669500	3.97459500	-1.58816200
H	-2.96724700	3.12072500	-0.26738600

H	-4.47213400	4.89901100	-1.02358500
H	-4.96766800	3.88099300	-2.49332000
H	-3.97069000	1.56521900	-2.77774900
C	-0.75489700	-3.84398000	1.00941700
C	-1.41306000	-5.09804100	0.63016800
H	-1.36132000	-2.81652300	0.38980600
C	-2.40813200	-5.70782100	1.28374500
H	-1.06599000	-5.53953800	-0.31268400
H	-2.87293900	-6.61514600	0.90489500
H	-2.79221400	-5.31704100	2.22784600
C	0.54657400	-3.55418700	0.47349900
H	0.76795700	-4.00961900	-0.50180500
C	1.45464900	-2.64390700	0.95064400
H	1.37034700	-2.31112700	1.98836200
H	2.42552500	-2.52556300	0.46697700
H	-0.88971100	-3.55440100	2.06370600
C	-3.95895100	-1.83587900	-0.68237100
C	-4.20608300	-2.35710700	0.59047700
C	-5.05601200	-1.47896000	-1.47001900
C	-5.50568200	-2.50589200	1.06443800
H	-3.36254600	-2.64471300	1.21611200
C	-6.35672600	-1.61104800	-0.99425400
H	-4.90256600	-1.08377100	-2.47423900
C	-6.58811200	-2.12446200	0.27777700
H	-5.67070700	-2.91950200	2.05885900
H	-7.19421500	-1.31177300	-1.62350600
H	-7.60545400	-2.23100300	0.65166900
C	-2.24033700	-3.01064700	-2.02361000
H	-1.18553500	-3.01645200	-2.34365400
H	-2.43702900	-3.91356300	-1.43158000
H	-2.87956400	-3.04983800	-2.91706300

**(R)-TS4**

P	-1.50278900	-0.96987500	0.16007800
C	-0.61762500	-2.44854800	0.78507700
C	-2.80025500	-1.57907200	-0.97149300
C	-2.41227600	-0.36173700	1.61697500
C	0.49258900	-2.21789800	1.64527200
C	-0.92014000	-3.73665600	0.34560600
C	-2.43409900	-2.29623400	-2.10530300
C	-4.11349600	-1.12303400	-0.87500100
C	-3.24369000	-1.18353800	2.36491000
C	-2.24761200	0.96948800	1.99025300
C	0.78009500	-0.93961300	2.35950800



C	1.25303300	-3.32981400	1.94582900
C	-0.14314900	-4.85132000	0.69003100
H	-1.78968900	-3.89043300	-0.29099600
C	-3.32357300	-2.56596300	-3.14962800
H	-1.40487000	-2.64955200	-2.19114400
C	-5.02658200	-1.26447400	-1.91894100
H	-4.41205900	-0.59572400	0.02584700
C	-4.01710200	-0.69416000	3.42235400
H	-3.30739100	-2.23819800	2.09418600
C	-2.98591500	1.52895700	3.03044900
H	-1.54230900	1.57751200	1.42360700
C	1.54223600	0.16305600	1.87821500
C	0.31741300	-0.82756700	3.65568600
C	0.95395100	-4.60602800	1.47790200
H	-0.38960300	-5.85376200	0.34801400
C	-4.58410200	-1.93268400	-3.08521600
C	-3.94381800	0.69662900	3.65935700
P	1.91662100	0.22288800	0.07697800
C	1.82032000	1.24376200	2.71475200
C	0.58622800	0.26715800	4.47045500
C	3.03142400	1.65489600	-0.12882300
C	2.98596600	-1.23776100	-0.15943100
C	1.35731700	1.31587700	4.03644700
H	2.40299000	2.07844300	2.32907100
C	4.35538800	1.55558500	-0.53110700
C	2.46700800	2.92284000	0.02301300
C	4.12336700	-1.44492900	0.61141600
C	2.63290300	-2.19140600	-1.11135000
H	1.57949200	2.16604900	4.67693200
C	5.16023900	2.67970100	-0.75046000
H	4.76871500	0.56814300	-0.71250000
C	3.23589400	4.08122500	-0.06578300
H	1.39864800	2.98860000	0.22847400
C	5.00285900	-2.50754800	0.37763300
H	4.34119800	-0.73434400	1.40943400
C	3.44383300	-3.29061500	-1.38477100
H	1.68688300	-2.06099200	-1.63405100
C	4.60007200	3.93370600	-0.42203100
C	4.68563700	-3.35254300	-0.70653900
C	2.91084900	-4.67757800	2.47158000
H	3.70228100	-4.58236100	1.70299100
H	3.29968800	-5.10894000	3.39956800
O	2.36539800	-3.39430000	2.73413000
O	1.86795000	-5.49199800	1.96629000

H	-0.92012900	-1.64014500	6.35575100
C	-0.90772500	-0.99058300	5.47495300
H	-1.91429200	-0.58218700	5.25470700
O	-0.00347800	0.08042500	5.68636300
O	-0.44688300	-1.72134500	4.34962300
O	-5.42756600	-1.97143200	-4.17057800
O	-4.82663000	1.29299100	4.53120600
O	5.60130600	-4.28598400	-1.13839400
O	5.34679300	5.08785200	-0.50907100
C	-6.08493900	1.55479800	3.94282800
H	-6.66032800	2.14097200	4.66748800
H	-5.97954400	2.12985100	3.01084400
H	-6.63511100	0.62935800	3.71485700
C	-2.70187600	2.96588100	3.49496200
C	-4.85447800	-1.72219300	4.21026100
C	-6.46480000	-0.75365400	-1.74571200
C	-5.06336600	-1.08722700	-5.21543700
H	-5.66522900	-1.36022200	-6.08898700
H	-5.26632500	-0.03912400	-4.94977100
H	-3.99662300	-1.16946900	-5.46797200
C	-2.82729200	-3.54233900	-4.23526200
C	6.22000600	-2.63392100	1.31724600
C	2.96039600	-4.41067600	-2.31924600
C	6.57952000	-3.72557900	-1.99191700
H	7.19809200	-2.97771400	-1.47253400
H	7.21928800	-4.54878600	-2.32749300
H	6.11810700	-3.24106800	-2.86536400
C	6.56455600	2.45314400	-1.34548400
C	2.57719700	5.45106800	0.15848700
C	6.29530100	5.33515800	0.50519100
H	6.23981600	6.39601800	0.77932600
H	6.09637700	4.72917600	1.40117900
H	7.31604800	5.13181400	0.15082100
Cu	-0.13303500	0.52416800	-1.01609300
C	-1.81818500	2.90096900	-1.51715500
O	-0.72870400	2.48171700	-0.99248700
C	-1.88404500	2.02318100	-3.53384200
C	-3.26928000	2.06244100	-3.96221400
C	-3.90241200	3.06514300	-4.59103500
H	-3.85510100	1.17625200	-3.67610600
H	-3.37411500	3.97122800	-4.89165000
H	-4.96304600	3.00723900	-4.83395200
C	-1.29175800	0.74971000	-3.34515400
C	0.04849300	0.47366000	-3.16466100

H	-1.98522600	-0.09606000	-3.26657900
H	0.39445500	-0.56252600	-3.22459300
H	0.79855700	1.24379900	-3.36344700
C	-1.82985300	4.30674300	-2.01943900
C	-2.99479700	5.07545000	-2.09536500
C	-0.62739900	4.87915400	-2.45901200
C	-2.95847000	6.37744400	-2.59200800
H	-3.94388900	4.66731100	-1.75517200
C	-0.59230200	6.16907500	-2.96331700
H	0.27817400	4.27109400	-2.40570300
C	-1.76209900	6.92762900	-3.03184300
H	-3.87726700	6.96112900	-2.63576600
H	0.35135700	6.59059700	-3.30943200
H	-1.73531900	7.94232300	-3.42655300
C	-3.12128800	2.34779600	-0.98781400
H	-3.32233400	2.76635100	0.01304000
H	-3.97988900	2.56974100	-1.63069800
H	-3.04267200	1.26012900	-0.88496900
H	-1.22726800	2.79893100	-3.93636500
C	1.11637900	5.30304500	0.59924800
H	0.49711100	4.75335600	-0.12038200
H	1.04019900	4.79505000	1.57405900
H	0.67299500	6.30239500	0.70802100
C	3.27687500	6.25543900	1.26306500
H	3.44677100	5.64053800	2.15940800
H	4.23290800	6.67040300	0.93509600
H	2.64161000	7.10242400	1.55864100
C	2.60761300	6.24641600	-1.15200300
H	2.10099100	7.21412900	-1.01888500
H	3.63550400	6.43338100	-1.48329900
H	2.08094800	5.70015700	-1.94632200
C	6.97060100	3.56656000	-2.32060300
H	7.07699000	4.54698900	-1.85258700
H	7.92998300	3.30772700	-2.79036900
H	6.22196400	3.66898500	-3.11858500
C	6.60232700	1.15469900	-2.17166300
H	6.50610300	0.24618700	-1.55982700
H	5.81212300	1.13788800	-2.93463200
H	7.57112600	1.08656300	-2.68509900
C	7.61142300	2.29283600	-0.23494900
H	7.35999300	1.43871700	0.40971800
H	8.60155600	2.10115000	-0.67452700
H	7.69717800	3.17502100	0.40746800
C	5.75473500	-2.50576900	2.77935400

H	5.19936200	-1.58558800	2.98941300
H	5.11288400	-3.34795200	3.06891300
H	6.63271100	-2.51717600	3.43998200
C	6.97617100	-3.96648700	1.24866000
H	7.55367300	-4.10005400	0.32949300
H	7.68802200	-4.00281300	2.08555500
H	6.29911300	-4.82501300	1.34490300
C	7.19893300	-1.48713100	1.03344600
H	7.58180300	-1.51584600	0.00292000
H	6.71765600	-0.50951100	1.18198200
H	8.06229800	-1.54318500	1.71230900
C	2.99422400	-5.74424500	-1.55899000
H	2.35036200	-5.70665800	-0.66845100
H	2.62462700	-6.55291800	-2.20647800
H	4.01022700	-6.00130800	-1.24022900
C	1.51063900	-4.17948900	-2.76312600
H	0.82156600	-4.11106500	-1.90559700
H	1.40000700	-3.27296300	-3.37729700
H	1.18679200	-5.02963900	-3.38004300
C	3.80569200	-4.53035200	-3.59340400
H	3.89760900	-3.56067600	-4.10391800
H	4.80810500	-4.91789900	-3.38602500
H	3.32343800	-5.22912800	-4.29179900
C	-2.25993000	-4.78730300	-3.52474100
H	-1.39610200	-4.56596800	-2.88550400
H	-3.02942100	-5.26542300	-2.90198400
H	-1.92582300	-5.51999200	-4.27307200
C	-3.90354600	-4.07561800	-5.18795200
H	-4.76723800	-4.47580400	-4.64290700
H	-4.26926600	-3.32988100	-5.89938400
H	-3.46650500	-4.89342600	-5.77812900
C	-1.70464300	-2.89976200	-5.05995500
H	-0.87286200	-2.55580500	-4.42873600
H	-1.30042700	-3.62815000	-5.77851000
H	-2.06002700	-2.03037400	-5.63016100
C	-7.43211000	-1.94094100	-1.84611400
H	-8.46847400	-1.59373800	-1.72209700
H	-7.35229400	-2.44173300	-2.81727300
H	-7.22652000	-2.67842900	-1.05704300
C	-6.84213800	0.30249000	-2.79366600
H	-6.98159500	-0.13969500	-3.78431400
H	-7.79185800	0.77935600	-2.51198100
H	-6.07927000	1.09398800	-2.86235200
C	-6.67287200	-0.10569000	-0.37141500

H	-6.46235400	-0.79722500	0.45715700
H	-6.05229000	0.79272200	-0.23520800
H	-7.72318300	0.20236500	-0.28033300
C	-3.97441500	-2.94468800	4.52945500
H	-3.59741400	-3.45830800	3.63811400
H	-3.10487900	-2.66203400	5.13854800
H	-4.56084500	-3.67729600	5.10085700
C	-5.38562000	-1.23476700	5.56316600
H	-6.17678100	-0.48453200	5.48192500
H	-5.80849100	-2.09448800	6.10215300
H	-4.58676600	-0.80863100	6.18405100
C	-6.03129100	-2.19949600	3.34909000
H	-6.72862600	-1.38225000	3.11952600
H	-5.68611600	-2.61998000	2.39335800
H	-6.59690500	-2.98173700	3.87614200
C	-2.35465500	2.93855600	4.98997100
H	-1.48012500	2.29754300	5.17184200
H	-2.10872800	3.95253700	5.33782500
H	-3.18886800	2.56142200	5.59233400
C	-3.88352000	3.91420200	3.25777600
H	-4.73329300	3.69237600	3.91069500
H	-3.57156500	4.94754900	3.46615000
H	-4.22039900	3.87651400	2.21113800
C	-1.49687400	3.56332600	2.75707100
H	-0.59075300	2.95133500	2.87902700
H	-1.67177600	3.69728900	1.67903800
H	-1.28369200	4.55671000	3.17597900

