

*Supporting Information*

**Understanding the mechanism and stereoselectivity of NHC-Catalyzed [3 + 2]  
cycloaddition of 3-bromoaldehydes and isatin N-Boc ketimines**

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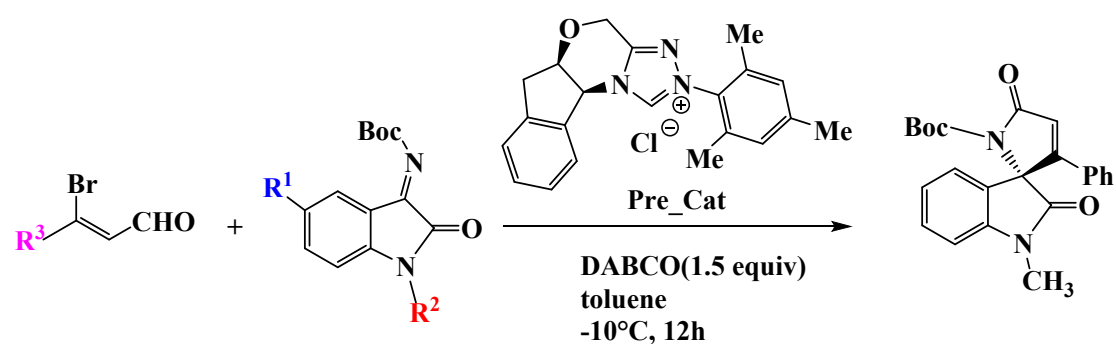
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Table S1. Single-point energies (in kcal/mol) at SMD(toluene)/M06-2X/6-311++G(d,p) level, based on the optimized geometries at different levels of theory.

Species	M06-2X/ 6-31G(d,p)	B3LYP-D3/ 6-31G(d,p)	M06-2X-D3/ 6-31G(d,p)
R1+R2+Cat	0.0	0.0	0.0
TS3(RR)	12.0	11.0	12.6
TS3(RS)	13.5	10.4	13.9
TS3(SR)	10.9	9.1	11.0
TS3(SS)	7.2	6.0	7.4

Table S2. Comparison of the Gibbs free energies (a.u.) of the stereoselective transition states.



Entry	$R^1$	$R^2$	$R^3$	TS3(SS)	TS3(SR)	$\Delta\Delta G(\text{kcal/mol})$
1	5-CH <sub>3</sub>	CH <sub>3</sub>	Ph	-4847.627188	-4847.620725	4.1
2	5-Cl	CH <sub>3</sub>	Ph	-5267.959831	-5267.954738	3.2
3	H	Ac	Ph	-4921.675193	-4921.67258	1.6
4	H	H	Ph	-4769.070085	-4769.064543	3.5
5	H	CH <sub>3</sub>	4-FC <sub>6</sub> H <sub>4</sub>	-4907.597463	-4907.591953	3.5
6	H	CH <sub>3</sub>	4-MeC <sub>6</sub> H <sub>4</sub>	-4847.627247	-4847.622047	3.3
7	H	CH <sub>3</sub>	4-MeOC <sub>6</sub> H <sub>4</sub>	-4922.829649	-4922.821918	4.9
8	H	CH <sub>3</sub>	4-NO <sub>2</sub> C <sub>6</sub> H <sub>4</sub>	-5012.842624	-5012.836462	3.9

We have examined the dependence of substrate on the stereoselectivity by considering a series of substrates with different substituent groups (3-aryl-3-bromoaldehydes and isatin N-Boc ketimines). As depicted in Table S2, the energy differences between **TS3(SS)** and **TS3(SR)**, associated with the S- and R- configured products respectively, are close to the range of 1.5 ~ 2.9 kcal/mol (which can be obtained from the experimentally reported *ee* values with the range of 86% ~ 99%).

These results demonstrate that the stereoselectivity can be explained by our calculated results.

Table S3. Total (a.u.) and relative free energies in parentheses (kcal/mol) of the reactant, intermediates, transition states and products at SMD(toluene)/M06-2X/6-311++G(d,p) level.

species	Gsol	$\Delta G$	species	Gsol	$\Delta G$
<b>R1+R2+Cat</b>	-4048.220044	0.0	<b>TS4(SR)</b>	-4808.379273	-13.4
<b>Re-TS1</b>	-4808.329748	17.6	<b>TS4(SS)</b>	-4808.389557	-19.9
<b>Re-IM1</b>	-4048.198507	13.5	<b>IM4(RR)</b>	-4808.393042	-22.1
<b>Si-TS1</b>	-4808.273679	52.8	<b>IM4(RS)</b>	-4808.412573	-34.3
<b>Si-IM1</b>	-4808.330791	17.0	<b>IM4(SR)</b>	-4808.401411	-27.3
<b>Re-TS2</b>	-4808.326804	19.5	<b>IM4(SS)</b>	-4808.402446	-28.0
<b>Re-TS2<sub>d</sub></b>	-4808.300279	36.1	<b>TS5(RR)</b>	-4808.344694	8.3
<b>Re-TS2<sub>w</sub></b>	-4808.311375	29.2	<b>TS5(RS)</b>	-4808.379835	-13.8
<b>Re-TS2<sub>2w</sub></b>	-4808.323971	21.3	<b>TS5(SS)</b>	-4808.381584	-14.9
<b>Re-IM2</b>	-4808.336309	13.5	<b>IM5(RR)</b>	-4808.389005	-19.6
<b>TS3-RR</b>	-4808.338667	12.0	<b>IM5(RS)</b>	-4808.400983	-27.1
<b>TS3(RS)</b>	-4808.336397	13.5	<b>IM5(SR)</b>	-4808.393561	-22.4
<b>TS3(SR)</b>	-4808.340517	10.9	<b>IM5(SS)</b>	-4808.400998	-27.1
<b>TS3(SS)</b>	-4808.346403	7.2	<b>TS6(RR)</b>	-4808.383542	-16.1
<b>IM3(RR)</b>	-4808.396719	-24.4	<b>TS6(RS)</b>	-4808.38942	-19.8
<b>IM3(RS)</b>	-4808.391609	-21.2	<b>TS6(SR)</b>	-4808.38268	-15.6
<b>IM3(SR)</b>	-4808.392298	-21.6	<b>TS6(SS)</b>	-4808.386567	-18.0
<b>IM3(SS)</b>	-4808.394903	-23.3	<b>P(R)</b>	-4808.425559	-42.5
<b>TS4(RR)</b>	-4808.390724	-20.6	<b>P(S)</b>	-4808.425559	-42.5
<b>TS4(RS)</b>	-4808.374488	-10.4			



Fig.S1 Free energy profiles and optimized transition states of direct and DABCO- and H<sub>2</sub>O-assisted proton transfer. The solvation-corrected relative free energies at SMD(toluene)/M06-2X/6-311++G(d,p) level are given in kcal/mol. Key bond lengths are given in Å.

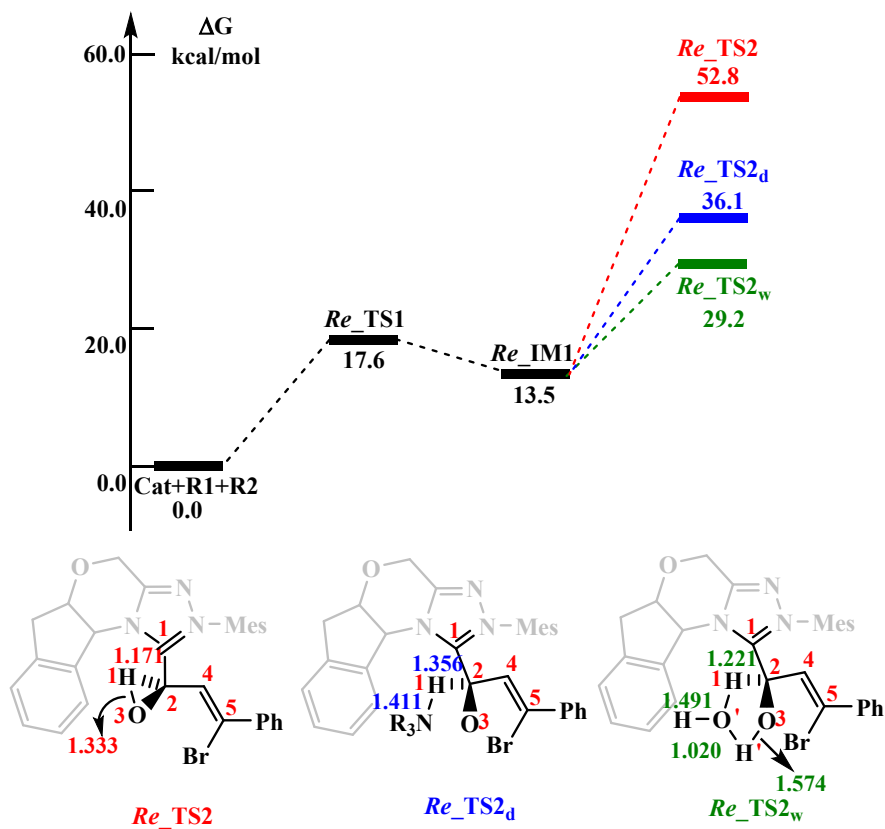


Fig.S2 Free energy profiles of the *RR*-, *RS*- and *SR*-configurational pathways. The solvation-corrected relative free energies at SMD(toluene)/M06-2X/6-311++G(d,p) level are given in kcal/mol.