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P	-1.49836900	-1.04085000	0.15649500
C	-0.59417900	-2.45232300	0.89017500
C	-2.74722400	-1.75982900	-0.96124000
C	-2.44575200	-0.34316700	1.54449600
C	0.49959500	-2.13870100	1.74421600
C	-0.86284500	-3.77190400	0.52959100
C	-2.33317400	-2.49540900	-2.06788100
C	-4.08016900	-1.36172000	-0.89428900
C	-3.24915200	-1.12513400	2.36298100
C	-2.33067400	1.02278200	1.78970400
C	0.74232800	-0.80137000	2.36216600
C	1.27991400	-3.21100900	2.12643300
C	-0.06449200	-4.84324800	0.95265800
H	-1.72170000	-3.98494300	-0.10484200
C	-3.19288800	-2.82428800	-3.11948500

H	-1.29381400	-2.82680700	-2.11661500
C	-4.96718800	-1.56141000	-1.95059500
H	-4.41036400	-0.82093500	-0.01241000
C	-4.03495800	-0.57188900	3.37853000
H	-3.27149300	-2.20127700	2.18914700
C	-3.08491800	1.64393600	2.78391900
H	-1.66099900	1.60567600	1.15416900
C	1.48018000	0.28499000	1.80816200
C	0.25018900	-0.60010200	3.63705000
C	1.01510500	-4.52118100	1.73703600
H	-0.28247200	-5.87159000	0.67401000
C	-4.47487900	-2.23264100	-3.09301200
C	-4.00368400	0.83708400	3.49828800
P	1.88309700	0.23422100	0.01044700
C	1.71666700	1.43255600	2.56472400
C	0.47644600	0.56201900	4.36849600
C	2.97761600	1.66764700	-0.27482000
C	2.98718300	-1.21621500	-0.09745500
C	1.23000800	1.59357600	3.86882900
H	2.28433000	2.25023600	2.12536200
C	4.31000500	1.56968500	-0.65125300
C	2.39083700	2.93152000	-0.18734600
C	4.11047900	-1.32802600	0.71166800
C	2.67971000	-2.25298500	-0.97385300
H	1.41924100	2.49609100	4.44499200
C	5.10092800	2.69558500	-0.90882700
H	4.74090700	0.58137900	-0.78260700
C	3.15173600	4.09493400	-0.29043200
H	1.31487700	2.98794900	-0.01664700
C	5.01808100	-2.38486300	0.59158600
H	4.28975300	-0.54590900	1.44999200
C	3.52561900	-3.34762300	-1.14069600
H	1.74081700	-2.19003700	-1.52072700
C	4.52032800	3.95331100	-0.63016600
C	4.74897500	-3.32504000	-0.42651700
C	2.95889400	-4.48702200	2.76227000
H	3.76823000	-4.42712500	2.00813200
H	3.33397600	-4.85104900	3.72438400
O	2.38337700	-3.20079100	2.92967100
O	1.94405500	-5.35358000	2.28779100
H	-1.04498900	-1.22007100	6.36477700
C	-1.01291600	-0.64235400	5.43581800
H	-2.01511400	-0.26543800	5.14999400
O	-0.12862200	0.45450200	5.58604700

O	-0.50570400	-1.45528000	4.38797800
O	-5.28407900	-2.30543700	-4.20349100
O	-4.87758200	1.47966300	4.34625800
O	5.69436900	-4.27115600	-0.75397500
O	5.25085900	5.11420900	-0.75362700
C	-6.16605400	1.66238300	3.79606900
H	-6.67783300	2.40683400	4.41593800
H	-6.11176500	2.02896200	2.76018800
H	-6.75365500	0.73171600	3.80611000
C	-2.84191500	3.12562500	3.11159700
C	-4.84059700	-1.54891400	4.25794800
C	-6.42384000	-1.09300200	-1.81894100
C	-4.90471900	-1.41129700	-5.23151700
H	-5.48480400	-1.67903200	-6.12136400
H	-5.12569100	-0.36871700	-4.95799800
H	-3.83146400	-1.48276400	-5.46106500
C	-2.65203600	-3.81658900	-4.16740600
C	6.20829500	-2.40247000	1.57269300
C	3.09838900	-4.54841000	-1.99885700
C	6.69104300	-3.76465900	-1.61937800
H	7.30673300	-2.99369800	-1.13152000
H	7.33079500	-4.60907600	-1.89764300
H	6.24921200	-3.32675400	-2.52681800
C	6.51042000	2.46873500	-1.49304400
C	2.47799600	5.45995900	-0.08421600
C	6.21337500	5.39992200	0.23712400
H	6.11195800	6.45241400	0.53005300
H	6.07213000	4.77306800	1.12924100
H	7.23135800	5.25351800	-0.15173700
Cu	-0.18122400	0.51606400	-1.00864500
C	-1.90533900	2.64472100	-1.84167000
O	-0.86868900	2.38610500	-0.98994800
C	-1.57372800	2.04947300	-3.30637800
C	-2.72226300	2.17575800	-4.25802800
C	-2.90547100	3.17591800	-5.11729700
H	-3.47845200	1.38317200	-4.18581700
H	-2.18531400	3.99131000	-5.19986000
H	-3.78520400	3.23185000	-5.75587000
C	-1.12839700	0.62586400	-3.23139200
C	0.16310500	0.22805400	-3.26700900
H	-1.91179800	-0.14172700	-3.18226900
H	0.44089800	-0.82725300	-3.28992300
H	0.97180200	0.95045900	-3.39787000
C	-2.05208000	4.15980600	-2.02850500

C	-3.24659700	4.86175100	-1.86004500
C	-0.91828600	4.89060100	-2.39903200
C	-3.31025500	6.23890500	-2.06645700
H	-4.15419700	4.33558800	-1.56782300
C	-0.97609400	6.25956100	-2.62015900
H	0.03024000	4.35878100	-2.49746600
C	-2.17900500	6.94363300	-2.45623700
H	-4.25762500	6.75920200	-1.92682600
H	-0.07585300	6.79905700	-2.91519000
H	-2.22996900	8.01808000	-2.62784300
C	-3.21980000	2.01152900	-1.37042500
H	-3.46027200	2.34413300	-0.35059200
H	-4.07519500	2.24056300	-2.02269000
H	-3.11084100	0.92126400	-1.34384700
H	-0.72663900	2.65225500	-3.66709400
C	1.04601700	5.29672700	0.44002000
H	0.39245800	4.71209300	-0.21930000
H	1.04003900	4.81612700	1.43189400
H	0.58743000	6.28953900	0.54866500
C	3.21327900	6.32094500	0.95377000
H	3.47037800	5.73768500	1.85074200
H	4.12472200	6.77082900	0.55322900
H	2.55949800	7.14471200	1.27298500
C	2.43452200	6.21035000	-1.42004500
H	1.94482000	7.18700600	-1.28788800
H	3.44253700	6.37954000	-1.81639900
H	1.86085700	5.64395700	-2.16637900
C	6.88132500	3.53568800	-2.53214900
H	6.92679800	4.54846700	-2.12715100
H	7.86097800	3.29570900	-2.96911900
H	6.14385200	3.54656400	-3.34695600
C	6.58007400	1.12663400	-2.24326200
H	6.51767100	0.25443700	-1.57643100
H	5.78564100	1.03978200	-2.99705900
H	7.54668800	1.05817100	-2.76083700
C	7.56977800	2.39364400	-0.38517600
H	7.33425000	1.58096000	0.31605400
H	8.55670000	2.18209200	-0.82288900
H	7.65658500	3.31610100	0.19684700
C	5.69851600	-2.15091200	3.00389000
H	5.13695800	-1.21688400	3.11600800
H	5.04738600	-2.96464000	3.34818700
H	6.55648100	-2.10007000	3.68828900
C	6.98942900	-3.72023100	1.64171300



H	7.59515500	-3.92099800	0.75356600
H	7.67832700	-3.67161900	2.49698200
H	6.32688400	-4.58208000	1.79255900
C	7.17312800	-1.26507500	1.21268400
H	7.58985400	-1.38113600	0.20169600
H	6.66656000	-0.28986000	1.25429100
H	8.01504200	-1.23695100	1.91970500
C	3.13583000	-5.81642900	-1.13426300
H	2.46634700	-5.72118900	-0.26728700
H	2.80250500	-6.68294700	-1.72405000
H	4.14701300	-6.02290600	-0.76681100
C	1.66171700	-4.38887300	-2.51151000
H	0.93718800	-4.26498400	-1.69084800
H	1.55712200	-3.53983600	-3.20448500
H	1.37935600	-5.29445300	-3.06668500
C	3.98834200	-4.74401600	-3.23338400
H	4.07717900	-3.81245600	-3.81117400
H	4.99095300	-5.09236300	-2.96800900
H	3.54330900	-5.50252300	-3.89316300
C	-2.08366800	-5.03419400	-3.41252600
H	-1.24864700	-4.78047200	-2.74710600
H	-2.86431000	-5.51676300	-2.80764300
H	-1.70758100	-5.77404000	-4.13360300
C	-3.69293400	-4.38763000	-5.13714500
H	-4.55995500	-4.79973300	-4.60663000
H	-4.05972900	-3.65991500	-5.86708200
H	-3.22342100	-5.20380900	-5.70430300
C	-1.51855300	-3.17563900	-4.97718500
H	-0.69012100	-2.84929200	-4.33345000
H	-1.11231200	-3.89979200	-5.69860100
H	-1.86178800	-2.29681800	-5.54065000
C	-7.35824300	-2.30448500	-1.93371300
H	-8.40523700	-1.98218100	-1.83425600
H	-7.24663300	-2.80914000	-2.89931800
H	-7.15244000	-3.03217300	-1.13596800
C	-6.79798300	-0.05300500	-2.88326700
H	-6.90463700	-0.50273500	-3.87475600
H	-7.76315600	0.40769200	-2.62853400
H	-6.04793200	0.75145200	-2.93373200
C	-6.68218700	-0.43987000	-0.45592000
H	-6.46915100	-1.11887400	0.38204800
H	-6.09036800	0.47776100	-0.31710400
H	-7.74294100	-0.16283800	-0.39101500
C	-3.97104800	-2.77538500	4.59255400

H	-3.70048500	-3.37180300	3.71391000
H	-3.03633300	-2.48490000	5.09040300
H	-4.52513200	-3.43967500	5.26969100
C	-5.28279400	-0.97697300	5.61027800
H	-6.06912900	-0.22198900	5.53543700
H	-5.67707200	-1.79660300	6.22739200
H	-4.44065500	-0.52385800	6.15092100
C	-6.06689600	-2.05061100	3.48417700
H	-6.74016300	-1.23147800	3.19855600
H	-5.76673400	-2.56765600	2.56127400
H	-6.64195100	-2.76116400	4.09606300
C	-2.43002900	3.24104800	4.58649200
H	-1.53134500	2.63944500	4.79087400
H	-2.19549700	4.28823300	4.82811600
H	-3.22708400	2.90575500	5.25928500
C	-4.06940500	4.00723600	2.85074800
H	-4.88343000	3.80996800	3.55524500
H	-3.78909100	5.06427800	2.96279500
H	-4.44342400	3.87642600	1.82438600
C	-1.69674000	3.69834300	2.26785000
H	-0.76016500	3.14043600	2.41354900
H	-1.90663200	3.70506000	1.18818400
H	-1.51598300	4.73780300	2.57628400

**(R)-TS5**

P	-1.90560800	-0.12645800	-0.08877800
C	-1.38801200	-1.06442300	-1.58632200
C	-3.16274100	1.07829700	-0.66434300
C	-2.94368600	-1.40534000	0.72267000
C	-0.50265300	-2.16240900	-1.39175000
C	-1.82761700	-0.72552300	-2.86475200
C	-2.83066100	2.03646600	-1.61654200
C	-4.44333500	1.10712300	-0.11665300
C	-3.93782900	-2.03265100	-0.01652000
C	-2.76475400	-1.77628100	2.05289300
C	-0.08660900	-2.72804100	-0.07267200
C	-0.12086300	-2.82401100	-2.54310300
C	-1.42237900	-1.41912900	-4.01289600
H	-2.53477600	0.09167800	-2.98199600
C	-3.74096600	2.99153800	-2.08259800
H	-1.82568900	2.01818900	-2.03802700
C	-5.38238900	2.07112900	-0.47579000
H	-4.71367700	0.35076600	0.61115200
C	-4.83753900	-2.93949200	0.54659500

H	-4.02146900	-1.79378500	-1.07700200
C	-3.65133400	-2.64098800	2.69833600
H	-1.90266800	-1.38329400	2.58388700
C	0.94685300	-2.24799800	0.78654400
C	-0.71349400	-3.88612000	0.34121600
C	-0.55460600	-2.46375300	-3.81439200
H	-1.77716700	-1.14704300	-5.00430900
C	-4.98928400	3.04479000	-1.42449300
C	-4.74630800	-3.12282900	1.94204000
P	1.69597600	-0.62441500	0.35453500
C	1.26187100	-2.92847400	1.96076700
C	-0.38784500	-4.55794900	1.51379600
C	3.22820000	-0.40040200	1.34011800
C	2.42113100	-1.03821500	-1.27696100
C	0.60239700	-4.10603200	2.35059300
H	2.05822700	-2.54543100	2.59812200
C	4.44087300	-0.15638600	0.70585300
C	3.17078300	-0.23394800	2.72633600
C	3.21411100	-2.17175900	-1.41446600
C	2.21401100	-0.21409500	-2.37784600
H	0.86491000	-4.63729500	3.26240300
C	5.61314800	0.16004200	1.39977100
H	4.48313700	-0.19065600	-0.37926500
C	4.31002300	-0.00060100	3.49289900
H	2.20043300	-0.28474200	3.21274100
C	3.90988400	-2.46426500	-2.59079600
H	3.31084300	-2.83633400	-0.55661100
C	2.86037500	-0.44811000	-3.59200200
H	1.51737400	0.61474300	-2.26791300
C	5.54361500	0.10823900	2.80393700
C	3.79278100	-1.51402000	-3.62938800
C	0.98269100	-4.02275400	-4.03027200
H	1.96707700	-3.55885500	-4.23064300
H	0.97089100	-5.07689500	-4.32636000
O	0.69288000	-3.91436900	-2.64559000
O	-0.02229900	-3.31658400	-4.73544000
H	-2.31773800	-6.48487600	0.11919700
C	-2.16622000	-5.52683600	0.62849000
H	-3.10359000	-5.16807600	1.09470700
O	-1.16588100	-5.67483700	1.62345900
O	-1.70934200	-4.55920200	-0.30207000
O	-5.89363500	4.03925000	-1.72049200
O	-5.73897300	-3.80541000	2.60859200
O	4.58821600	-1.61274200	-4.74947300

O	6.69496400	0.20184500	3.55360700
C	-6.88209700	-3.00693000	2.84206400
H	-7.58066900	-3.61423200	3.42755000
H	-6.62596900	-2.09783100	3.40709600
H	-7.36979000	-2.70127400	1.90332400
C	-3.39291500	-3.09054300	4.14586800
C	-5.78852900	-3.66414200	-0.42614100
C	-6.81622500	1.96576300	0.07122100
C	-5.60810500	5.28541300	-1.11735400
H	-4.64209500	5.69502800	-1.44428300
H	-6.40940000	5.96955600	-1.41758400
H	-5.59335600	5.20656000	-0.01949600
C	-3.30327700	3.84792700	-3.29103300
C	4.70789500	-3.78631500	-2.64325200
C	2.49190000	0.35894000	-4.84688900
C	5.88144800	-1.07770800	-4.55450700
H	6.49848400	-1.71957700	-3.90751700
H	6.35365900	-1.00940000	-5.54070200
H	5.83522400	-0.07460800	-4.10358600
C	6.83091500	0.56549700	0.54265400
C	4.19436200	0.24927400	5.00536100
C	7.41958400	-1.00858500	3.60351400
H	8.33311900	-0.81072300	4.17493400
H	6.84372500	-1.80209700	4.10384800
H	7.69312100	-1.36449700	2.59902000
Cu	-0.10351900	0.88618300	0.95337000
C	2.74984700	0.10959900	5.49537100
H	2.07104500	0.83637400	5.02846500
H	2.34923600	-0.90165200	5.32579600
H	2.72079200	0.29767800	6.57684800
C	5.03451200	-0.72740200	5.83855600
H	4.81549400	-1.77137700	5.56919600
H	6.10710900	-0.54863200	5.72557600
H	4.79202400	-0.60300000	6.90347200
C	4.64255700	1.68874500	5.29900000
H	4.54120800	1.90232800	6.37323100
H	5.68805200	1.85260400	5.01367100
H	4.01927500	2.41005700	4.75007000
C	7.99143400	1.20680100	1.31348300
H	8.53986700	0.50374000	1.94785500
H	8.71013500	1.60993700	0.58577600
H	7.65269900	2.03683300	1.94575800
C	6.38671200	1.62066100	-0.48971000
H	5.61641000	1.25168800	-1.18233100

H	5.99402400	2.52189600	0.00067600
H	7.25222600	1.91650000	-1.09966000
C	7.34947500	-0.65055700	-0.23315400
H	6.58005600	-1.04034700	-0.91525600
H	8.22332900	-0.36915800	-0.83979200
H	7.65176500	-1.47305200	0.43163700
C	3.88774300	-4.91004900	-1.98140900
H	3.72705300	-4.75315900	-0.90826700
H	2.89948300	-5.02821900	-2.44154000
H	4.42953700	-5.86000800	-2.08543700
C	5.03165300	-4.27855400	-4.05962200
H	5.76669000	-3.66039500	-4.58170700
H	5.44432100	-5.29513300	-3.99306600
H	4.13345200	-4.32266900	-4.69097500
C	6.01161600	-3.65961700	-1.84528100
H	6.70328000	-2.92619300	-2.28111200
H	5.81457500	-3.35603100	-0.80679900
H	6.53149500	-4.62857300	-1.81980600
C	2.01925200	-0.60820700	-5.94309300
H	1.13808600	-1.18047700	-5.61533700
H	1.73497100	-0.04104300	-6.84174800
H	2.80533100	-1.31713200	-6.22373800
C	1.33562800	1.32563900	-4.56912900
H	0.45339900	0.81297700	-4.15719900
H	1.62203100	2.12919500	-3.87612200
H	1.03353000	1.79967000	-5.51305600
C	3.65780700	1.20541300	-5.37284500
H	4.08939100	1.82426900	-4.57220600
H	4.45228000	0.59596400	-5.81439000
H	3.29472400	1.88601600	-6.15647800
C	-2.58476200	2.94238800	-4.31182500
H	-1.63997200	2.52589300	-3.93769900
H	-3.22875500	2.10887500	-4.62879000
H	-2.33403400	3.53020600	-5.20548700
C	-4.46102100	4.48702000	-4.06869100
H	-5.23009600	3.74763800	-4.32708100
H	-4.95087600	5.30782100	-3.53872000
H	-4.06365800	4.90159000	-5.00582800
C	-2.31148900	4.93364400	-2.85723800
H	-1.42046100	4.50008600	-2.38297100
H	-1.98353600	5.51026800	-3.73479700
H	-2.74003600	5.63753000	-2.13140600
C	-7.77440000	1.70505500	-1.09948500
H	-8.80617000	1.61371600	-0.72889100

H	-7.74481600	2.51723100	-1.83292100
H	-7.51600900	0.76646900	-1.61099400
C	-7.26240200	3.22139900	0.82979400
H	-7.42901200	4.07056800	0.16158600
H	-8.21229500	3.02291300	1.34668900
H	-6.52347100	3.50895700	1.59236900
C	-6.96437500	0.79040200	1.04607000
H	-6.70858700	-0.17428900	0.58370100
H	-6.34402900	0.91450500	1.94592100
H	-8.01173200	0.73011900	1.37236300
C	-4.93914300	-4.26888700	-1.56100900
H	-4.34374800	-3.52905500	-2.11011900
H	-4.23807700	-5.01926000	-1.16957800
H	-5.59784300	-4.76714000	-2.28617300
C	-6.57406600	-4.83978600	0.16574600
H	-7.35549300	-4.53761100	0.86977600
H	-7.07096800	-5.37252600	-0.65768800
H	-5.91763500	-5.55301700	0.67996500
C	-6.77947900	-2.66487300	-1.03606000
H	-7.44829600	-2.23622900	-0.27505300
H	-6.26626400	-1.82990500	-1.53461200
H	-7.40941000	-3.16535000	-1.78566600
C	-3.27780100	-4.62077800	4.19376600
H	-2.42931200	-4.97602900	3.59039900
H	-3.10848500	-4.94739500	5.23034400
H	-4.19183500	-5.10597700	3.83305500
C	-4.49984400	-2.63605000	5.10608000
H	-5.43787700	-3.17360000	4.93721600
H	-4.19061800	-2.83390300	6.14236500
H	-4.68626400	-1.55590500	5.01651600
C	-2.07798500	-2.51790600	4.68345700
H	-1.21505200	-2.79268000	4.05904200
H	-2.10498100	-1.42277800	4.77556800
H	-1.89935700	-2.92461600	5.68796900
C	0.82896400	2.96554900	3.32753100
C	0.76554500	4.37671700	3.72516000
H	0.99278700	2.92258300	2.02271600
C	1.73222700	5.07979000	4.32618400
H	-0.15812800	4.89614700	3.43765300
H	1.62358400	6.14199100	4.53536500
H	2.66295200	4.60875100	4.64815700
C	-0.38964700	2.20829400	3.30515900
H	-1.29876500	2.81427100	3.19362000
C	-0.56204400	0.85109900	3.19385900

H	0.22013600	0.13909000	3.47348400
H	-1.58026200	0.46553100	3.20354500
H	1.72277900	2.41997500	3.66572300
C	1.05938600	3.76227500	-0.01986300
O	0.97690100	2.60059300	0.74122300
C	2.39299200	4.48253300	0.40259600
C	3.01541000	5.39876400	-0.61479300
C	3.35575600	6.66664300	-0.39107200
H	3.27088400	4.94508500	-1.57758900
H	3.14106500	7.14835400	0.56449400
H	3.86411600	7.26977800	-1.14125100
C	3.42750400	3.44437300	0.75432800
C	4.15618200	3.47831200	1.86743300
H	3.58622800	2.64216000	0.02409800
H	4.90067800	2.71188300	2.08992400
H	4.00956700	4.26215100	2.61382100
C	-0.16916900	4.65663600	0.21146600
C	-1.37922400	4.06897700	0.59041300
C	-0.14761400	6.04452300	0.04043000
C	-2.51844500	4.83217500	0.82240300
H	-1.42778700	2.98789700	0.71575600
C	-1.28278900	6.81548700	0.27827000
H	0.76994100	6.53650200	-0.27641800
C	-2.47302500	6.21589500	0.67914100
H	-3.44470700	4.33311800	1.11572200
H	-1.23062300	7.89692200	0.15588500
H	-3.35646500	6.82282100	0.87829000
C	1.09912800	3.35488300	-1.49303900
H	0.23572300	2.70226400	-1.69777900
H	1.05568500	4.21475200	-2.17791400
H	2.01114400	2.77471400	-1.70493100
H	2.18677700	5.06266600	1.31885800

**(R)-P<sub>b</sub>**

H	-1.96531500	-1.91912100	0.24703900
C	-0.63842200	-0.55068600	0.58365900
O	-0.99508100	-1.88013100	0.25464800
C	-1.43716900	0.42352500	-0.36646400
C	-1.10670700	1.86931000	-0.14182700
C	-0.22480600	2.56116500	-0.85765200
H	-1.63740500	2.36344300	0.67881400
H	0.32869500	2.09863000	-1.67652200
H	-0.00738600	3.60685700	-0.64906500
C	-2.91492300	0.19322200	-0.23830100

C	-3.62332200	-0.61199100	-1.03010500
H	-3.41847400	0.71348100	0.58298600
H	-4.69219000	-0.76490300	-0.89287500
H	-3.15638100	-1.13183500	-1.86831900
C	0.84018800	-0.41882400	0.27253600
C	1.36001600	-1.08684300	-0.83958700
C	1.69373100	0.39615600	1.01595200
C	2.69382200	-0.94054200	-1.20023500
H	0.70448600	-1.73872800	-1.41343500
C	3.03103500	0.54226200	0.65856500
H	1.31876100	0.93556300	1.88398600
C	3.53626000	-0.12333200	-0.45195400
H	3.07935900	-1.47333800	-2.06852100
H	3.67916400	1.18305500	1.25484300
H	4.58239700	-0.00878000	-0.73177200
C	-0.96825700	-0.29294500	2.04911100
H	-0.36075500	-0.94583600	2.68721200
H	-0.79544400	0.74900000	2.34810600
H	-2.02479500	-0.52387300	2.24070400
H	-1.12274300	0.13457000	-1.38254500

**(S)-TS4**

P	-1.44181100	-0.89379600	0.38870200
C	-0.51473200	-2.04755000	1.47376200
C	-2.62149100	-1.93407800	-0.54556400
C	-2.44045600	0.12808300	1.51637400
C	0.56006400	-1.49927500	2.22781400
C	-0.71421600	-3.42649700	1.42223600
C	-2.08659400	-2.87568300	-1.42212200
C	-3.99365500	-1.68942000	-0.60030300
C	-3.34093300	-0.40167300	2.43095300
C	-2.26931700	1.50909500	1.44582000
C	0.75608600	-0.04971200	2.52127800
C	1.39396500	-2.41765100	2.83333400
C	0.14232700	-4.33543800	2.05988700
H	-1.55356600	-3.82028400	0.85179700
C	-2.84740100	-3.52525800	-2.39571800
H	-1.01966600	-3.10029500	-1.35964300
C	-4.80214100	-2.25169900	-1.59163500
H	-4.43503200	-1.01576100	0.13163600
C	-4.17224400	0.41348700	3.20705600
H	-3.40943100	-1.48683900	2.52165000
C	-3.06378000	2.38359400	2.18216000
H	-1.52507800	1.89835600	0.75232900



C	1.55690900	0.86499900	1.77907100
C	0.18447700	0.45044500	3.67249400
C	1.20720000	-3.79407600	2.73648900
H	-0.01698800	-5.40998300	2.00908300
C	-4.17421000	-3.07417500	-2.55436300
C	-4.08371800	1.80531100	2.97353400
P	2.01114000	0.37170600	0.06683500
C	1.78302000	2.15302400	2.26238500
C	0.39872300	1.74770600	4.12869100
C	3.04572400	1.72662300	-0.59145900
C	3.18306300	-1.00561300	0.30959200
C	1.21962700	2.61994400	3.45936400
H	2.39916900	2.83800000	1.68263500
C	4.34248600	1.54381700	-1.05145400
C	2.43227800	2.96474400	-0.79228800
C	4.31349000	-0.87187200	1.10449800
C	2.93900800	-2.22319600	-0.31936600
H	1.40132400	3.62761500	3.82537200
C	5.07154000	2.56386600	-1.67490500
H	4.79487600	0.56160000	-0.95026400
C	3.13345900	4.05640800	-1.29921500
H	1.37826000	3.06090500	-0.53687900
C	5.28593800	-1.87290100	1.19756900
H	4.45021000	0.06384000	1.64736300
C	3.85345100	-3.27296400	-0.26356200
H	1.99962200	-2.33543600	-0.85773900
C	4.47489900	3.84201800	-1.70441500
C	5.07488800	-3.02426900	0.40879100
C	3.16486300	-3.42380600	3.65737600
H	3.93228500	-3.46240300	2.85706800
H	3.60690200	-3.56012300	4.64939800
O	2.49739900	-2.17416900	3.60073900
O	2.19572800	-4.43327600	3.42517600
H	-1.23972100	0.47877900	6.39741200
C	-1.17319400	0.83042300	5.36309300
H	-2.16412500	1.13141100	4.97072700
O	-0.28618500	1.93541600	5.29238700
O	-0.63977600	-0.19851800	4.54434100
O	-4.89546900	-3.44357900	-3.66376800
O	-5.01620500	2.65473100	3.52358000
O	6.06927300	-3.96787700	0.28534400
O	5.15748800	4.93356100	-2.19373800
C	-6.22211900	2.69391100	2.78615900
H	-6.83884300	3.48477900	3.22668000