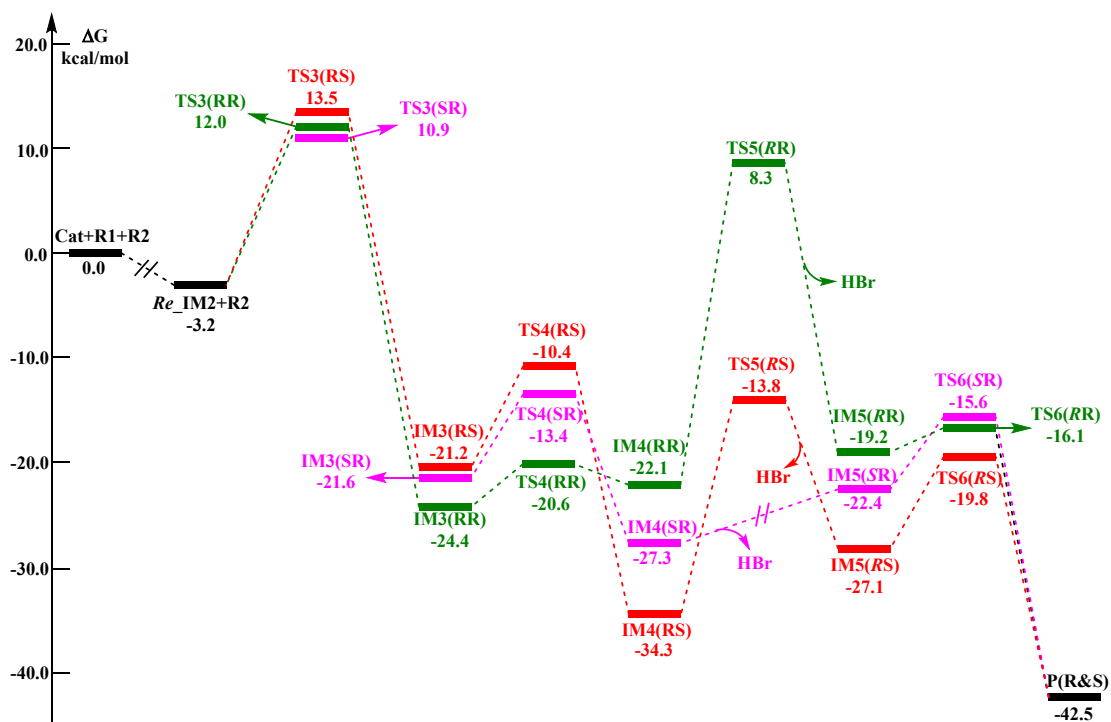




Fig. S3 Superposition of the optimized geometry **R2** (magenta) with the corresponding **R2**-parts in **TS3(SS)/TS3(SR)** (cyan).

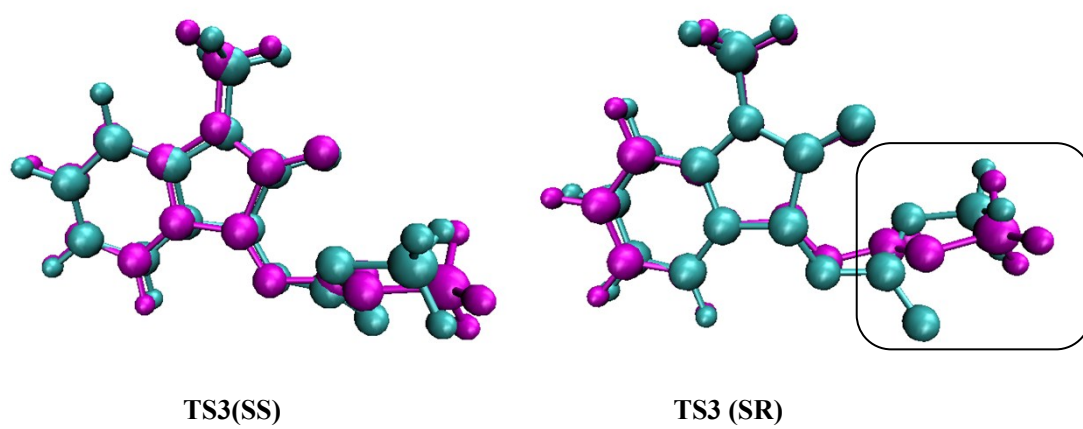


Fig. S4 Superposition of the optimized geometry **Re-IM2** (yellow) with the corresponding **Re-IM2**-parts in **TS3(SS)/TS3(SR)** (cyan).

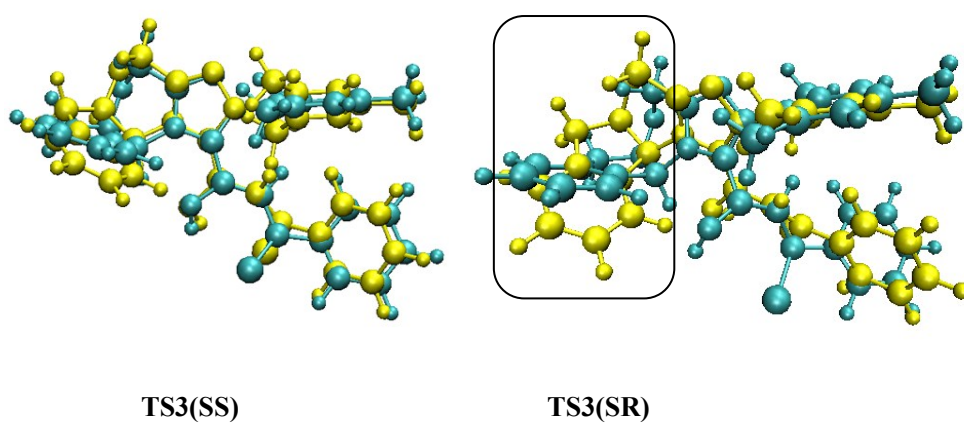
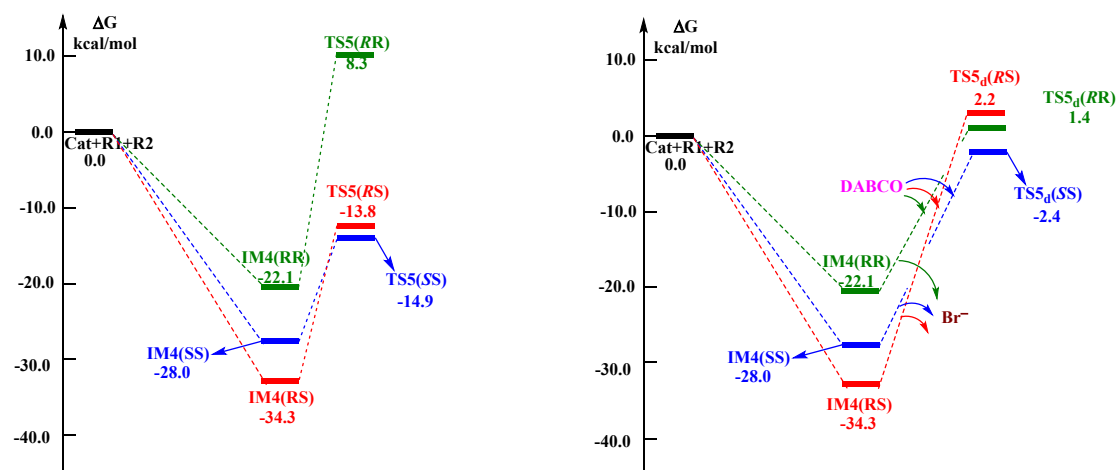




Fig.S5 Comparison between Br<sup>-</sup> (left) and DABCO (right) assisted deprotonation. The solvation-corrected relative free energies at SMD(toluene)/M06-2X/6-311++G(d,p) level are given in kcal/mol.



## Cartesian coordinates

### DABCO

C	-0.78666700	1.30696900	-0.42007200
C	0.77165600	1.31294700	-0.42865600
H	-1.19527900	1.51709100	-1.41419600
H	-1.18752300	2.06047200	0.26636300
H	1.16739900	1.52549100	-1.42764300
H	1.17370500	2.07049400	0.25259000
C	-0.78036000	-1.02530600	-0.91838100
H	-1.17663500	-1.99582500	-0.60087500
H	-1.18777700	-0.81309700	-1.91246700
C	0.77842300	-1.01964300	-0.92615700
H	1.18516100	-1.98676700	-0.61134100
H	1.17493600	-0.80499700	-1.92417900
C	0.78777600	-0.28423400	1.34256000
H	1.19428500	-1.25273900	1.65240100
H	1.18984600	0.47462200	2.02242400
C	-0.77075700	-0.29066500	1.35068100
H	-1.16638200	-1.26230500	1.66482900
H	-1.17268900	0.46509600	2.03425500
N	-1.28414700	-0.00491200	0.00661800
N	1.28422200	0.00520600	-0.00690600