H	-6.03635000	2.92372200	1.72601300
H	-6.76899200	1.74011200	2.84438000
C	-2.78541500	3.89398700	2.14734600
C	-5.08275700	-0.28603900	4.23527100
C	-6.31524400	-1.98839700	-1.60908900
C	-4.52088900	-2.74615900	-4.83868600
H	-5.08148500	-3.19658900	-5.66446500
H	-4.76235000	-1.67490700	-4.77102000
H	-3.44313000	-2.83218700	-5.04221400
C	-2.17003300	-4.67645600	-3.16255700
C	6.47827200	-1.60455200	2.13677100
C	3.49777800	-4.65218600	-0.84050600
C	7.04017800	-3.62230900	-0.68207400
H	7.63322100	-2.74736200	-0.37535100
H	7.70805500	-4.48427200	-0.78500100
H	6.57627100	-3.40172700	-1.65494300
C	6.44036300	2.19547400	-2.28390800
C	2.42235800	5.40949400	-1.45834900
C	6.14715400	5.49625000	-1.35991800
H	6.11588800	6.58574300	-1.48222800
H	5.96706100	5.25331200	-0.30246000
H	7.15318400	5.15421500	-1.64225800
Cu	-0.00019800	0.20423700	-1.13428400
C	-1.44227000	2.48696900	-2.60190300
O	-0.69824600	2.07824300	-1.64654800
C	-1.70029400	0.83462700	-4.04820800
C	-3.11531300	0.66956400	-4.34560900
C	-3.83189500	1.29603200	-5.28896800
H	-3.64591400	-0.01580900	-3.66747200
H	-3.36950900	1.99555300	-5.98798500
H	-4.90618400	1.14389600	-5.38586900
C	-1.04149900	-0.26600400	-3.43853500
C	0.30658500	-0.39785400	-3.17467500
H	-1.69053500	-1.07045400	-3.07353500
H	0.71163300	-1.37851800	-2.90540400
H	1.02454000	0.31721900	-3.58604700
H	-1.11742600	1.37211900	-4.80084000
C	1.01253600	5.36625600	-0.86191800
H	0.37474300	4.59371300	-1.31136700
H	1.04419800	5.18568700	0.22385500
H	0.52326100	6.33716100	-1.02235300
C	3.15740000	6.54266600	-0.72946200
H	3.39500200	6.26263400	0.30771100
H	4.08082400	6.83293500	-1.23590200

H	2.51316600	7.43269200	-0.69218400
C	2.30417800	5.75129100	-2.94882000
H	1.78137300	6.71121200	-3.07519500
H	3.28989400	5.83233800	-3.42112900
H	1.72837700	4.98053400	-3.47856400
C	6.76810200	3.00207000	-3.54720400
H	6.90378200	4.07080400	-3.37243700
H	7.69494100	2.61340900	-3.99193200
H	5.96687500	2.89406800	-4.29130200
C	6.44932800	0.72170800	-2.73116800
H	6.42424100	0.01400900	-1.89069100
H	5.60306400	0.49518500	-3.39405800
H	7.37700600	0.51948100	-3.28365400
C	7.55410400	2.34151600	-1.23911700
H	7.35360500	1.69356500	-0.37410800
H	8.52026900	2.03807800	-1.66899300
H	7.66257000	3.36493200	-0.86397000
C	5.95743500	-1.09077400	3.49175900
H	5.33752700	-0.19100600	3.41577600
H	5.36480800	-1.85724900	4.00880900
H	6.81191700	-0.84376000	4.13688200
C	7.34693500	-2.82324600	2.47154600
H	7.96379900	-3.16894500	1.63703200
H	8.03207300	-2.54683800	3.28538600
H	6.74337800	-3.67373400	2.81355200
C	7.35878500	-0.50772800	1.52405400
H	7.76241800	-0.80487900	0.54524600
H	6.78950700	0.42207900	1.37920500
H	8.20933700	-0.28291100	2.18382000
C	3.61204000	-5.70129200	0.27483600
H	2.94811300	-5.45438500	1.11580300
H	3.31835400	-6.68926400	-0.10869700
H	4.63655700	-5.77306200	0.65627700
C	2.05100400	-4.68309500	-1.34580500
H	1.33475700	-4.42194600	-0.55141300
H	1.88929500	-4.00719500	-2.19964000
H	1.81168300	-5.70003600	-1.68662700
C	4.39187600	-5.05738100	-2.01840200
H	4.41890500	-4.27145200	-2.78705600
H	5.41604600	-5.27932100	-1.70292500
H	3.99093600	-5.96721900	-2.48747200
C	-1.54606100	-5.62392300	-2.12032100
H	-0.78707200	-5.13661500	-1.49534600
H	-2.31907000	-6.03454500	-1.45507300

H	-1.05456200	-6.46521700	-2.62996300
C	-3.11316700	-5.55030600	-3.99777400
H	-3.97260900	-5.89711400	-3.41079600
H	-3.49661700	-5.05034500	-4.89208000
H	-2.55535500	-6.43554000	-4.33517500
C	-1.05348000	-4.14322400	-4.06799900
H	-0.29183800	-3.59129100	-3.49997500
H	-0.55056900	-4.97817100	-4.57771400
H	-1.43946900	-3.46256100	-4.83907700
C	-7.08987800	-3.30734700	-1.74820000
H	-8.17017300	-3.10332100	-1.72831700
H	-6.85533300	-3.82862100	-2.68078700
H	-6.86147600	-3.97910200	-0.90822600
C	-6.69336900	-1.03412800	-2.74886800
H	-6.55888800	-1.50494800	-3.72880500
H	-7.75239200	-0.74943800	-2.66219700
H	-6.09155500	-0.11197300	-2.71724000
C	-6.78725200	-1.35920800	-0.29434500
H	-6.51780300	-1.98028700	0.57198800
H	-6.38420500	-0.35069100	-0.12961100
H	-7.88183300	-1.26919100	-0.31300000
C	-4.25120600	-1.32066800	5.01577200
H	-3.81601500	-2.10165700	4.38237900
H	-3.42674800	-0.83821400	5.55888700
H	-4.89110100	-1.82106800	5.75556600
C	-5.69372300	0.63274300	5.29989600
H	-6.45916400	1.31086700	4.91283900
H	-6.17066500	0.00683800	6.06756700
H	-4.92732200	1.24463900	5.79369900
C	-6.20562500	-1.03194400	3.50451100
H	-6.85136400	-0.34647100	2.93789700
H	-5.80140500	-1.76572000	2.79187500
H	-6.83880200	-1.57240100	4.22320500
C	-2.53142500	4.38125200	3.58064800
H	-1.68182800	3.84735000	4.03178000
H	-2.28977800	5.45432200	3.57427200
H	-3.40962200	4.23177800	4.21907800
C	-3.93095000	4.70008000	1.52284700
H	-4.82588500	4.70697400	2.15322900
H	-3.61294700	5.74527500	1.39847900
H	-4.19311400	4.31157300	0.52737500
C	-1.52984600	4.20585600	1.32413000
H	-0.63691600	3.69935900	1.72235700
H	-1.63571400	3.92802800	0.26424600

H	-1.34152500	5.28788200	1.36653500
C	-2.89140000	2.71078300	-2.30959800
C	-3.55258900	1.84009000	-1.44034500
C	-3.61491500	3.77623100	-2.85006900
C	-4.88527000	2.02693600	-1.11185600
H	-3.00224600	0.98899200	-1.04497300
C	-4.95763600	3.96598800	-2.52727600
H	-3.13077100	4.47273400	-3.53248400
C	-5.60060800	3.09437100	-1.65615700
H	-5.36749300	1.33805500	-0.41568400
H	-5.50232900	4.80210500	-2.96397700
H	-6.65011500	3.24139400	-1.40311500
C	-0.79483300	3.43907100	-3.58625700
H	-0.71548100	4.44211500	-3.13502600
H	0.22300500	3.08332100	-3.79517500
H	-1.34400400	3.53689400	-4.53111200

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P	-1.51073800	-0.65228600	0.25558400
C	-0.68854900	-2.04167200	1.13721900
C	-2.85242600	-1.41005600	-0.73238900
C	-2.40747200	0.21443600	1.58485500
C	0.40625500	-1.70405800	1.98305900
C	-1.01316100	-3.37656800	0.89946800
C	-2.54174400	-2.35126400	-1.70935200
C	-4.16762200	-0.95201400	-0.65197800
C	-3.29497100	-0.44173600	2.42657200
C	-2.22359000	1.58654500	1.72554100
C	0.71580600	-0.32197100	2.45205000
C	1.12751100	-2.76999300	2.48241900
C	-0.27217700	-4.43939500	1.43567000
H	-1.87406600	-3.61228000	0.27684400
C	-3.48101300	-2.83236900	-2.62654400
H	-1.52180600	-2.73284100	-1.76643700
C	-5.14750200	-1.35316500	-1.55796700
H	-4.42034400	-0.23655600	0.12416800
C	-4.11107200	0.24934600	3.32858800
H	-3.37124000	-1.52784400	2.35361900
C	-3.02117300	2.34825300	2.57669900
H	-1.44101100	2.05716800	1.13196400
C	1.54062400	0.63120900	1.79000500
C	0.19589600	0.07856700	3.66655600
C	0.80987900	-4.09731200	2.20770000
H	-0.53227900	-5.47772400	1.24294500

C	-4.75379600	-2.23042600	-2.59430900
C	-4.03736700	1.65988400	3.28402900
P	2.01406400	0.28045000	0.04840300
C	1.80317600	1.86782900	2.37916600
C	0.45253400	1.32215600	4.23405500
C	3.15934600	1.62254300	-0.41591000
C	3.07536100	-1.19628400	0.19923400
C	1.26938100	2.23945300	3.62188600
H	2.42939000	2.58632100	1.85294200
C	4.50692600	1.44729200	-0.69613600
C	2.58842900	2.88076900	-0.60753000
C	4.15496000	-1.23337700	1.07186700
C	2.78978200	-2.32040500	-0.57087900
H	1.47825100	3.20753800	4.07132100
C	5.32458400	2.49703500	-1.13111000
H	4.92916100	0.45101800	-0.60594500
C	3.36114800	3.99384500	-0.92583400
H	1.50882600	2.97299100	-0.51245800
C	5.04632000	-2.31067900	1.11214800
H	4.31423900	-0.37838600	1.72914300
C	3.61684800	-3.44085400	-0.57056900
H	1.88394300	-2.30339900	-1.17352400
C	4.74427800	3.78514100	-1.15474600
C	4.80577200	-3.35612900	0.19439900
C	2.75249600	-4.05141500	3.23313600
H	3.55539100	-4.08406200	2.46798300
H	3.12261800	-4.34885700	4.21938600
O	2.22136900	-2.73691800	3.29969100
O	1.69885400	-4.91529000	2.84063400
H	-1.11326800	-0.13262000	6.43737600
C	-1.09108400	0.31789700	5.43982200
H	-2.09522100	0.66775000	5.13191000
O	-0.19140000	1.41396500	5.43273000
O	-0.61690600	-0.63310700	4.49961000
O	-5.66296400	-2.48212800	-3.59641700
O	-4.97316500	2.41397700	3.95385500
O	5.73538400	-4.35803100	0.02911100
O	5.49156800	4.89547200	-1.48001700
C	-6.18895100	2.52622900	3.24029300
H	-6.85014400	3.16390700	3.83685900
H	-6.03393500	2.98569200	2.25176300
H	-6.67024100	1.54736800	3.08836800
C	-2.72808700	3.84263000	2.78190400
C	-4.99136700	-0.59830000	4.27072500