### R1

C	0.42745300	0.37964200	0.08261400
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C	1.04634000	1.54904900	0.31725800
C	2.49775800	1.82656300	0.33700600
H	0.40735900	2.40098200	0.53522600
H	2.73915300	2.88734000	0.55102100
O	3.38184800	1.02393000	0.14730800
C	-1.04572900	0.24554600	0.04397900
C	-1.68899700	-0.88883800	0.55075200
C	-1.81776300	1.28687700	-0.48532800
C	-3.07618100	-0.96519300	0.55240400
C	-3.20488200	1.20121500	-0.49289900
H	-1.32462600	2.15018100	-0.92071900
C	-3.83803000	0.07750000	0.03103100
H	-3.56331600	-1.84457400	0.96052300
H	-3.79048200	2.00883200	-0.91975400
H	-1.09458200	-1.70467900	0.94750500
H	-4.92099200	0.01001000	0.02411200
Br	1.39122500	-1.21067700	-0.22792200
<b>R2</b>			
N	-1.17058700	-1.33283100	0.17827000
C	-2.49055300	-0.83579900	0.31125800
O	-3.08422400	-0.79460800	1.35370900
O	-2.99292100	-0.53741200	-0.88951000
C	-4.29576900	0.04592200	-0.83767800
H	-4.57513200	0.23526100	-1.87250300
H	-5.00261000	-0.63813200	-0.36427500

H	-4.25651200	0.97818200	-0.27034700
C	3.96267500	-0.64776600	-0.18367200
C	3.32474800	-1.88698100	-0.14883100
C	1.93412800	-1.95973100	-0.04761900
C	1.21674200	-0.77740300	0.01592900
C	1.86988100	0.46469500	-0.01924800
C	3.24794700	0.55308600	-0.11960700
H	5.04445800	-0.60895000	-0.26274600
H	3.91275100	-2.79634000	-0.19908400
H	1.41236800	-2.91080000	-0.01695000
H	3.75579500	1.51101200	-0.14797000
C	-0.21755800	-0.50196400	0.12189400
C	-0.34525300	1.02895400	0.14772000
O	-1.36552300	1.67343200	0.22718000
N	0.93966200	1.51261000	0.05907300
C	1.26802900	2.91868800	0.05556300
H	1.90347700	3.16836800	0.91046000
H	1.78342700	3.19194500	-0.87004400
H	0.32970900	3.46949200	0.12677000
<b>Cat</b>			
C	4.50346300	2.66808700	-0.22040300
C	4.97758000	1.39409100	0.08250700
C	4.16708400	0.29345800	-0.18401100
C	2.42325200	1.74689000	-1.04638400
C	3.23511700	2.84553700	-0.77981700

H	5.12326500	3.53461200	-0.01246800
H	5.96039900	1.26353100	0.52627700
H	1.42858800	1.86187400	-1.46987100
H	2.88140400	3.84680800	-1.00325700
C	2.90879700	0.47897000	-0.74734100
C	2.18721800	-0.83590500	-0.94363900
C	3.09613800	-1.88988800	-0.20928800
H	2.07776000	-1.07865700	-2.00391700
C	4.44434800	-1.17026800	0.05074800
H	3.23177400	-2.77107000	-0.83858200
H	4.78938500	-1.38998800	1.06625700
H	5.21372600	-1.53892600	-0.63638900
N	0.85345700	-0.80027500	-0.37821800
O	2.52257500	-2.40439300	0.98142800
C	0.65795500	-0.98723900	0.96405500
C	1.82341700	-1.45569000	1.76937700
H	2.47175500	-0.61079200	2.04716900
H	1.49180400	-1.96109900	2.67670700
N	-0.58001500	-0.78176300	1.28175400
C	-0.30634900	-0.42114200	-1.00241400
N	-1.13949200	-0.42986200	0.06443900
C	-2.52916500	-0.09380400	0.02278300
C	-2.96061400	1.05696100	0.68911000
C	-3.40747600	-0.92213300	-0.67940000
C	-4.31756800	1.36819500	0.64069600

C	-4.75542700	-0.56528200	-0.70660200
C	-5.22796700	0.57205300	-0.05446600
H	-4.67037900	2.26079700	1.15292200
H	-5.45410100	-1.19877000	-1.24823000
C	-1.98248600	1.93382700	1.42445100
H	-1.61390400	1.43795100	2.32643000
H	-1.11048200	2.15053100	0.79879500
H	-2.45137100	2.87803400	1.70833900
C	-2.91306200	-2.15789900	-1.38223100
H	-2.22770600	-1.89224900	-2.19108000
H	-2.35935000	-2.80209000	-0.69201300
H	-3.74976300	-2.72624400	-1.79315000
C	-6.68440700	0.95429900	-0.12258500
H	-6.85191900	1.71149100	-0.89568000
H	-7.30943200	0.09124000	-0.36300000
H	-7.02877900	1.37276000	0.82662400

**Re\_TS1**

C	2.24360800	1.14705100	0.83338000
C	1.09402100	0.67046500	1.31698600
C	-0.32261700	1.09256300	1.01977900
H	1.16811200	-0.11806100	2.06500200
H	-0.89971800	1.08793100	1.97386600
O	-0.62307400	1.91204700	0.12568000
C	3.57668400	0.69124000	1.30222500
C	3.72691100	0.19905100	2.60563700



C	4.69854500	0.70832000	0.46593800
C	4.94856900	-0.29831600	3.04390100
C	5.92078400	0.21253100	0.90627000
H	4.60083200	1.11104700	-0.53620400
C	6.05104000	-0.30047700	2.19390600
H	5.04241800	-0.67042600	4.05918500
H	6.77602300	0.23008100	0.23737100
H	2.88631900	0.23080500	3.29094400
H	7.00662000	-0.68257300	2.53829600
Br	2.26994500	2.44637000	-0.55389700
C	-6.07395600	2.47629300	-0.56718600
C	-6.54997300	1.33220500	0.06958400
C	-5.63246700	0.44543300	0.62403200
C	-3.77747700	1.85208000	-0.08853900
C	-4.70377500	2.73367100	-0.64363800
H	-6.77723000	3.17561300	-1.00866800
H	-7.61630300	1.13386800	0.12679000
H	-2.70473600	2.04555000	-0.13671700
H	-4.35317700	3.63205400	-1.14125900
C	-4.26755000	0.71004800	0.53763600
C	-3.46413600	-0.38959600	1.20306100
C	-4.51377100	-1.53650000	1.44321800
H	-3.03007600	-0.05970500	2.15133500
C	-5.88972100	-0.83984800	1.37026200
H	-4.34706500	-2.01060900	2.41220800

H	-6.61203000	-1.50026600	0.88142100
H	-6.26654200	-0.63423100	2.37885000
N	-2.37071900	-0.87158000	0.37082500
O	-4.41262100	-2.60330200	0.51072500
C	-2.62502200	-1.70912200	-0.68347500
C	-4.01429400	-2.23973500	-0.80194600
H	-4.68997000	-1.49234300	-1.23965100
H	-4.02783000	-3.14262900	-1.41216000
N	-1.53475700	-2.00326600	-1.32093200
C	-1.04277900	-0.60197700	0.41363300
N	-0.57514000	-1.29849800	-0.62988700
C	0.79867100	-1.37114800	-1.04226800
C	1.24112800	-0.49805800	-2.03445100
C	1.63441000	-2.28377700	-0.39510000
C	2.59402700	-0.55363600	-2.37065700
C	2.97453200	-2.30328200	-0.76757800
C	3.46823400	-1.44603300	-1.75374500
H	2.97386600	0.13698000	-3.11985500
H	3.65337100	-2.98976200	-0.26703900
C	0.29790700	0.48582900	-2.66954800
H	-0.54256300	-0.03436000	-3.13995800
H	-0.09659800	1.17002100	-1.90949000
H	0.81621400	1.07000600	-3.43256300
C	1.09918900	-3.18348900	0.68649200
H	0.78860700	-2.60143200	1.56107200

H	0.22329300	-3.73952800	0.33870800
H	1.86022300	-3.89727800	1.00611900
C	4.92176200	-1.49903000	-2.14625800
H	5.54804800	-1.75253800	-1.28722700
H	5.08814800	-2.25600400	-2.91994000
H	5.25863600	-0.53823900	-2.54462400

**Si\_TS1**

C	0.20153400	2.00322100	1.01057100
C	-0.18269700	0.92774500	1.70146800
C	0.65919300	-0.26080300	2.16637400
H	-1.24959600	0.85723900	1.92384200
H	0.02540700	-0.85847800	2.87613600
O	1.88741500	-0.15632300	2.37698600
C	-0.74586000	3.04051100	0.53783600
C	-0.61020400	3.62476900	-0.72730500
C	-1.85683600	3.38153100	1.32023700
C	-1.57656300	4.50331400	-1.20690200
C	-2.81919800	4.26227200	0.83988500
H	-1.95127700	2.96525200	2.31811000
C	-2.68655100	4.82303700	-0.42814800
H	-1.45795900	4.94326700	-2.19207600
H	-3.66927800	4.51997600	1.46334900
H	0.26241400	3.38467200	-1.32564700
H	-3.43521400	5.51460100	-0.80083800
Br	2.00248900	2.19987900	0.44533900

C	-4.95435000	0.45310100	-1.41279700
C	-5.27893800	-0.79480100	-0.88224100
C	-4.32230900	-1.48132600	-0.14091300
C	-2.72286900	0.31175900	-0.48971400
C	-3.68488900	1.00230800	-1.22320700
H	-5.69430400	0.99842600	-1.98980600
H	-6.26099600	-1.22644300	-1.05141800
H	-1.72901800	0.72757000	-0.35946500
H	-3.43632900	1.97260400	-1.64252000
C	-3.06468000	-0.91764800	0.06291300
C	-2.20601400	-1.82847500	0.91917200
C	-2.96550600	-3.19955900	0.88878900
H	-2.11949200	-1.46029300	1.94670200
C	-4.42140300	-2.83272200	0.52424900
H	-2.90141900	-3.69561600	1.85880800
H	-4.84971900	-3.60806800	-0.11717500
H	-5.03676100	-2.77941500	1.42961500
N	-0.86166900	-1.97909700	0.39151100
O	-2.40100100	-4.13406900	-0.02018800
C	-0.63912500	-2.75524200	-0.71439000
C	-1.77889300	-3.60186700	-1.17821500
H	-2.48084300	-3.01094800	-1.78274200
H	-1.41589400	-4.44276800	-1.76894700
N	0.59265000	-2.66018900	-1.10571000
C	0.28561700	-1.34227500	0.72133200

N	1.14536700	-1.77335800	-0.20472200
C	2.50057600	-1.33678000	-0.41769000
C	2.71885000	-0.43189500	-1.45521900
C	3.52138300	-1.84643100	0.38412700
C	4.03001000	-0.02031500	-1.68357900
C	4.81433000	-1.40403400	0.11633900
C	5.08570200	-0.49292900	-0.90522300
H	4.22702700	0.69293500	-2.48022500
H	5.63144100	-1.77831800	0.72826800
C	1.57123200	0.09987600	-2.27121700
H	1.15699900	-0.67376800	-2.92457000
H	0.76775300	0.45670200	-1.61703300
H	1.89914300	0.93967800	-2.88700600
C	3.22866800	-2.79521500	1.51105600
H	2.77406100	-2.22063900	2.32539400
H	2.53605500	-3.58318200	1.19984200
H	4.14782500	-3.26436600	1.86701200
C	6.49390700	-0.00963000	-1.13878400
H	6.76571900	0.75426100	-0.40335300
H	7.21280500	-0.82741500	-1.04310800
H	6.60387300	0.42943100	-2.13280700

**Re\_IM1**

C	-2.21868500	-0.98722300	0.91637800
C	-1.12022400	-0.34488300	1.31292600
C	0.35649000	-0.66717400	1.08077700

H	-1.29261800	0.53515000	1.93667300
H	0.78152500	-0.59403900	2.12418800
O	0.71173700	-1.72530500	0.38694900
C	-3.58495500	-0.57731200	1.32753100
C	-3.79296800	-0.03037000	2.59971200
C	-4.68062100	-0.69458200	0.46480800
C	-5.05149500	0.41777200	2.98620000
C	-5.93839500	-0.24657700	0.85271600
H	-4.53383100	-1.14021300	-0.51388600
C	-6.12982700	0.31669100	2.11238300
H	-5.19167800	0.83196400	3.97973700
H	-6.77469600	-0.34364400	0.16655400
H	-2.96435700	0.01727200	3.29914300
H	-7.11405000	0.65869000	2.41581000
Br	-2.15111400	-2.47618500	-0.26142300
C	6.01114900	-2.37376900	-0.82387500
C	6.48757700	-1.28869800	-0.09162100
C	5.57060500	-0.46966200	0.55993300
C	3.71645800	-1.83407300	-0.24253700
C	4.64268000	-2.64458600	-0.89563200
H	6.71366400	-3.01881500	-1.34265700
H	7.55268200	-1.08409400	-0.03412600
H	2.64157100	-2.02638100	-0.25363300
H	4.29629600	-3.50146800	-1.46439200
C	4.20832400	-0.74522200	0.47139400

C	3.40094100	0.27951300	1.24166100
C	4.44430300	1.40279600	1.59998800
H	2.94520300	-0.14353700	2.14059600
C	5.82744300	0.73946800	1.42384500
H	4.28708000	1.76019400	2.61895300
H	6.52810100	1.45795700	0.98769800
H	6.23233400	0.44165500	2.39763600
N	2.32612300	0.85050000	0.43296200
O	4.31041400	2.57007100	0.80078900
C	2.59958700	1.76165400	-0.55025000
C	3.97545600	2.34132600	-0.55709500
H	4.68822500	1.66416900	-1.04731000
H	3.97965300	3.30410900	-1.06829000
N	1.53687800	2.05575700	-1.23404300
C	1.01398400	0.54690000	0.36076000
N	0.56028800	1.28148900	-0.65859700
C	-0.78282100	1.29928100	-1.17219200
C	-1.15831000	0.29712100	-2.06308300
C	-1.65257500	2.28623000	-0.70035700
C	-2.49574400	0.28533200	-2.46474000
C	-2.97095000	2.23239800	-1.13439200
C	-3.40878000	1.23284300	-2.00913200
H	-2.82997500	-0.50328500	-3.13434300
H	-3.68024500	2.97031300	-0.76739300
C	-0.17142700	-0.74076400	-2.52030800

H	0.68129800	-0.26492100	-3.01705700
H	0.19823700	-1.30884200	-1.65515700
H	-0.64376800	-1.42839400	-3.22415600
C	-1.17227300	3.33399300	0.26716500
H	-0.83719100	2.87884700	1.20625000
H	-0.32560300	3.89108400	-0.14487800
H	-1.97208200	4.03857800	0.50043000
C	-4.84952300	1.19443300	-2.44688100
H	-5.08967000	0.24559700	-2.93263900
H	-5.51567000	1.31894000	-1.58822100
H	-5.06420900	2.00008400	-3.15638700

#### Si\_IM1

C	0.20921900	1.97940000	0.98840100
C	-0.24446800	0.87930300	1.59201500
C	0.54719900	-0.38658400	2.00698800
H	-1.32072300	0.85163100	1.77548000
H	-0.12799200	-0.88146800	2.77365100
O	1.79747900	-0.29397100	2.28755500
C	-0.67954600	3.08023000	0.54243200
C	-0.45586900	3.74042400	-0.67147600
C	-1.81757900	3.41330100	1.28862300
C	-1.36107100	4.68730200	-1.13874400
C	-2.71817900	4.36409900	0.82166000
H	-1.98027700	2.93784700	2.25083100
C	-2.49725800	5.00151100	-0.39696900



H	-1.17442400	5.18494200	-2.08522100
H	-3.58915300	4.61651500	1.41808000
H	0.43791700	3.50384300	-1.23895900
H	-3.19808200	5.74679300	-0.75919700
Br	2.04142000	2.15776800	0.52417300
C	-5.02728100	0.42104800	-1.46645400
C	-5.33687700	-0.81450000	-0.90055600
C	-4.36934600	-1.47231600	-0.14878400
C	-2.78780900	0.32496300	-0.55252800
C	-3.76147300	0.98503400	-1.29903600
H	-5.77556700	0.94493600	-2.05251700
H	-6.31597600	-1.25993600	-1.05028100
H	-1.79935300	0.75902700	-0.43841900
H	-3.52568100	1.94571100	-1.74617200
C	-3.11413100	-0.89380400	0.03398800
C	-2.25181900	-1.78322100	0.91212000
C	-2.99603800	-3.16260100	0.89391800
H	-2.17783700	-1.40115200	1.93565200
C	-4.45738600	-2.80709900	0.54970200
H	-2.91086700	-3.65762600	1.86306000
H	-4.89822100	-3.59733200	-0.06439200
H	-5.05384400	-2.73092400	1.46626500
N	-0.90027400	-1.93779900	0.40066400
O	-2.43647900	-4.08989600	-0.02675800
C	-0.66239000	-2.71830100	-0.69690500

C	-1.80300900	-3.55454800	-1.17655400
H	-2.49443300	-2.95513700	-1.78410300
H	-1.43818300	-4.39393900	-1.76854300
N	0.58030100	-2.64574300	-1.05762800
C	0.25681600	-1.33627400	0.75013600
N	1.13787900	-1.77351900	-0.15089600
C	2.49800500	-1.34534300	-0.37833700
C	2.69948400	-0.43594300	-1.41346300
C	3.53189000	-1.89616000	0.37840300
C	4.01280400	-0.05234700	-1.68189300
C	4.82347000	-1.48170900	0.06989800
C	5.08162200	-0.56109000	-0.94839900
H	4.19836700	0.66761600	-2.47520200
H	5.65235200	-1.88440000	0.64725700
C	1.54125300	0.12551400	-2.19449800
H	1.10894000	-0.62881600	-2.85935900
H	0.75195600	0.48021400	-1.52204700
H	1.86712500	0.97507100	-2.79786200
C	3.24717600	-2.84949900	1.50172300
H	2.75355600	-2.27694200	2.29563800
H	2.58404900	-3.65856300	1.17788400
H	4.17173800	-3.29136000	1.87789100
C	6.49345600	-0.11204800	-1.22377900
H	6.82977500	0.59413100	-0.45791700
H	7.18520900	-0.95864600	-1.21493900

H	6.57140800	0.38400000	-2.19377700
<b>Re_TS2</b>			
C	2.20281000	-0.98873200	-0.96082800
C	1.20724500	-0.14799700	-1.27335200
C	-0.25218400	-0.32336000	-1.23085500
H	1.53239100	0.83352400	-1.62198800
H	-0.77994900	-0.70838600	-2.20317800
O	-0.88622600	-1.62950200	-1.24615000
C	3.62733200	-0.64350500	-1.14082700
C	4.01684900	0.16501100	-2.21773700
C	4.60568100	-1.04792300	-0.22406300
C	5.33446800	0.58736900	-2.35131100
C	5.92359800	-0.62856700	-0.36285500
H	4.31675000	-1.68695000	0.60404000
C	6.29454500	0.19716800	-1.42176100
H	5.61491900	1.20905200	-3.19590600
H	6.66488600	-0.94839200	0.36369000
H	3.28094300	0.44269700	-2.96587600
H	7.32504600	0.51966200	-1.53050100
Br	1.84459700	-2.62845900	-0.07533800
C	-5.58220400	-2.40992600	1.40486900
C	-6.20409100	-1.41599400	0.65402100
C	-5.42472800	-0.62097600	-0.18264000
C	-3.41950500	-1.83095000	0.47335000
C	-4.20419500	-2.62042500	1.30995900