C	-6.61658200	-0.95384800	-1.33541800
C	-5.42332400	-1.69001400	-4.74455600
H	-6.26584900	-1.84988200	-5.42629800
H	-5.35508600	-0.62086100	-4.48907000
H	-4.49203700	-1.98222200	-5.25398500
C	-3.03273100	-3.99033300	-3.53982500
C	6.18705000	-2.24540000	2.14761400
C	3.19726000	-4.72467900	-1.30193300
C	6.78773500	-3.99212600	-0.84085200
H	7.46201600	-3.25287700	-0.38238900
H	7.35633300	-4.90294300	-1.05786700
H	6.40138800	-3.57081300	-1.78097200
C	6.76269100	2.15069200	-1.56879800
C	2.67953600	5.36238300	-1.07630400
C	6.38262100	5.39157000	-0.50612500
H	6.31414800	6.48648900	-0.50070700
H	6.13206500	5.01819400	0.49757000
H	7.42158400	5.11889800	-0.74308300
Cu	0.01482000	0.49838500	-1.14951700
C	-0.90164300	2.43240700	-3.08342400
O	-0.20545100	2.30858300	-1.91338700
C	-0.44658000	1.25364500	-4.04605100
C	-1.07257100	1.17061000	-5.40721200
C	-0.50358700	1.60548400	-6.53062000
H	-2.06055000	0.70013100	-5.45648500
H	0.48253900	2.07270800	-6.51979600
H	-0.99459200	1.52119500	-7.49848000
C	-0.62124100	-0.06655200	-3.36619100
C	0.39400200	-0.88879600	-3.03312800
H	-1.65542600	-0.38750700	-3.18458300
H	0.21694400	-1.87848700	-2.60706700
H	1.43053100	-0.63126600	-3.26083000
H	0.63447100	1.43947300	-4.16839200
C	1.19949500	5.28781600	-0.68059300
H	0.63083300	4.55813500	-1.27334800
H	1.08053900	5.02263400	0.38297400
H	0.74091400	6.27590400	-0.82711500
C	3.31633200	6.42927600	-0.17503400
H	3.44323800	6.05959100	0.85358100
H	4.28555000	6.76976900	-0.54774500
H	2.65933900	7.30954800	-0.13132900
C	2.75472000	5.81372100	-2.53938000
H	2.26758300	6.79309000	-2.65761800
H	3.79199400	5.90222200	-2.88232000

H	2.23205900	5.09873200	-3.18917000
C	7.23249200	3.00229000	-2.75562700
H	7.31833800	4.06695800	-2.53005800
H	8.21577400	2.64578500	-3.09393100
H	6.53212900	2.90533400	-3.59693800
C	6.84412500	0.69204900	-2.05692400
H	6.70737600	-0.04543200	-1.25241300
H	6.09996200	0.48677400	-2.83870900
H	7.84089700	0.51298600	-2.48296300
C	7.74114800	2.26978900	-0.39323300
H	7.43584600	1.60880600	0.42984800
H	8.75055700	1.96755800	-0.70950400
H	7.80950200	3.28492800	0.01060500
C	5.62258700	-1.77278600	3.50036800
H	5.17377600	-0.77429700	3.46420700
H	4.85702900	-2.46008500	3.88204200
H	6.43591700	-1.73263100	4.23775400
C	6.88370200	-3.58029700	2.43645800
H	7.51453100	-3.93417800	1.61678600
H	7.53400400	-3.45205900	3.31317600
H	6.16093000	-4.37425800	2.66677600
C	7.22837200	-1.21433600	1.69431800
H	7.69141100	-1.48648500	0.73551700
H	6.77077800	-0.22180700	1.57122000
H	8.03067000	-1.12453700	2.44119800
C	3.16739900	-5.88333700	-0.29475400
H	2.46334000	-5.67555300	0.52343500
H	2.83917900	-6.80611400	-0.79519100
H	4.15608900	-6.06493700	0.14104300
C	1.78584300	-4.59511600	-1.88855900
H	1.03808500	-4.33185700	-1.12352200
H	1.74050100	-3.84996500	-2.69707700
H	1.48921500	-5.56042800	-2.32107400
C	4.12889100	-5.08343600	-2.46595800
H	4.25221700	-4.23478200	-3.15425500
H	5.11585300	-5.40608900	-2.12115000
H	3.69523000	-5.91546000	-3.03896100
C	-2.38047700	-5.07279000	-2.65795400
H	-1.47433700	-4.72649200	-2.14283500
H	-3.08648500	-5.43360300	-1.89620100
H	-2.08696700	-5.93045800	-3.27952500
C	-4.16116300	-4.70220700	-4.29460900
H	-4.96283600	-5.02375100	-3.61856400
H	-4.61151700	-4.09413900	-5.08419500



H	-3.74336300	-5.59845700	-4.77520700
C	-1.99160600	-3.49817500	-4.55158600
H	-1.09894900	-3.09212800	-4.05635300
H	-1.66849500	-4.32917400	-5.19538600
H	-2.39104500	-2.70565400	-5.20040400
C	-7.39871900	-2.23241700	-1.00077000
H	-8.45578300	-1.99156400	-0.81372600
H	-7.35462700	-2.95582100	-1.82322600
H	-6.99484500	-2.70919300	-0.09561700
C	-7.26880100	-0.26701100	-2.54221100
H	-7.43556700	-0.96435600	-3.36789600
H	-8.24806200	0.13614500	-2.24555800
H	-6.65564600	0.57155800	-2.89911900
C	-6.76902900	0.00128300	-0.14573900
H	-6.38951100	-0.43266100	0.78954000
H	-6.25342700	0.95768700	-0.31470800
H	-7.83614000	0.21686100	0.00392900
C	-4.12165900	-1.69274600	4.91702300
H	-3.60415000	-2.33202400	4.19345100
H	-3.35982800	-1.25535000	5.57666000
H	-4.75641100	-2.34346700	5.53463300
C	-5.62110600	0.16273800	5.44292100
H	-6.42529200	0.84150700	5.14539700
H	-6.05625900	-0.56940700	6.13828300
H	-4.87499300	0.74841100	5.99542600
C	-6.10292500	-1.28891500	3.47062500
H	-6.79408100	-0.56177900	3.02176700
H	-5.69457700	-1.90652200	2.65694700
H	-6.69269600	-1.94466100	4.12744000
C	-2.38066500	4.06754800	4.26137800
H	-1.50872700	3.46752500	4.56429600
H	-2.13698100	5.12648000	4.43263300
H	-3.22211900	3.80458800	4.91383300
C	-3.90407200	4.74652700	2.39277600
H	-4.75259500	4.63629600	3.07437200
H	-3.58431400	5.79762600	2.43256500
H	-4.23830900	4.54574200	1.36406600
C	-1.52898400	4.29412600	1.94077200
H	-0.61851900	3.72108300	2.16798600
H	-1.71923500	4.21570600	0.85943700
H	-1.31658900	5.34973100	2.15923900
C	-2.42470400	2.45206400	-2.85407900
C	-2.88533200	2.44071100	-1.53873100
C	-3.37359200	2.59836000	-3.87278000

C	-4.23643000	2.56330400	-1.23469200
H	-2.13250900	2.34890400	-0.76148700
C	-4.73017100	2.71452800	-3.57874900
H	-3.05266300	2.65089700	-4.91263700
C	-5.16934700	2.70655900	-2.25664400
H	-4.55343300	2.54593300	-0.18803200
H	-5.44991500	2.83651600	-4.38887900
H	-6.23019900	2.81640800	-2.02836400
C	-0.51945900	3.75524700	-3.76026200
H	-0.79710000	4.59077400	-3.10348800
H	0.57186400	3.77322800	-3.89895500
H	-1.00081100	3.90388700	-4.73596800

**(S)-TS5**

P	-1.92688600	-0.05290800	-0.24367800
C	-1.23079100	-0.44716100	-1.90398400
C	-3.40947100	1.02012300	-0.45212100
C	-2.73841900	-1.65437100	0.15110600
C	-0.23601500	-1.46880900	-1.97097300
C	-1.55726100	0.28426300	-3.04390900
C	-3.38913700	2.22601600	-1.14599000
C	-4.59177800	0.65635900	0.19886200
C	-3.65551400	-2.18192200	-0.74892100
C	-2.49829800	-2.33473400	1.33983500
C	0.17288500	-2.40830700	-0.88624200
C	0.35542500	-1.64757600	-3.20597900
C	-0.91719500	0.09493800	-4.27869300
H	-2.35090400	1.02531900	-2.98854900
C	-4.52519800	3.04014800	-1.27249300
H	-2.46388400	2.56052300	-1.61275400
C	-5.72658100	1.46024500	0.19682400
H	-4.62096200	-0.28775100	0.73042200
C	-4.42408200	-3.31419800	-0.46725300
H	-3.79469700	-1.66750500	-1.69929100
C	-3.23350700	-3.46480700	1.70122100
H	-1.70751100	-1.97002400	1.98734600
C	1.14223500	-2.12636400	0.11693500
C	-0.29819900	-3.70485000	-0.91824100
C	0.05536900	-0.87375300	-4.32114500
H	-1.18300000	0.68128500	-5.15530700
C	-5.64928400	2.68685300	-0.50222600
C	-4.26415200	-3.87365100	0.82014800
P	1.73522900	-0.38370300	0.18149700
C	1.56324600	-3.12527200	0.99410700

C	0.12126100	-4.68862500	-0.02972300
C	3.07582300	-0.33278200	1.43559400
C	2.77672000	-0.36965500	-1.34413500
C	1.06075800	-4.43474100	0.93896900
H	2.32283200	-2.89630500	1.73963000
C	4.26994400	0.30116000	1.11907800
C	2.88787900	-0.74628500	2.75579100
C	3.68404800	-1.40793100	-1.51017000
C	2.73691400	0.64747400	-2.29743500
H	1.39786200	-5.20939800	1.62367300
C	5.31173800	0.46590600	2.03638800
H	4.40352900	0.68198900	0.10919000
C	3.90298000	-0.68224400	3.70865600
H	1.92169000	-1.14706200	3.04595600
C	4.62936800	-1.43184100	-2.53530300
H	3.66641900	-2.22816300	-0.79424200
C	3.66848000	0.70137400	-3.34080300
H	1.97310200	1.41929200	-2.21113300
C	5.14470600	-0.13905200	3.29656800
C	4.67825700	-0.29004500	-3.35859300
C	1.76304300	-2.18932700	-4.82566700
H	2.74234900	-1.68410000	-4.72092000
H	1.83817000	-3.07204900	-5.47004900
O	1.29146500	-2.57835600	-3.54590300
O	0.81577300	-1.28268400	-5.37522100
H	-1.67430700	-6.24310800	-1.98253800
C	-1.56229200	-5.48567900	-1.20034700
H	-2.49732900	-5.35562600	-0.62196900
O	-0.51593900	-5.86007300	-0.31915500
O	-1.20227000	-4.24439700	-1.78608400
O	-6.73001200	3.53587800	-0.41899500
O	-5.10087900	-4.87861900	1.25018100
O	5.72699900	-0.11259900	-4.23330300
O	6.19435200	-0.20637800	4.18583300
C	-6.34976000	-4.41767600	1.72363000
H	-6.84097200	-5.26913900	2.20725900
H	-6.22637000	-3.60640200	2.45617500
H	-6.99256600	-4.05386700	0.90821000
C	-2.87238200	-4.25225800	2.97099300
C	-5.35510900	-3.82357300	-1.58609400
C	-7.02575400	0.95315800	0.84290100
C	-6.51593700	4.63213500	0.44572300
H	-5.65289400	5.23874400	0.13547700
H	-7.42261000	5.24617300	0.41212400

H	-6.34280600	4.29833200	1.48096600
C	-4.44804100	4.19483700	-2.29395800
C	5.48114200	-2.70669000	-2.67284400
C	3.56058900	1.74600100	-4.46383800
C	6.89350800	0.36795400	-3.59772800
H	7.35202400	-0.39362600	-2.94755700
H	7.60304900	0.63317800	-4.38903100
H	6.67830900	1.25922700	-2.98704200
C	6.52012400	1.29228300	1.55354400
C	3.63713200	-1.14614200	5.15085500
C	7.12539400	-1.22493200	3.88891800
H	7.79544300	-1.30615200	4.75197700
H	6.62720200	-2.19192000	3.72410100
H	7.72542900	-0.98950300	2.99724200
Cu	-0.23921800	0.84486600	1.07166700
C	2.18206200	-1.58838300	5.34285400
H	1.46620200	-0.78432900	5.12188300
H	1.92474300	-2.46662500	4.73012100
H	2.03502400	-1.87152700	6.39369100
C	4.51514400	-2.34337900	5.53916700
H	4.45124000	-3.14436600	4.78749000
H	5.56473000	-2.06452800	5.66997100
H	4.16683400	-2.75773500	6.49607800
C	3.88717800	0.00958100	6.12995700
H	3.74966700	-0.34596600	7.16190600
H	4.90364400	0.40657500	6.03894800
H	3.17184000	0.82834400	5.96790400
C	7.42954800	1.81494300	2.67091700
H	8.00531700	1.03508300	3.17561400
H	8.15199500	2.52014000	2.23611800
H	6.85299100	2.35209300	3.43465600
C	6.00502100	2.54525600	0.81916000
H	5.45850500	2.30681900	-0.10425000
H	5.33714900	3.14049200	1.45794100
H	6.85578900	3.17923600	0.53201800
C	7.34037400	0.47131600	0.54980300
H	6.71902100	0.16411400	-0.30535000
H	8.17896500	1.06929200	0.16226800
H	7.75673700	-0.44181700	0.99766200
C	4.54675300	-3.92668700	-2.55391700
H	4.07559900	-4.02400100	-1.56804100
H	3.73786900	-3.87858500	-3.29638700
H	5.11982900	-4.84762300	-2.72981800
C	6.18798900	-2.85751000	-4.02442400