H	-6.17721800	-3.03440700	2.06401900
H	-7.27769600	-1.26445500	0.71897900
H	-2.35205200	-1.99695900	0.33840600
H	-3.74138400	-3.41428200	1.88731200
C	-4.04969100	-0.82469400	-0.25268000
C	-3.39664300	0.16013600	-1.19987900
C	-4.56119900	1.14303500	-1.61204500
H	-2.96363400	-0.34677300	-2.06437400
C	-5.86654300	0.47915600	-1.11321000
H	-4.56510000	1.27962900	-2.69419800
H	-6.50260400	1.23169700	-0.63540800
H	-6.43402500	0.07126600	-1.95648500
N	-2.32264300	0.90689000	-0.55039500
O	-4.40699200	2.45757800	-1.10097400
C	-2.57616000	1.98929300	0.25130800
C	-3.97456900	2.50783600	0.24602500
H	-4.61984900	1.90753000	0.90323000
H	-3.99501700	3.54788600	0.57085500
N	-1.49943600	2.46485700	0.79163400
C	-0.98065500	0.69049700	-0.52733400
N	-0.50517500	1.63456500	0.32037000
C	0.75974700	1.53340200	0.99367300
C	0.97494400	0.40203100	1.78609100
C	1.74601000	2.48628900	0.74007400
C	2.25695300	0.21832100	2.29964300

C	3.00649500	2.26639000	1.28910500
C	3.28217800	1.13281200	2.05597500
H	2.46220300	-0.67551000	2.88417800
H	3.80054800	2.98199800	1.09029800
C	-0.11266300	-0.61737800	2.00692300
H	-1.06351500	-0.13409400	2.25790700
H	-0.26636200	-1.23540200	1.11272700
H	0.16021200	-1.28629400	2.82551500
C	1.45331000	3.67109300	-0.13989900
H	1.18503900	3.34828300	-1.15226600
H	0.60891700	4.24870400	0.24634900
H	2.32419800	4.32490800	-0.20953100
C	4.66056900	0.91375600	2.62229900
H	4.85606600	-0.15006500	2.77943100
H	5.42561100	1.30283600	1.94611800
H	4.77007600	1.42057000	3.58701200

**Re\_TS2<sub>d</sub>**

C	2.05922600	0.02590300	-1.40724500
C	1.13095400	0.53992900	-0.59283000
C	-0.35815400	0.40623500	-0.65297500
H	1.53192100	1.09208400	0.25636900
H	-0.80314900	1.61381100	-0.22525800
O	-1.01226900	0.29967200	-1.78909600
C	3.50834500	0.17597700	-1.16201800
C	3.99991800	1.35913200	-0.59328300

C	4.40243600	-0.87843400	-1.38486700
C	5.33613400	1.47315100	-0.22993300
C	5.74006700	-0.76103100	-1.02281600
H	4.03331400	-1.79352500	-1.83536300
C	6.21383000	0.41204700	-0.44042100
H	5.69677400	2.39978100	0.20622100
H	6.41627800	-1.59228800	-1.19778200
H	3.32582700	2.19778400	-0.44832100
H	7.25893300	0.50231100	-0.16138600
Br	1.55922300	-1.16341700	-2.80724500
C	-1.83638700	-4.94926300	-1.16593000
C	-2.91303300	-4.70613400	-0.31361200
C	-3.29925700	-3.39017300	-0.08000600
C	-1.55437600	-2.57477100	-1.56634500
C	-1.16285900	-3.89398300	-1.78472700
H	-1.51974800	-5.97178700	-1.34891500
H	-3.43520800	-5.53051200	0.16384300
H	-1.06378000	-1.72015600	-2.03116900
H	-0.31880000	-4.09490100	-2.43831900
C	-2.62043200	-2.34398600	-0.70464300
C	-3.16342000	-1.00233500	-0.26839400
C	-4.49515200	-1.37737200	0.44254700
H	-3.28358300	-0.30746600	-1.09852300
C	-4.38781200	-2.87393800	0.82661700
H	-5.29947000	-1.25439600	-0.28595000

H	-4.10506800	-3.00342400	1.87739000
H	-5.34405300	-3.38696500	0.69296000
N	-2.27510500	-0.36275000	0.72406900
O	-4.83013700	-0.49650400	1.50061100
C	-2.51580900	-0.40189200	2.07917400
C	-3.92460800	-0.52275100	2.58071300
H	-4.03578800	-1.42496300	3.19494100
H	-4.16283000	0.33776700	3.21014100
N	-1.44564900	-0.26504800	2.78771400
C	-0.92518500	-0.11182100	0.56892900
N	-0.43053800	-0.15096500	1.84872700
C	0.93488800	-0.28523900	2.23187500
C	1.67855600	-1.36322800	1.73379300
C	1.51371500	0.72400300	3.01111700
C	3.05079600	-1.36917600	1.98660300
C	2.88308300	0.66061800	3.25173200
C	3.67150900	-0.36652700	2.72868800
H	3.65351600	-2.17501600	1.57309000
H	3.35220100	1.44814100	3.83759700
C	1.05198400	-2.45230200	0.90417800
H	0.00916600	-2.63161500	1.18293500
H	1.06595600	-2.19675900	-0.16231000
H	1.60682200	-3.38514200	1.02973200
C	0.67524900	1.86419800	3.52251900
H	0.06650100	2.28601300	2.71520600

H	-0.02238100	1.52572500	4.29379000
H	1.30524900	2.65352300	3.93760600
C	5.15716800	-0.40312900	2.97506600
H	5.67478500	-0.89252200	2.14670000
H	5.56386800	0.60623800	3.07805100
H	5.38885700	-0.95186800	3.89437000
C	-1.37882300	4.63860700	-2.19721700
C	-0.65882300	3.36847000	-1.66742600
H	-1.80245500	4.46339400	-3.19046400
H	-0.68675200	5.48251900	-2.27699800
H	-0.61113100	2.54312400	-2.38320800
H	0.35886400	3.58428300	-1.32442100
C	-3.47554600	3.94799100	-1.29032900
H	-4.26050000	4.22435200	-0.57904500
H	-3.93315400	3.89100800	-2.28230500
C	-2.81403600	2.59457000	-0.90684100
H	-3.32277200	2.10356900	-0.06968100
H	-2.75075200	1.88246600	-1.73256800
C	-1.38301400	3.84311000	0.59156600
H	-1.97830200	3.44361100	1.41995400
H	-0.34746200	3.93987800	0.93408900
C	-1.94900800	5.19073100	0.05425300
H	-2.75255300	5.56212500	0.69739400
H	-1.16871600	5.95757800	0.02148800
N	-2.47546100	5.02078700	-1.30024700



N	-1.41420500	2.85560000	-0.49961800
<b>Re_TS2<sub>w</sub></b>			
C	-1.88461100	-1.09455800	0.64797700
C	-1.26074800	-0.28841000	1.50733700
C	0.22026500	-0.03675000	1.56107300
H	-1.88490900	0.19964000	2.25323900
H	1.40310400	-0.99263300	2.61603300
O	0.96706600	-1.21997300	1.72278400
C	-3.33484800	-1.38123700	0.63817900
C	-4.04511000	-1.37452600	1.84489100
C	-4.03208100	-1.61345200	-0.55316100
C	-5.42257100	-1.56662400	1.85566100
C	-5.40819400	-1.80886800	-0.53898900
H	-3.48486100	-1.63389700	-1.48951200
C	-6.11042900	-1.78287800	0.66462100
H	-5.95581300	-1.56556300	2.80074900
H	-5.93402800	-1.98423000	-1.47226900
H	-3.50866500	-1.24519000	2.77922500
H	-7.18367700	-1.94306200	0.67478800
Br	-0.86120300	-1.88273100	-0.75198200
C	5.18349100	-2.81200300	-1.29610300
C	5.88917200	-1.73578200	-0.76319800
C	5.19192600	-0.76353000	-0.05244400
C	3.10034100	-1.95110300	-0.40139000
C	3.80249200	-2.91794700	-1.11735100

H	5.71247800	-3.57571200	-1.85744200
H	6.96295400	-1.65469300	-0.90451800
H	2.02834500	-2.02215900	-0.24310700
H	3.27089000	-3.76590400	-1.53675600
C	3.81449200	-0.87717300	0.12076500
C	3.27446000	0.29113100	0.91481200
C	4.47075000	1.30988100	0.97486400
H	2.95750500	0.02124900	1.92640900
C	5.72343200	0.47492400	0.62449000
H	4.53830100	1.74338200	1.97400900
H	6.39876400	1.06614600	-0.00150100
H	6.27075100	0.21295700	1.53654500
N	2.11785400	0.90528800	0.25271900
O	4.32910600	2.43742000	0.11951700
C	2.28620700	1.78875600	-0.77798300
C	3.68681400	2.17712700	-1.11263600
H	4.18974400	1.37934900	-1.67712100
H	3.69414400	3.09663500	-1.69770400
N	1.15313400	2.24445300	-1.21287900
C	0.78783300	0.76729700	0.46058500
N	0.22469100	1.59888800	-0.43538200
C	-1.17570600	1.81136000	-0.64915300
C	-1.75925400	1.30389300	-1.81193000
C	-1.90205800	2.47011700	0.34643100
C	-3.14757800	1.38655600	-1.90914400