H	7.00178900	-2.14378600	-4.17911900
H	6.62044700	-3.86619200	-4.08548300
H	5.48244100	-2.74284200	-4.85903300
C	6.51650400	-2.77732700	-1.54306200
H	7.26845700	-1.97939400	-1.62509400
H	6.04247500	-2.68108100	-0.55527100
H	7.04903900	-3.73927500	-1.57388600
C	3.51678900	1.03709600	-5.82583900
H	2.62116300	0.40285900	-5.90086600
H	3.45571000	1.78721800	-6.62803300
H	4.40617400	0.42226000	-6.00321000
C	2.26842600	2.55361400	-4.34350700
H	1.37709300	1.90656900	-4.33173000
H	2.25318500	3.18060500	-3.44226700
H	2.18255700	3.21990800	-5.21327400
C	4.71974100	2.74925300	-4.43638800
H	4.83489900	3.18608300	-3.43374000
H	5.66869500	2.29762600	-4.74081600
H	4.50984800	3.57257300	-5.13450600
C	-3.88623800	3.62262600	-3.61045000
H	-2.86073800	3.24803500	-3.51401400
H	-4.51678000	2.80179100	-3.98159500
H	-3.86704400	4.40908200	-4.37750200
C	-5.79314200	4.82261400	-2.68307300
H	-6.52948600	4.06406400	-2.97633800
H	-6.23768100	5.44050700	-1.89809400
H	-5.62562500	5.48096600	-3.54724100
C	-3.50449000	5.29488200	-1.79649000
H	-2.50289000	4.90308300	-1.57098000
H	-3.39869100	6.07428400	-2.56604400
H	-3.87673200	5.77178400	-0.87970000
C	-8.11377200	0.84713900	-0.23496400
H	-9.05059300	0.48211300	0.21150300
H	-8.31265800	1.81609100	-0.70489400
H	-7.81512700	0.13539100	-1.01840200
C	-7.51374500	1.86203500	1.97766000
H	-7.89693700	2.81607500	1.60404500
H	-8.33437400	1.36933300	2.51892800
H	-6.70966600	2.06112000	2.70170700
C	-6.84599700	-0.44689100	1.44018200
H	-6.50960800	-1.17784500	0.68979900
H	-6.12732300	-0.45853600	2.27336000
H	-7.81166600	-0.79559900	1.83208400
C	-4.60640300	-3.77081100	-2.93185600

H	-4.34251300	-2.75390400	-3.24446400
H	-3.67706900	-4.35442800	-2.90123400
H	-5.24688700	-4.18988600	-3.71979500
C	-5.81449400	-5.27807400	-1.42883700
H	-6.52333100	-5.43527300	-0.61199800
H	-6.31518700	-5.59009500	-2.35613200
H	-4.96379200	-5.95353000	-1.26490700
C	-6.57890800	-2.90474300	-1.70217300
H	-7.20127900	-2.91970300	-0.79655600
H	-6.27675400	-1.86106200	-1.87664200
H	-7.21142600	-3.21743700	-2.54590800
C	-2.54758500	-5.70488300	2.59609500
H	-1.69726600	-5.75177300	1.90111500
H	-2.27340300	-6.27000700	3.49902900
H	-3.40266100	-6.20495400	2.12862100
C	-3.99685200	-4.23272100	4.01469000
H	-4.85586800	-4.83867400	3.71119000
H	-3.62522900	-4.64653800	4.96294300
H	-4.33772800	-3.20577200	4.21237100
C	-1.62903400	-3.67060200	3.65298000
H	-0.75923700	-3.64595800	2.98000600
H	-1.79731800	-2.65490900	4.03967300
H	-1.36339500	-4.30394500	4.51026100
C	0.80530100	1.91714900	3.99752900
C	0.89662000	2.99283900	4.98962000
H	0.83663600	2.41591100	2.76780900
C	2.02135700	3.47581300	5.53022200
H	-0.05722300	3.46113200	5.26346000
H	2.01273500	4.30764500	6.23105400
H	2.99699400	3.05785400	5.27307500
C	-0.45950400	1.26187900	3.81789100
H	-1.32899500	1.88463200	4.06844000
C	-0.73668100	0.07498400	3.19345700
H	0.01757900	-0.70919400	3.08133800
H	-1.77471000	-0.24901900	3.11714200
H	1.69163400	1.26687500	3.93899600
C	0.71330100	3.93056500	1.14590200
O	0.76706500	2.57773600	1.46795500
C	1.16935000	4.10345900	-0.33633900
C	0.32063600	3.32583000	-1.29843300
C	-0.18864800	3.83234200	-2.41988800
H	0.17433200	2.26386600	-1.06603500
H	-0.05282400	4.88172600	-2.68999900
H	-0.73346800	3.21278600	-3.13399300

C	2.60745000	3.69066100	-0.49870200
C	3.53095000	4.44413200	-1.09248400
H	2.87336400	2.71055000	-0.08609600
H	4.56825500	4.12214400	-1.18580200
H	3.28768600	5.42584800	-1.50363900
H	1.09052900	5.17246100	-0.60249400
C	1.70169100	4.68836700	2.04644400
H	1.32621400	4.75565200	3.07473100
H	2.65451700	4.14217900	2.07335800
H	1.90491900	5.70406500	1.68017800
C	-0.68723000	4.52916300	1.32631800
C	-0.89165800	5.91379100	1.26117800
C	-1.79552900	3.72456800	1.59087100
C	-2.14461600	6.47040200	1.48881100
H	-0.05259500	6.57730600	1.05011000
C	-3.05838100	4.27354100	1.80093600
H	-1.67413300	2.64231300	1.64227100
C	-3.23609700	5.65144900	1.76871700
H	-2.26815300	7.55231000	1.45221400
H	-3.90545400	3.60888300	1.98546700
H	-4.21635700	6.09009100	1.95846300

**(S)-P<sub>b</sub>**

C	-0.57629200	-0.75477000	0.37860300
O	-0.84330300	-0.75886200	1.77544800
H	-0.37034300	-1.51104600	2.16031000
C	0.88831100	-0.44534200	0.09852900
C	1.41373000	-0.57474700	-1.18996400
C	1.72882000	0.00912600	1.11442600
C	2.74481900	-0.27312700	-1.45256200
H	0.77654700	-0.91110100	-2.00831400
C	3.06377900	0.30547600	0.85615700
H	1.31882800	0.14801000	2.11313900
C	3.57848100	0.16359500	-0.42707400
H	3.13400300	-0.38278700	-2.46387100
H	3.70307500	0.65722100	1.66489900
H	4.62252200	0.39672000	-0.63028100
C	-0.97064000	-2.11031100	-0.20038300
H	-1.99121600	-2.36256300	0.10899000
H	-0.94030400	-2.12239100	-1.29735500
H	-0.28408600	-2.89015500	0.15974300
C	-1.46705200	0.37735500	-0.20395900
C	-2.92788300	0.08806900	-0.00797600
C	-3.79754700	-0.08626700	-0.99892700

H	-3.25910700	0.03257600	1.03213900
H	-3.48739000	-0.03458600	-2.04393000
H	-4.85237700	-0.28136200	-0.81402600
C	-1.12884600	1.70637100	0.41019800
C	-0.59804600	2.72579100	-0.25732800
H	-1.34879500	1.80008700	1.47648600
H	-0.37106800	3.67480000	0.22479700
H	-0.35780900	2.64717100	-1.31883700
H	-1.25586300	0.42298600	-1.28591100

**(S)-TS4'**

C	3.41308400	0.66806900	1.67282200
C	0.98759200	0.33005900	2.90579800
C	2.19357000	0.47476600	3.82723300
C	3.20046500	1.31751600	3.05607800
H	4.11891500	-0.17320800	1.77869200
H	0.53845200	1.32429500	2.74404500
H	1.91888200	0.92802600	4.79106600
H	2.63828600	-0.50954100	4.04959900
H	2.79073900	2.32999500	2.91084300
H	4.15818100	1.43406700	3.58234300
C	-0.10570900	-0.63839500	3.24833900
C	-1.33991500	-0.48962700	2.60123900
C	0.07082800	-1.73568100	4.09419700
C	-2.34214300	-1.44137800	2.73538900
H	-1.49031900	0.38557800	1.96865100
C	-0.94206600	-2.68213200	4.24843300
H	1.00695200	-1.86558000	4.63783800
C	-2.14196200	-2.55143200	3.55601200
H	-3.28171500	-1.31111200	2.19534000
H	-0.78586600	-3.53111300	4.91295100
H	-2.92481300	-3.30018000	3.67127800
C	3.93941600	1.62884900	0.64124900
C	5.29454700	1.63096800	0.30883100
C	3.09378600	2.55768300	0.02165200
C	5.80144100	2.53003800	-0.62573400
H	5.95931700	0.90805600	0.78571300
C	3.59806700	3.45349300	-0.91462600
H	2.02458700	2.56735900	0.25845700
C	4.95202000	3.44204000	-1.24412700
H	6.86206700	2.51509900	-0.87337300
H	2.92583800	4.16646700	-1.39128200
H	5.34267600	4.14440600	-1.97879600
P	1.73872800	-0.06512900	1.22018300



C	0.96480700	-2.69870700	-2.08379600
C	-1.40409000	-3.31387900	-0.84868100
C	-0.98789100	-4.15581600	-2.07660300
C	0.52769200	-4.15686200	-2.18759300
H	0.57058300	-2.16052800	-2.96423800
H	-1.36326100	-3.94305300	0.05519400
H	-1.41113800	-5.16752000	-2.01161000
H	-1.41592500	-3.69530800	-2.98060700
H	0.95706700	-4.74925500	-1.36458800
H	0.87669200	-4.61658900	-3.12398800
C	-2.79465400	-2.76462800	-1.00079000
C	-3.07675000	-1.79164600	-1.96625400
C	-3.85287600	-3.29291500	-0.26045300
C	-4.38278800	-1.38903800	-2.21271800
H	-2.25620300	-1.34552200	-2.53523700
C	-5.16510700	-2.89415900	-0.50561000
H	-3.64597600	-4.04708000	0.50079000
C	-5.43470100	-1.95234400	-1.49243400
H	-4.58045900	-0.62661200	-2.96489200
H	-5.97918900	-3.33046200	0.07132500
H	-6.45955900	-1.64240200	-1.69012000
C	2.43137000	-2.39736500	-1.95692700
C	2.87495700	-1.08384800	-2.15983500
C	3.36987600	-3.36100600	-1.58136100
C	4.20205200	-0.73290100	-1.95296700
H	2.15884400	-0.32083100	-2.46522300
C	4.70508900	-3.01399500	-1.37962600
H	3.06291900	-4.39644600	-1.43569800
C	5.12304200	-1.69868300	-1.55027600
H	4.51602100	0.30075800	-2.09737600
H	5.42011200	-3.78062400	-1.08400000
H	6.16435800	-1.42583300	-1.38348900
P	-0.04557200	-2.01566600	-0.63742800
C	2.05166200	-1.89393300	1.32316700
C	0.86374800	-2.72662600	0.83084800
H	2.31939500	-2.19503900	2.34791000
H	2.93290700	-2.08557300	0.69451000
H	1.18940600	-3.75470900	0.60852100
H	0.10500500	-2.80112800	1.62471600
Cu	0.08358100	0.33500600	-0.51490700
C	-1.31962800	2.93729500	0.31008200
O	-0.48006600	2.00276900	0.53665300
C	-2.77896900	2.61567800	0.38007900
C	-3.74009400	3.59418100	0.66172800

C	-3.21144600	1.29422400	0.21750500
C	-5.08443100	3.25878300	0.78800700
H	-3.43710400	4.63147400	0.78765300
C	-4.55061700	0.95559300	0.35713700
H	-2.47870000	0.51979000	-0.01795000
C	-5.49552500	1.93830300	0.64494400
H	-5.81384900	4.03703500	1.00933900
H	-4.85327000	-0.08522200	0.23911700
H	-6.54628600	1.67436700	0.75716700
C	-0.89779600	4.31601300	0.76478800
H	-1.38321500	5.12934200	0.21220300
H	-1.14130000	4.43724300	1.83173900
H	0.19000300	4.40348700	0.65367600
C	-1.15017600	3.35545000	-1.82058800
C	-1.04719400	2.06180300	-2.36919600
C	0.10062700	1.29158700	-2.44252500
H	-1.98808600	1.59148000	-2.68639700
H	1.07448100	1.78588700	-2.35065600
H	0.08311200	0.39255500	-3.06445300
C	-2.29002600	4.18402600	-2.17180200
C	-2.32119600	5.52424300	-2.19270600
H	-3.21054300	3.63623800	-2.40558700
H	-3.22686000	6.07401800	-2.43943500
H	-1.42746900	6.11629200	-1.98807200
H	-0.19728800	3.87979100	-1.67581400

**(S)-D'**

C	3.20168700	0.91592000	1.81345500
C	0.75307000	0.26053300	2.87877400
C	1.85582100	0.65229600	3.85871400
C	2.77253900	1.61385600	3.11499300
H	3.92474400	0.12224300	2.06815000
H	0.10056500	1.12886400	2.68674800
H	1.43875700	1.09251300	4.77597400
H	2.44309900	-0.22924000	4.16572300
H	2.22110800	2.53635100	2.86887700
H	3.65043600	1.91407300	3.70449500
C	-0.12517500	-0.91459300	3.20435100
C	-1.40240700	-0.97559700	2.62553000
C	0.30142100	-1.98733300	3.99229000
C	-2.20365700	-2.09849300	2.79444000
H	-1.74226600	-0.12070700	2.03234700
C	-0.50767300	-3.10871100	4.16794700
H	1.27705800	-1.95661800	4.47823100

C	-1.75634300	-3.17669500	3.55740400
H	-3.18537500	-2.12854900	2.32034800
H	-0.15653400	-3.93428100	4.78622700
H	-2.38518400	-4.05646200	3.69142100
C	3.82066900	1.82574400	0.79133900
C	5.19520100	1.79606800	0.55325800
C	3.03872200	2.72406300	0.05717000
C	5.77554600	2.63209100	-0.39719800
H	5.81663400	1.09794200	1.11692400
C	3.61007700	3.55414300	-0.89930500
H	1.96025700	2.75643600	0.23211500
C	4.98392700	3.50901300	-1.13259500
H	6.85065000	2.59277600	-0.56805900
H	2.97798400	4.23675000	-1.46782000
H	5.43382600	4.15816900	-1.88192000
P	1.62768100	0.06004100	1.21542900
C	1.16465400	-2.53582700	-2.25682400
C	-1.13831400	-3.38330900	-1.02198800
C	-0.72215900	-4.08124500	-2.33354700
C	0.79086000	-4.00140800	-2.46470400
H	0.75502900	-1.95476300	-3.10246700
H	-0.99574200	-4.07972600	-0.17935600
H	-1.09671800	-5.11340700	-2.35922700
H	-1.19064300	-3.55565500	-3.18049600
H	1.25690200	-4.63043700	-1.68963500
H	1.14880600	-4.37617900	-3.43487000
C	-2.56287400	-2.90919300	-1.03142200
C	-2.97304000	-1.89873200	-1.90836600
C	-3.51520900	-3.49392100	-0.19749000
C	-4.30165600	-1.49972100	-1.96420000
H	-2.23565000	-1.40895800	-2.55114800
C	-4.84890300	-3.09667000	-0.24847500
H	-3.20353500	-4.27316600	0.50051100
C	-5.24639800	-2.10503800	-1.13813300
H	-4.60058600	-0.69952100	-2.64003100
H	-5.57927600	-3.56800500	0.40753800
H	-6.29010300	-1.79723700	-1.18542700
C	2.61517100	-2.18126200	-2.08991500
C	2.99465800	-0.83657000	-2.18362500
C	3.59830100	-3.12205600	-1.77623000
C	4.29867100	-0.43376000	-1.93410100
H	2.23998500	-0.09024900	-2.42927400
C	4.91188300	-2.72346800	-1.53084700
H	3.34617900	-4.18031600	-1.71655600

C	5.26433800	-1.38003100	-1.59509800
H	4.55815700	0.62329900	-1.99028700
H	5.66218100	-3.47391600	-1.28560800
H	6.28760000	-1.06737200	-1.39044800
P	0.12189500	-2.00363600	-0.77140400
C	2.17573000	-1.71933400	1.19614400
C	1.10326600	-2.67115600	0.66258100
H	2.49309900	-2.04029700	2.20081100
H	3.06563500	-1.74382800	0.54831700
H	1.54897100	-3.64066200	0.39049000
H	0.35779800	-2.87165500	1.44630100
Cu	-0.24334200	0.24869500	-0.40538300
C	-1.75675800	2.65812100	0.35162000
O	-1.30683400	1.43177000	0.76012200
C	-3.26825400	2.64198000	0.07520300
C	-4.01260500	3.81410600	-0.11012200
C	-3.94888300	1.42322600	0.04534000
C	-5.38488900	3.77026900	-0.32980000
H	-3.51536000	4.78330400	-0.07707000
C	-5.32398700	1.37679400	-0.17032900
H	-3.37563300	0.50949200	0.21192200
C	-6.04922000	2.54755000	-0.36058000
H	-5.93898100	4.69855900	-0.46718400
H	-5.83156900	0.41208800	-0.17661700
H	-7.12591300	2.50973200	-0.52237800
C	-1.44499700	3.68366400	1.44860900
H	-1.70936100	4.71727500	1.18869100
H	-1.98252900	3.40310900	2.36371200
H	-0.36499100	3.64755900	1.66158500
C	-0.96025000	3.06569800	-0.94825200
C	-0.97571100	1.90468000	-1.89731100
C	0.12240300	1.38898900	-2.48314800
H	-1.96488600	1.50157600	-2.14592600
H	1.10934700	1.82035700	-2.29465600
H	0.05741600	0.59690400	-3.23087100
C	-1.38677200	4.31380800	-1.66021600
C	-0.72326800	5.46764100	-1.60341700
H	-2.30458100	4.24721400	-2.25141100
H	-1.06461400	6.35925100	-2.12605100
H	0.18996500	5.56521000	-1.01249900
H	0.08048500	3.21099900	-0.60695700
<b>(S)-TS5'</b>			
C	-1.52066400	3.10654500	-1.44403600

C	-2.95711800	0.97749700	-2.42768500
C	-3.55765300	2.36533100	-2.65042700
C	-2.39690900	3.34048700	-2.69093300
H	-1.96636500	3.63275100	-0.58327300
H	-2.36378400	0.71446000	-3.32108500
H	-4.16654900	2.39177000	-3.56595900
H	-4.22441400	2.63371200	-1.81648400
H	-1.78915100	3.15094000	-3.58957000
H	-2.72011300	4.38907500	-2.74564200
C	-3.92017000	-0.14252400	-2.15332100
C	-3.57627600	-1.45368700	-2.50254800
C	-5.15660800	0.06641500	-1.53161900
C	-4.41632800	-2.52067200	-2.20813200
H	-2.63319000	-1.63883500	-3.01592400
C	-5.99800700	-1.00071900	-1.23205500
H	-5.47760700	1.07529600	-1.27579500
C	-5.62878900	-2.30098800	-1.55961000
H	-4.12184000	-3.52918100	-2.49651100
H	-6.95386700	-0.81078200	-0.74582000
H	-6.28927500	-3.13512100	-1.32860700
C	-0.11592200	3.59593400	-1.65994200
C	0.32331500	4.78218100	-1.07229300
C	0.74721000	2.91740400	-2.52656000
C	1.58932400	5.28953700	-1.35424400
H	-0.33958300	5.31640100	-0.38863900
C	2.00647700	3.42367300	-2.81554800
H	0.43378700	1.96776500	-2.96931500
C	2.43058800	4.61599900	-2.23222300
H	1.91832200	6.21579900	-0.88482100
H	2.66957200	2.86954200	-3.47965600
H	3.42253400	5.00831600	-2.45011300
P	-1.65139600	1.25958600	-1.06645300
C	-0.91399100	-0.38011200	3.28555800
C	-1.61348500	-2.64000500	1.88388700
C	-1.12518900	-2.81812900	3.32476700
C	-1.51727500	-1.54689600	4.06663600
H	0.17402300	-0.39744700	3.44387200
H	-2.71621500	-2.65353500	1.90422700
H	-1.55401000	-3.72360200	3.77529900
H	-0.02940400	-2.93587200	3.34774300
H	-2.61640400	-1.47649500	4.09015100
H	-1.17454600	-1.54187800	5.11092900
C	-1.14530100	-3.62833800	0.85997800
C	0.20888900	-3.94137400	0.70539500

C	-2.06809400	-4.21572500	-0.00789800
C	0.62311800	-4.82748900	-0.28212400
H	0.95244900	-3.47405900	1.35566700
C	-1.65501200	-5.09931000	-1.00114400
H	-3.12726800	-3.97099500	0.09697600
C	-0.30658800	-5.40897500	-1.14117000
H	1.68276500	-5.05806400	-0.39254200
H	-2.39062500	-5.55046800	-1.66632700
H	0.02195200	-6.09786200	-1.91716300
C	-1.39689600	1.01408700	3.56237000
C	-0.56955500	2.08850800	3.20996800
C	-2.66410500	1.29727600	4.07816000
C	-1.00682000	3.40073700	3.33119100
H	0.43523300	1.89138500	2.83453700
C	-3.10154500	2.61367200	4.20851300
H	-3.32582500	0.48732100	4.38531100
C	-2.28164700	3.66992800	3.82598200
H	-0.33889100	4.21193300	3.04178500
H	-4.09250200	2.81142900	4.61506300
H	-2.62933400	4.69694700	3.92547300
P	-1.13309900	-0.86628800	1.45572000
C	-2.71996200	1.24032000	0.45592700
C	-2.80288900	-0.16792800	1.03744400
H	-3.72498400	1.63687200	0.24974500
H	-2.25083800	1.92370900	1.17871400
H	-3.45387200	-0.18596800	1.92471500
H	-3.23769100	-0.86865200	0.30523000
Cu	0.14235700	-0.30799900	-0.45165600
C	3.33756800	0.52807900	0.01701900
O	2.10008000	0.29598000	-0.58850000
C	2.22389600	-0.95236600	-2.88361400
C	3.56064000	-1.45473900	-3.21562600
H	2.31127300	-0.26927900	-1.74728300
C	4.41249700	-0.90478600	-4.08860200
H	3.89082600	-2.32710600	-2.63815800
H	5.41478600	-1.29884000	-4.24124700
H	4.13016500	-0.03333200	-4.68321700
C	1.23147700	-1.86497900	-2.38469000
H	1.61885500	-2.76124500	-1.88360200
C	-0.11708700	-1.64422400	-2.29449100
H	-0.57031000	-0.86696600	-2.91636400
H	-0.78183900	-2.41858400	-1.90784000
H	1.83689600	-0.19094400	-3.57937200
C	4.07007000	-0.78163800	0.33698500

C	5.43450600	-0.80473600	0.63807800
C	3.37144200	-1.98879900	0.39178700
C	6.08045400	-1.99217900	0.96664800
H	6.01253600	0.11860600	0.61982500
C	4.01136400	-3.17903000	0.72249200
H	2.30573200	-1.97953900	0.16720800
C	5.37270300	-3.18856000	1.00828600
H	7.14654000	-1.98077900	1.19088100
H	3.43997200	-4.10801600	0.76378300
H	5.87751600	-4.11927700	1.26325400
C	4.17761800	1.39980700	-0.92069800
H	3.62632800	2.32193000	-1.13886100
H	5.14328800	1.68436600	-0.48230200
H	4.37052000	0.86732900	-1.86322900
C	3.12992500	1.29976600	1.35509100
C	2.32415000	2.55291000	1.13289000
C	2.57066900	3.70843800	1.74693400
H	1.50133500	2.46890600	0.41394300
H	3.38930800	3.81373200	2.46190800
H	1.97002800	4.59792300	1.55689200
C	2.49447000	0.41805500	2.38924300
C	2.89694100	0.33042700	3.65458500
H	1.64764300	-0.17688400	2.03390200
H	2.40973000	-0.32379600	4.37746400
H	3.74514800	0.91095100	4.02154200
H	4.12309400	1.59422400	1.73821600

**(R)-TS4'**

C	-2.26432200	-2.40980700	1.55662800
C	-0.28244700	-0.91741000	2.73643500
C	-1.01711900	-1.91455400	3.62805600
C	-1.46904500	-3.04299500	2.71287800
H	-3.25757300	-2.11512700	1.93654700
H	0.65221700	-1.37854000	2.37669200
H	-0.37798100	-2.26770600	4.45017800
H	-1.90468400	-1.44878300	4.08738900
H	-0.58593900	-3.55892800	2.30030700
H	-2.07088800	-3.80365700	3.22962200
C	0.04224400	0.44409900	3.27821900
C	1.08999100	1.16596400	2.68996000
C	-0.70094100	1.06008900	4.28817400
C	1.35946500	2.47392000	3.07047400
H	1.67570600	0.68030300	1.90893700
C	-0.42794900	2.37120500	4.67539800

H	-1.50600000	0.51678800	4.78341800
C	0.59340100	3.08840400	4.06017700
H	2.17461800	3.01223900	2.58600700
H	-1.01948200	2.83300100	5.46496700
H	0.80346400	4.11372600	4.36251300
C	-2.44226600	-3.32095300	0.37446900
C	-3.66761300	-3.94970100	0.14972900
C	-1.38614700	-3.57882000	-0.50695000
C	-3.84435900	-4.80952100	-0.93087400
H	-4.49780800	-3.75074700	0.83002600
C	-1.56107500	-4.43091600	-1.59137500
H	-0.42086600	-3.08700200	-0.35400800
C	-2.79157300	-5.04797400	-1.80868700
H	-4.80939000	-5.28934600	-1.08942300
H	-0.73077800	-4.61192800	-2.27300200
H	-2.92658800	-5.71426000	-2.65905200
P	-1.32677200	-0.82364200	1.16146000
C	-2.53104000	2.22589400	-1.71130900
C	-0.68461700	3.81813300	-0.46126600
C	-1.61517900	4.47803500	-1.50094600
C	-2.91931100	3.69466500	-1.57038600
H	-2.01532900	2.09877700	-2.67964700
H	-0.91117800	4.20742200	0.54504300
H	-1.77511700	5.53827400	-1.26361500
H	-1.12783700	4.44949900	-2.48732400
H	-3.49320900	3.85268600	-0.64373800
H	-3.55980700	4.02694800	-2.40063800
C	0.78085700	4.00909700	-0.73695800
C	1.34719600	3.57402300	-1.94066600
C	1.61569300	4.60123300	0.21062200
C	2.70352800	3.73751000	-2.19265200
H	0.71702900	3.08338900	-2.68683800
C	2.97699700	4.76205300	-0.03468300
H	1.18958700	4.94184600	1.15604000
C	3.52515800	4.33373000	-1.23861200
H	3.12497200	3.38108800	-3.13228600
H	3.61034200	5.22819100	0.71902600
H	4.58918000	4.45771000	-1.43243600
C	-3.59810800	1.17605300	-1.59185600
C	-3.29382800	-0.14191800	-1.95765300
C	-4.86610000	1.44250100	-1.07154600
C	-4.21302500	-1.16674000	-1.78116600
H	-2.30828800	-0.36999300	-2.36618200
C	-5.79321000	0.41591700	-0.89666900