C	-3.28576000	2.52118400	0.20165800
C	-3.92639200	1.95529100	-0.90143800
H	-3.63487000	0.97431000	-2.78973600
H	-3.87824000	3.00423900	0.97472400
C	-0.93651700	0.72654900	-2.93302300
H	-0.56399700	1.52921100	-3.57667600
H	-0.07664100	0.16956500	-2.55968500
H	-1.54420000	0.04984600	-3.53754400
C	-1.21390400	3.08237300	1.53858200
H	-0.86813100	2.32396900	2.24997900
H	-0.33884500	3.66161500	1.22994300
H	-1.89678800	3.74879300	2.06805900
C	-5.42890100	1.92198200	-0.97798800
H	-5.80561200	1.04564300	-0.43838600
H	-5.87134700	2.81231900	-0.52472700
H	-5.77436800	1.85101400	-2.01185500
O	1.54134300	0.14660000	3.69334300
H	2.20276700	0.83523600	3.81396200
H	0.60537600	0.49924800	2.58794400
<b>Re_TS2<sub>2w</sub></b>			
C	1.90885100	1.02647100	0.69806500
C	1.28578500	0.09319900	1.41736800
C	-0.19184700	-0.19031000	1.43152700
H	1.90112800	-0.49800700	2.09438700
O	-0.94116600	0.95142000	1.79212400

C	3.35625100	1.32495100	0.74633500
C	4.05795000	1.13061100	1.94202800
C	4.05930500	1.75195300	-0.38615300
C	5.43235200	1.33543300	1.99696400
C	5.43255500	1.95946500	-0.32724900
H	3.51970200	1.91760600	-1.31259700
C	6.12594500	1.74999700	0.86321400
H	5.95822500	1.18637100	2.93446600
H	5.96324400	2.28815800	-1.21547400
H	3.51712100	0.84204900	2.83740000
H	7.19684000	1.91982900	0.90903600
Br	0.88946900	2.01287700	-0.57305500
C	-5.05934500	3.05285700	-1.13532300
C	-5.79166600	1.91780400	-0.79559900
C	-5.13009100	0.84394500	-0.20716800
C	-3.02096900	2.04795700	-0.29123500
C	-3.68674700	3.11730700	-0.88541300
H	-5.56052100	3.89581000	-1.60073300
H	-6.85910600	1.87052100	-0.99079600
H	-1.95592500	2.08401700	-0.08118200
H	-3.13362000	4.01185400	-1.15296300
C	-3.76090700	0.91606400	0.03556600
C	-3.25753200	-0.35792700	0.67700500
C	-4.46707000	-1.35875200	0.56708700
H	-2.99111200	-0.21793100	1.72710400

C	-5.69713500	-0.47200600	0.26266900
H	-4.57912600	-1.89962400	1.50767400
H	-6.33586600	-0.96602300	-0.47641200
H	-6.29677700	-0.33369900	1.16890100
N	-2.08653900	-0.89033400	-0.03040300
O	-4.29645000	-2.38073500	-0.40639500
C	-2.23793000	-1.62733500	-1.17442200
C	-3.63091000	-1.96849800	-1.58334000
H	-4.12575100	-1.10735000	-2.05482900
H	-3.62296000	-2.80766100	-2.27900600
N	-1.10029900	-2.02697500	-1.64731000
C	-0.75728900	-0.79091600	0.21767400
N	-0.18198500	-1.49689200	-0.77516500
C	1.22169700	-1.67374400	-1.00246200
C	1.81026700	-0.99358000	-2.07271700
C	1.94433500	-2.47149300	-0.11232100
C	3.19830000	-1.05118800	-2.17199900
C	3.33075500	-2.49066700	-0.25590900
C	3.97428200	-1.76215500	-1.25525300
H	3.68904900	-0.51220300	-2.97931700
H	3.92150100	-3.08435900	0.43750300
C	0.98777700	-0.26575500	-3.10336300
H	0.59469200	-0.97474700	-3.83839700
H	0.14045000	0.25459600	-2.65441500
H	1.60175400	0.47171000	-3.62510500

C	1.26261400	-3.26921800	0.96863200
H	1.04247600	-2.67876200	1.86739500
H	0.31518200	-3.68198200	0.60847800
H	1.90024100	-4.10287000	1.27053300
C	5.47693100	-1.71347800	-1.32302700
H	5.84694900	-0.87657300	-0.71981900
H	5.92342900	-2.63189700	-0.93473300
H	5.82551500	-1.56484100	-2.34789600
O	-2.25662100	-0.17701900	3.77019500
O	-0.45343100	-1.82694400	3.47396100
H	-0.34326700	-1.08212100	2.31660100
H	-1.40692900	0.72283900	2.63931300
H	-2.29327700	0.21702600	4.64625900
H	-1.51644400	-0.94070200	3.78681200
H	-0.86421800	-2.67203700	3.25274900

**Re\_IM2**

C	2.00048700	-1.29343100	-0.88122800
C	1.21272600	-0.24392700	-1.18591200
C	-0.22651400	-0.20451500	-1.29856500
H	1.74558500	0.70166600	-1.26844400
H	-0.66535100	-2.06006000	-1.63610800
O	-0.93373900	-1.19443000	-1.97755600
C	3.45939200	-1.22847400	-0.73075100
C	4.18554700	-0.28973100	-1.48114500
C	4.15098300	-2.01044500	0.20461200

C	5.54995000	-0.12082700	-1.27980800
C	5.51723800	-1.84326800	0.39725300
H	3.60739000	-2.74465600	0.78906800
C	6.22521500	-0.89698600	-0.34013300
H	6.09097000	0.60917600	-1.87368000
H	6.03130100	-2.45727800	1.12993700
H	3.67690200	0.29266600	-2.24216800
H	7.29309400	-0.77333800	-0.19232200
Br	1.14868500	-2.92691900	-0.34021900
C	-4.57348600	-2.52408000	2.10068100
C	-5.48079200	-1.71967800	1.41624800
C	-5.01961300	-0.91798600	0.37516000
C	-2.75909300	-1.73885700	0.70081900
C	-3.22267900	-2.53386500	1.74576800
H	-4.91868900	-3.14951400	2.91776500
H	-6.53092100	-1.71467300	1.69387500
H	-1.70813400	-1.74937000	0.42485600
H	-2.52795600	-3.16768200	2.28745000
C	-3.67146400	-0.92946000	0.02674600
C	-3.38468600	0.03085900	-1.10744700
C	-4.75049000	0.77599300	-1.35357900
H	-3.06318400	-0.49570100	-2.00466800
C	-5.80553800	0.01968200	-0.50599200
H	-4.99738400	0.73929900	-2.41517700
H	-6.41155900	0.73684600	0.05788200

H	-6.49222300	-0.53442200	-1.15427200
N	-2.33684100	0.98543400	-0.76127800
O	-4.71408800	2.16139900	-1.05940500
C	-2.61878000	2.09940300	-0.00498900
C	-4.05581000	2.46697300	0.15254800
H	-4.49896200	1.91807200	0.99790600
H	-4.15710300	3.53689500	0.33490200
N	-1.56999500	2.68954000	0.44724100
C	-0.95865500	0.80896700	-0.73356200
N	-0.51804600	1.89782300	0.00350900
C	0.78469600	2.06937100	0.55351300
C	1.26065300	1.15523400	1.50263200
C	1.58292600	3.10470400	0.05431200
C	2.59850600	1.25324700	1.88207100
C	2.90841200	3.17334800	0.47716800
C	3.44079900	2.23677100	1.36537600
H	2.99789400	0.52775200	2.58798200
H	3.54740600	3.96062100	0.08429900
C	0.39553600	0.05226400	2.05091200
H	-0.66725600	0.30062800	1.99287100
H	0.55991300	-0.87610500	1.49130300
H	0.64881500	-0.13910200	3.09648000
C	1.01778700	4.07300000	-0.94940900
H	0.66645200	3.54314900	-1.84110500
H	0.15559000	4.60364000	-0.53633000



H	1.77092600	4.80290200	-1.25191200
C	4.89842200	2.26068700	1.74433700
H	5.42529500	1.42851100	1.26480000
H	5.37645800	3.19142900	1.43099300
H	5.02749800	2.15563900	2.82507800

**TS3(RR)**

H	-0.53295600	-1.09023900	-2.30658500
C	1.73466300	0.08359200	-0.72713200
C	0.42752900	0.58331900	-0.48362600
C	-0.73217600	0.43831700	-1.18445800
H	0.30988500	1.13030000	0.44302700
O	-0.99449400	-0.23059300	-2.34147600
C	2.86161500	0.61264000	0.06522400
C	2.64433600	1.14370400	1.35311500
C	4.18905900	0.54989000	-0.38895100
C	3.69700500	1.62858600	2.11874700
C	5.24102600	1.02123200	0.38865700
H	4.39241400	0.12341000	-1.36471300
C	5.00700500	1.57707900	1.64263300
H	3.48865200	2.04223600	3.10224400
H	6.25379300	0.95080200	0.00398200
H	1.64968600	1.15068300	1.78836700
H	5.82830500	1.95432300	2.24349300
Br	2.09217600	-0.16293900	-2.59967700
C	-4.32916000	-2.14806900	2.90145600

C	-5.36065700	-2.05292000	1.96826700
C	-5.09152400	-1.49035100	0.72237100
C	-2.76720400	-1.14338500	1.34793500
C	-3.04236900	-1.69810900	2.59450800
H	-4.52789000	-2.58332100	3.87600800
H	-6.35858500	-2.40601900	2.21199200
H	-1.74896800	-0.84201800	1.11144100
H	-2.23362800	-1.80000500	3.31096700
C	-3.80642800	-1.04630100	0.42782200
C	-3.74036500	-0.45302700	-0.96145500
C	-5.23407100	-0.36463900	-1.42475100
H	-3.11446900	-1.04999500	-1.63003400
C	-6.01802400	-1.27695100	-0.45011900
H	-5.33009400	-0.69773400	-2.45822400
H	-6.96942500	-0.80583100	-0.18219500
H	-6.25433100	-2.22911300	-0.93668900
N	-3.16506300	0.89595500	-0.87122300
O	-5.73838800	0.96723400	-1.44846500
C	-3.89553600	1.93928800	-0.37774300
C	-5.38035000	1.76439700	-0.34215800
H	-5.67888100	1.30492300	0.61210400
H	-5.88093000	2.72802500	-0.44397900
N	-3.13900400	2.92909600	-0.00909900
C	-1.86551700	1.23619800	-0.76628300
N	-1.86868700	2.48566900	-0.26444300

C	-0.71806600	3.28241200	0.06589700
C	-0.47056000	3.50921000	1.42601200
C	0.16350500	3.67515300	-0.94493500
C	0.70830400	4.16812900	1.76249100
C	1.33400400	4.32132700	-0.54731200
C	1.62998200	4.56456700	0.79180200
H	0.92930600	4.34443100	2.81246600
H	2.04680600	4.61823500	-1.31297200
C	-1.40429800	2.98697100	2.48697500
H	-0.97561800	3.14463100	3.47788300
H	-2.37813500	3.48106100	2.44315900
H	-1.57898700	1.91086700	2.36089000
C	-0.04421400	3.34050100	-2.39788800
H	0.53555400	2.44573200	-2.65602900
H	-1.09120900	3.14481100	-2.63890300
H	0.30447700	4.16294000	-3.02648000
C	2.94572300	5.17927200	1.18622100
H	3.70584300	4.39504400	1.27788200
H	3.29151400	5.89499500	0.43681100
H	2.87342900	5.69224100	2.14809500
N	0.35482100	-2.42870600	-1.01274300
C	-0.85737100	-2.89233300	-0.62107000
O	-1.87316500	-2.81187600	-1.30321900
O	-0.84571100	-3.59989100	0.53999400
C	-2.02252600	-4.35829100	0.78764100

H	-1.90581200	-4.77044600	1.79032300
H	-2.91769100	-3.73610900	0.73661500
H	-2.11039500	-5.16678800	0.05561300
C	5.42090600	-3.12894400	-0.17268800
C	4.77272700	-3.26268100	-1.39973600
C	3.41342000	-2.96155500	-1.52289900
C	2.73714800	-2.50225100	-0.40389100
C	3.39701800	-2.39054400	0.82882400
C	4.73951000	-2.69810900	0.97007300
H	6.47608300	-3.37219000	-0.09648800
H	5.32729300	-3.61397000	-2.26335400
H	2.88630300	-3.06680000	-2.46440700
H	5.24376100	-2.60371500	1.92605900
C	1.34101100	-2.10170000	-0.20055000
C	1.24603400	-1.73968000	1.28087900
O	0.30295700	-1.26248300	1.89164300
N	2.49932100	-1.95516200	1.80935600
C	2.86349100	-1.63424700	3.16691400
H	3.15300300	-2.53676900	3.71461300
H	3.69062100	-0.91716300	3.17517900
H	1.98818800	-1.18588400	3.63889000

**TS3(RS)**

H	-1.01101500	-1.73673200	-1.87441600
C	1.52612100	-0.23488300	-0.63446000
C	0.21669400	0.29234600	-0.35283100

C	-1.00552800	0.02776000	-0.89072300
H	0.19637000	1.02773700	0.44238700
O	-1.42022400	-0.79895300	-1.86737600
C	2.67714200	0.61825500	-0.22811800
C	2.63599000	1.32512500	0.98825100
C	3.85751400	0.70527500	-0.98597000
C	3.71303700	2.09770100	1.40925800
C	4.93057900	1.48054800	-0.56128500
H	3.92436200	0.16250300	-1.92044400
C	4.86849100	2.18783800	0.63744500
H	3.64259300	2.62639200	2.35605600
H	5.82428900	1.52705100	-1.17637400
H	1.76630200	1.26236600	1.63724100
H	5.70649900	2.79513000	0.96545900
Br	1.63380800	-0.87503300	-2.45734500
C	-3.69335400	-2.90024700	2.76082400
C	-4.78226600	-2.05108900	2.56411200
C	-4.84835700	-1.30967400	1.39144100
C	-2.77286500	-2.29426400	0.60159800
C	-2.70040000	-3.02259400	1.78876100
H	-3.62531300	-3.48037400	3.67588200
H	-5.56492900	-1.97236800	3.31301000
H	-2.00548300	-2.41971800	-0.15090900
H	-1.85213500	-3.68269300	1.94088300
C	-3.84262200	-1.42546800	0.42719100

C	-4.13033400	-0.51641500	-0.74552700
C	-5.64136100	-0.21178500	-0.56022500
H	-3.87777900	-0.94170000	-1.71661700
C	-5.91190100	-0.33622100	0.95501500
H	-6.18438900	-1.00309800	-1.08150700
H	-5.79002200	0.62352300	1.47130400
H	-6.92982200	-0.68019900	1.15386500
N	-3.39939300	0.77479300	-0.64284900
O	-6.06083100	0.99000500	-1.17249000
C	-4.00583400	1.99478600	-0.50994700
C	-5.49310600	2.14866600	-0.61403800
H	-5.91891500	2.38768200	0.36885800
H	-5.71703300	2.97708300	-1.28889000
N	-3.13645100	2.94703800	-0.34417300
C	-2.06398000	0.98848200	-0.57706100
N	-1.93017200	2.31526100	-0.39642500
C	-0.71647700	3.09183700	-0.34511600
C	-0.35482200	3.63693000	0.89030700
C	0.07041600	3.20934600	-1.49409700
C	0.84766600	4.33508100	0.95631100
C	1.26871800	3.91111900	-1.36686600
C	1.67614200	4.47188400	-0.15802100
H	1.16099800	4.75283100	1.90996100
H	1.91522700	3.99295600	-2.23737200
C	-1.20468600	3.41109400	2.11273100

H	-0.74688700	3.87657300	2.98677800
H	-2.20889400	3.82326600	1.98220600
H	-1.31148600	2.33889100	2.31887900
C	-0.27429500	2.54355800	-2.79863600
H	0.25110300	1.58372700	-2.87263500
H	-1.34476300	2.34998900	-2.90227900
H	0.04212500	3.16927400	-3.63591600
C	2.99027100	5.20023100	-0.06246500
H	3.76963700	4.65744000	-0.60302700
H	2.91134000	6.20390500	-0.49303300
H	3.30958500	5.30123000	0.97737800
N	0.32876100	-2.63737000	0.00109600
C	0.30052500	-3.35598400	-1.13358100
O	-0.61241000	-3.22526500	-1.97189900
O	1.24720500	-4.28719500	-1.29043200
C	1.43629500	-4.75085500	-2.62203900
H	2.23537400	-5.48876200	-2.56868800
H	0.52015100	-5.19465300	-3.01580000
H	1.74139800	-3.91263000	-3.25516300
C	1.98506000	-0.43192500	4.31161700
C	0.66109400	-0.54090100	3.88034400
C	0.36904100	-1.09156100	2.62898100
C	1.42125000	-1.50653200	1.82983400
C	2.74379600	-1.40079300	2.27422700
C	3.05003300	-0.86616200	3.51914100

H	2.19428100	-0.00411500	5.28743100
H	-0.14367100	-0.20563200	4.52668500
H	-0.65027200	-1.18954200	2.26479200
H	4.07718200	-0.77246300	3.85555800
C	1.43105300	-2.04623400	0.45717100
C	2.91716600	-2.30756000	0.16079000
O	3.45849300	-2.69927900	-0.84962400
N	3.60638900	-1.87588300	1.29406300
C	5.03728800	-1.69162900	1.31121200
H	5.27950500	-0.63039500	1.44305500
H	5.49799100	-2.27608500	2.11403300
H	5.41624000	-2.03414200	0.34769800

**TS3(SR)**

H	1.33080700	-1.37770400	-1.63599200
C	-1.76370500	-0.51801400	-0.83473700
C	-0.71411000	0.44500200	-0.59764700
C	0.60961600	0.36875100	-0.89235900
H	-0.96545500	1.22107300	0.11909300
O	1.32647400	-0.34459600	-1.77660800
C	-3.17718000	-0.08413100	-0.62156100
C	-3.48713000	0.83258000	0.39892600
C	-4.24651700	-0.63752900	-1.34329800
C	-4.80333100	1.19418500	0.66566800
C	-5.56023500	-0.26915400	-1.07619400
H	-4.03940600	-1.36266100	-2.12045300