H	-5.14083400	2.46045300	-0.79622200
C	-5.46731000	-0.89185900	-1.23866800
H	-3.94342900	-2.18689700	-2.05398000
H	-6.77654500	0.64477100	-0.48783000
H	-6.18889300	-1.69517800	-1.09428300
P	-1.16882900	1.99118900	-0.42807300
C	-2.59581300	0.48413400	1.54234600
C	-2.13536900	1.89486400	1.16523400
H	-2.88364800	0.45735500	2.60515300
H	-3.48856700	0.20922400	0.96066200
H	-2.99583700	2.58097300	1.13518600
H	-1.44768200	2.28137500	1.93233100
Cu	0.05991900	0.04157200	-0.63135600
C	2.89763100	-0.67627400	-0.21305100
O	1.69570800	-0.81648300	0.19975600
C	2.79200400	-1.30750900	-2.30110100
C	1.74121300	-0.48951100	-2.76488600
C	0.38145900	-0.70886500	-2.62868800
H	2.04700200	0.47039500	-3.20429500
H	0.01842000	-1.72418300	-2.43937100
H	-0.29904300	-0.06084000	-3.18666300
C	4.10870500	-1.14497900	-2.89231100
C	5.09900300	-2.04780600	-2.88645400
H	4.29239100	-0.17014300	-3.36211500
H	6.06809400	-1.84061200	-3.33559900
H	4.96624300	-3.03379900	-2.43806000
H	2.51363700	-2.32542900	-2.00329100
C	3.40700600	0.73765300	-0.37887000
H	2.58198100	1.37769700	-0.71818000
H	3.74707800	1.12484800	0.59706800
H	4.24171800	0.83604100	-1.08362700
C	3.86709500	-1.72704700	0.20310700
C	5.24903700	-1.51942700	0.20689100
C	3.37992500	-2.97591600	0.61281100
C	6.11967200	-2.52844600	0.61131300
H	5.65354000	-0.55934200	-0.10737500
C	4.24616600	-3.98655100	0.99884500
H	2.30097300	-3.13101700	0.61818300
C	5.62405100	-3.76600700	1.00189500
H	7.19329900	-2.34466400	0.61136900
H	3.84872500	-4.95227100	1.30965300
H	6.30532500	-4.55755800	1.31100000

**(R)-D'**

C	-2.00982200	-2.59748800	1.52532200
C	-0.18040800	-0.93677400	2.72210500
C	-0.83867900	-1.98086100	3.61899300
C	-1.19225000	-3.14874000	2.71069800
H	-3.04879200	-2.42294200	1.85383800
H	0.77712100	-1.33033100	2.34028800
H	-0.17676200	-2.27786200	4.44542300
H	-1.76228300	-1.58534700	4.07365500
H	-0.26525300	-3.60010900	2.32099000
H	-1.74357300	-3.94728900	3.22673800
C	0.06115300	0.44292100	3.26307900
C	1.04567800	1.22981600	2.64830300
C	-0.69484500	1.00312100	4.29556200
C	1.24123500	2.54973200	3.03359300
H	1.63328900	0.77247200	1.84773400
C	-0.49581100	2.32787900	4.68316100
H	-1.44958100	0.40713200	4.80934600
C	0.46333300	3.10968600	4.04680300
H	2.01148800	3.14078500	2.53650600
H	-1.09523300	2.74846900	5.48979300
H	0.61701500	4.14433600	4.35205800
C	-2.01236200	-3.51120700	0.33176800
C	-3.12878700	-4.29791300	0.04672000
C	-0.88978500	-3.61345900	-0.49915100
C	-3.13612000	-5.16252300	-1.04490500
H	-4.00949100	-4.22152300	0.68737000
C	-0.89688500	-4.47148300	-1.59298600
H	-0.00574000	-3.00037100	-0.29469600
C	-2.02126400	-5.24638900	-1.87277100
H	-4.01797300	-5.76723100	-1.25260600
H	-0.01535800	-4.53520300	-2.23084000
H	-2.02459000	-5.91547800	-2.73171700
P	-1.24478200	-0.91366500	1.16706300
C	-2.74626800	2.00380900	-1.66641300
C	-1.02611200	3.76795000	-0.46955600
C	-2.02719600	4.32980500	-1.50041200
C	-3.25836100	3.43481300	-1.53328700
H	-2.24412500	1.91206200	-2.64621700
H	-1.27746100	4.14669200	0.53453500
H	-2.27432800	5.37528600	-1.27243900
H	-1.55699600	4.33139500	-2.49566000
H	-3.82680600	3.55447200	-0.59757700
H	-3.94145000	3.69865400	-2.35409200
C	0.41365100	4.08152000	-0.76629900

C	1.00195500	3.67748400	-1.97068700
C	1.20837600	4.74750700	0.16569900
C	2.34115100	3.93499400	-2.23519100
H	0.40336300	3.13466700	-2.70764200
C	2.55206000	5.00687200	-0.09368400
H	0.76560700	5.06219500	1.11216200
C	3.12293400	4.60274000	-1.29486300
H	2.78121100	3.60047700	-3.17474100
H	3.15400000	5.52767000	0.64969900
H	4.17418700	4.79970900	-1.49730400
C	-3.71963000	0.86938600	-1.52134600
C	-3.32134300	-0.41610000	-1.90958900
C	-4.98677400	1.02434200	-0.95577300
C	-4.14440700	-1.51623100	-1.71404600
H	-2.33572600	-0.55922700	-2.35448800
C	-5.81707300	-0.07825100	-0.75753500
H	-5.33641800	2.01286400	-0.65959000
C	-5.39609700	-1.35221800	-1.12392700
H	-3.80095700	-2.50543000	-2.01503800
H	-6.80041200	0.06455000	-0.31128400
H	-6.04135900	-2.21456700	-0.96159100
P	-1.33672500	1.90319700	-0.41475000
C	-2.60943500	0.28088500	1.57788700
C	-2.24294800	1.72353700	1.20725000
H	-2.87678800	0.23047500	2.64475500
H	-3.48967600	-0.04894900	1.00542900
H	-3.14110700	2.36013300	1.21606700
H	-1.55225700	2.13562000	1.96061200
Cu	0.11610700	0.10535200	-0.51792800
C	2.93718200	-0.50177300	-0.44424300
O	1.76569300	-0.65043400	0.23995500
C	2.67049900	-0.89331200	-1.97696500
C	1.53329700	-0.09154700	-2.51568200
C	0.31022500	-0.56219400	-2.82726400
H	1.73754100	0.97238700	-2.68665400
H	0.05858500	-1.62072900	-2.73330800
H	-0.43825900	0.08307500	-3.28990800
C	3.85577900	-0.74042500	-2.87882800
C	4.67768800	-1.72671400	-3.23084300
H	4.05226600	0.27443900	-3.24342500
H	5.54457600	-1.55520100	-3.86612700
H	4.52553000	-2.74607100	-2.87195700
H	2.37093200	-1.95483300	-1.93465000
C	3.43547500	0.94624300	-0.35306900

H	2.59622500	1.61993600	-0.57837200
H	3.76580500	1.15954800	0.67353400
H	4.26452000	1.18934400	-1.03470200
C	3.97576100	-1.49349800	0.08176700
C	5.35082900	-1.25493000	0.05944300
C	3.53070100	-2.72245200	0.57695000
C	6.25355200	-2.21251500	0.51453700
H	5.73168700	-0.30896300	-0.32348500
C	4.42701600	-3.68506000	1.02532300
H	2.45531000	-2.89779200	0.61509200
C	5.79636900	-3.43402900	0.99606500
H	7.32211700	-2.00009200	0.49045600
H	4.05497200	-4.63581500	1.40736900
H	6.50195300	-4.18395600	1.35192600

**(R)-TS5'**

C	3.02008100	1.17165400	-1.39454300
C	0.89683500	1.96068500	-2.89897900
C	2.27317000	1.90823800	-3.58932800
C	3.13642900	0.87037700	-2.89026000
H	3.34987500	2.21596800	-1.24376600
H	0.24068800	1.22909600	-3.39177900
H	2.15245800	1.70518400	-4.66188800
H	2.76878100	2.88713200	-3.51245300
H	2.77146800	-0.15093000	-3.09360700
H	4.18488400	0.90647700	-3.21722500
C	0.21006400	3.29767600	-2.92908300
C	-1.14445000	3.38764100	-3.26736500
C	0.87866400	4.48292900	-2.59714100
C	-1.81621900	4.60550400	-3.23965600
H	-1.68217900	2.48486900	-3.55657900
C	0.21054000	5.70202600	-2.56552600
H	1.94305000	4.45812800	-2.35861100
C	-1.14372500	5.76816600	-2.87822400
H	-2.87039500	4.64339500	-3.51013100
H	0.75516500	6.60665700	-2.29888500
H	-1.66688100	6.72258200	-2.85422700
C	3.84404600	0.29125100	-0.50644600
C	4.89559400	0.84479100	0.22889200
C	3.64754400	-1.09158900	-0.45555400
C	5.74288200	0.04026700	0.98390000
H	5.05207400	1.92485400	0.20437700
C	4.49342400	-1.89825000	0.29787700
H	2.82594000	-1.54865400	-1.01075100

C	5.54628400	-1.33711300	1.01740300
H	6.56034700	0.49238400	1.54504600
H	4.31527400	-2.97274900	0.32111800
H	6.20972400	-1.97248000	1.60267400
P	1.15399700	1.21676900	-1.14676500
C	-0.61911800	1.52666000	3.16599800
C	-2.90810200	1.88950700	1.71703200
C	-2.95434800	2.21297200	3.22800100
C	-1.56287300	2.59807600	3.70055400
H	-0.89250000	0.56348800	3.63218300
H	-3.05664700	2.81673400	1.14031900
H	-3.70307800	2.98972000	3.43401600
H	-3.28138900	1.31236400	3.76993200
H	-1.29345800	3.58654400	3.29602400
H	-1.50231200	2.67689500	4.79610500
C	-3.96122800	0.88975600	1.32591100
C	-3.87969000	-0.43406500	1.77080400
C	-5.06067200	1.26374900	0.55357600
C	-4.85812600	-1.36198700	1.44447300
H	-3.02525600	-0.75043900	2.37173100
C	-6.05589100	0.34122900	0.23630400
H	-5.13832200	2.29204700	0.19666600
C	-5.95734100	-0.97338200	0.67975400
H	-4.75049000	-2.39402800	1.77729600
H	-6.90759100	0.65102400	-0.36719600
H	-6.72854100	-1.69777800	0.42225800
C	0.85715400	1.72965700	3.32868000
C	1.70626500	0.63540400	3.12573800
C	1.42665400	2.97088100	3.61689300
C	3.08479400	0.78374600	3.16285700
H	1.27294600	-0.34747300	2.93178100
C	2.81198100	3.11934300	3.66893800
H	0.79149100	3.83585000	3.80547300
C	3.64452100	2.03298100	3.42752600
H	3.72663500	-0.07620100	2.96730400
H	3.23949500	4.09505500	3.89641100
H	4.72710600	2.15228500	3.45206400
P	-1.13567400	1.32191100	1.35311700
C	1.02246100	2.61340200	0.06967300
C	-0.39596400	2.85354600	0.58331700
H	1.42930800	3.54009000	-0.35737800
H	1.69183800	2.32122400	0.89468600
H	-0.40451000	3.69668100	1.29063000
H	-1.05532300	3.13390600	-0.25554400

Cu	-0.62757300	-0.21122700	-0.40774200
C	-0.37393900	-3.39596000	-0.00549700
O	-0.99329400	-2.18733100	-0.30389700
C	-2.84344100	-2.02768200	-2.12646200
C	-3.98733800	-2.93730600	-2.01499400
H	-1.95582200	-2.28663200	-1.16605900
C	-4.18408500	-4.04760800	-2.73366000
H	-4.71125800	-2.68050500	-1.23257100
H	-5.03570500	-4.70220200	-2.56118200
H	-3.49264500	-4.34027800	-3.52591900
C	-3.00085200	-0.66032200	-1.72685000
H	-3.81009200	-0.46410000	-1.01655900
C	-2.14368800	0.37643700	-1.99690300
H	-1.44773300	0.28486100	-2.83577400
H	-2.39910300	1.39117800	-1.68533800
H	-2.22789800	-2.18120900	-3.02668300
C	0.07143300	-3.37934100	1.49152600
C	1.34648500	-2.61572300	1.70702300
C	2.27503500	-2.95622900	2.59781700
H	1.47568900	-1.71278900	1.09727400
H	2.16253900	-3.84477400	3.22231800
H	3.18380600	-2.37017300	2.73662900
C	-1.00042000	-2.77468800	2.35310600
C	-1.74030300	-3.44059700	3.23651700
H	-1.13433300	-1.69694100	2.22240500
H	-2.48974600	-2.94502100	3.85395000
H	-1.62776900	-4.51683600	3.37831900
H	0.22746400	-4.41916200	1.82774900
C	-1.38830600	-4.53059500	-0.19498800
H	-0.95095500	-5.50793000	0.05201500
H	-2.26368000	-4.35569700	0.44690000
H	-1.73496000	-4.56353500	-1.23632000
C	0.80527100	-3.66057600	-0.94370900
C	0.90213800	-2.95788000	-2.14646300
C	1.76573400	-4.64015100	-0.67311100
C	1.93189900	-3.21681500	-3.04833400
H	0.15648900	-2.19157400	-2.36017900
C	2.80121000	-4.89505400	-1.56639200
H	1.71235000	-5.20811800	0.25669700
C	2.89144100	-4.18130100	-2.75896900
H	1.98223800	-2.66100300	-3.98510600
H	3.54218700	-5.65842000	-1.33079900
H	3.70089600	-4.38101400	-3.45934300