C	-5.85052800	0.65314600	-0.07421600
H	-5.00525600	1.90031400	1.46535900
H	-6.36229500	-0.71086100	-1.65947300
H	-2.70477900	1.25163800	1.02536500
H	-6.87649000	0.94203000	0.13012400
Br	-1.48043900	-1.50199900	-2.47638800
C	6.82328200	-1.11468400	-1.34109700
C	6.64506900	-1.47764100	-0.00819500
C	5.39714500	-1.28808300	0.57791400
C	4.51623700	-0.39224300	-1.50236700
C	5.76796400	-0.57941000	-2.08300900
H	7.79223800	-1.25311700	-1.81004000
H	7.46659900	-1.89890700	0.56362300
H	3.67641000	0.00028300	-2.06847700
H	5.92355000	-0.31355300	-3.12333500
C	4.35300300	-0.74542100	-0.16685000
C	3.10097600	-0.62480800	0.67158300
C	3.57638100	-0.93038600	2.13818100
H	2.30764000	-1.31573900	0.36647200
C	4.94961200	-1.62066200	1.97953200
H	2.84405500	-1.56830100	2.63461500
H	5.63422100	-1.27021500	2.75804600
H	4.84324200	-2.70358900	2.10283100
N	2.54519200	0.72908300	0.61057100
O	3.65493700	0.22410800	2.96926600

C	3.05427200	1.76129100	1.34706100
C	4.11818200	1.39881900	2.33007700
H	5.08356000	1.24362100	1.82933900
H	4.21920500	2.17717500	3.08608300
N	2.37308100	2.85551400	1.17342500
C	1.47364800	1.19958900	-0.05093500
N	1.39805900	2.49317700	0.27981200
C	0.47446400	3.45567700	-0.25076100
C	0.58011600	3.79755400	-1.60108700
C	-0.49471600	3.98479300	0.60452100
C	-0.34155300	4.71903700	-2.09391000
C	-1.38948600	4.90262300	0.06053500
C	-1.33078000	5.27598600	-1.28313100
H	-0.28489900	5.00648000	-3.14060500
H	-2.15740100	5.32884700	0.70096500
C	1.63213200	3.18668200	-2.48934300
H	2.61297100	3.18836200	-2.00334600
H	1.38666400	2.14843600	-2.73985300
H	1.71282600	3.74835800	-3.42123600
C	-0.56984600	3.56192700	2.04707100
H	-0.59572300	2.46998100	2.14258200
H	0.30198000	3.91459500	2.60565600
H	-1.47084100	3.96051300	2.51637500
C	-2.33972900	6.23717100	-1.85504600
H	-2.67172500	6.95668600	-1.10327600

H	-1.92539400	6.78897600	-2.70159200
H	-3.22282000	5.69675400	-2.21043800
N	0.09338400	-2.15463700	0.32682700
C	0.47989200	-3.03697300	-0.59689300
O	1.45281500	-2.81159500	-1.35572200
O	-0.15009900	-4.21629300	-0.63489800
C	-0.04219100	-4.93849700	-1.85490700
H	-0.50269000	-4.35535600	-2.65766300
H	1.00144600	-5.14450700	-2.09835300
H	-0.59722600	-5.86293700	-1.70276600
C	-2.52141900	-0.01255700	4.13818500
C	-1.20953900	0.26582900	3.75205500
C	-0.67378100	-0.32361500	2.60123700
C	-1.47371800	-1.16992300	1.85328800
C	-2.77533300	-1.46912700	2.27150700
C	-3.32467100	-0.89387500	3.41024300
H	-2.92467800	0.45275100	5.03217600
H	-0.60035400	0.93301700	4.35357900
H	0.35304000	-0.13629600	2.29275200
H	-4.34017100	-1.11635500	3.72017400
C	-1.20307000	-1.88785500	0.58897500
C	-2.47108900	-2.73395000	0.36514900
O	-2.77551300	-3.47498400	-0.54259400
N	-3.34571100	-2.37855200	1.39276800
C	-4.73648200	-2.76095000	1.39975500

H	-4.97752500	-3.34887200	2.29125800
H	-5.37095600	-1.86848100	1.36329200
H	-4.90706300	-3.36463600	0.50780100
<b>TS3(SS)</b>			
H	0.75010000	-1.93185600	-0.64832600
C	-1.67148100	-0.39083800	-0.95303300
C	-0.49325500	0.34394600	-0.59122000
C	0.80234200	-0.06485500	-0.57183500
H	-0.68514600	1.26828400	-0.06838000
O	1.30948100	-1.23514600	-1.05764500
C	-2.96005900	0.33859500	-1.09100900
C	-3.12092700	1.64636500	-0.59496400
C	-4.09132000	-0.28873300	-1.63814900
C	-4.34678000	2.29668100	-0.66688200
C	-5.31764200	0.36423600	-1.70150800
H	-4.00325400	-1.30020800	-2.02039600
C	-5.45592200	1.66490200	-1.22496700
H	-4.43022000	3.30725300	-0.27597700
H	-6.16962700	-0.15320900	-2.13189000
H	-2.29400700	2.17855300	-0.14044300
H	-6.41101600	2.17689600	-1.28614500
Br	-1.39091800	-1.68662700	-2.35890800
C	6.59033700	-1.62967700	-2.68837300
C	6.87027000	-1.85709000	-1.34241900
C	5.88007100	-1.60425100	-0.39787000

C	4.33982100	-0.91822100	-2.14640200
C	5.33500100	-1.16706000	-3.08853100
H	7.35574100	-1.81528100	-3.43525200
H	7.84670800	-2.22081400	-1.03596500
H	3.35107900	-0.58142300	-2.44490200
H	5.13259400	-1.00464800	-4.14214700
C	4.63346700	-1.13450000	-0.80488300
C	3.72379400	-0.93976800	0.38423500
C	4.66382600	-1.06632500	1.63309800
H	2.93292800	-1.68034100	0.45743500
C	5.92166100	-1.79104500	1.09962800
H	4.14225200	-1.62540800	2.40974100
H	6.81797700	-1.37707500	1.57136300
H	5.88161600	-2.85589100	1.35438400
N	3.07464500	0.37568800	0.35857200
O	4.99907600	0.17078400	2.25132600
C	3.75271100	1.47970900	0.79154600
C	5.11051300	1.26831900	1.37209700
H	5.85153000	1.09099800	0.57954400
H	5.40533400	2.14130600	1.95459500
N	3.02135700	2.55027000	0.73527000
C	1.83632400	0.78104600	-0.00368200
N	1.83315900	2.10967300	0.22265500
C	0.77134600	3.05671800	0.02422600
C	0.53188500	3.53472500	-1.26647100

C	0.01946900	3.43108200	1.13909500
C	-0.51974700	4.43170700	-1.42503200
C	-1.01664300	4.34263600	0.92700000
C	-1.30046700	4.84638000	-0.34205700
H	-0.73968100	4.81347600	-2.41908800
H	-1.62527800	4.64710600	1.77436100
C	1.35227500	3.05240200	-2.43144800
H	2.42298600	3.11511100	-2.21517500
H	1.11438600	2.00639300	-2.65695300
H	1.14311000	3.64655700	-3.32223600
C	0.29444800	2.82172900	2.48640700
H	0.13664000	1.73769500	2.44524800
H	1.32336400	3.01632800	2.80240300
H	-0.38914700	3.22568000	3.23439200
C	-2.43667400	5.81135300	-0.56094800
H	-2.98265900	5.99915100	0.36593300
H	-2.06766500	6.76989100	-0.93783900
H	-3.14019500	5.41623300	-1.29982000
N	-0.42088900	-2.05739200	0.93129500
C	0.27657700	-1.70131800	2.03678700
O	1.47840600	-1.44519300	2.08286200
O	-0.46035900	-1.75447400	3.17944900
C	0.15758100	-1.18961000	4.32291400
H	1.11001600	-1.68006800	4.53487500
H	0.33277700	-0.11984900	4.17255900

H	-0.54123100	-1.33836600	5.14602600
C	-5.24644000	-3.76576200	-0.01765600
C	-4.07639200	-4.34469800	-0.50810900
C	-2.83748200	-3.73790100	-0.28634400
C	-2.80244400	-2.54227600	0.41288100
C	-3.98460900	-1.98303300	0.92012300
C	-5.22031100	-2.57606000	0.71581900
H	-6.19996200	-4.25219900	-0.19839600
H	-4.12959700	-5.27648100	-1.06081300
H	-1.91553400	-4.17244800	-0.65626700
H	-6.13081000	-2.13435400	1.10698600
C	-1.69186800	-1.65930600	0.79581400
C	-2.34410500	-0.55028600	1.62071900
O	-1.81826900	0.44547700	2.09095300
N	-3.69335300	-0.81453900	1.63082900
C	-4.68276600	0.11225200	2.12442000
H	-5.35905000	0.40565800	1.31464200
H	-5.25717400	-0.33206500	2.94354200
H	-4.14718200	0.99084800	2.48614000

**IM3(RR)**

H	0.00428400	-1.54878400	-1.66400400
C	1.53214700	0.19855600	-0.65548300
C	0.16305500	0.72828900	-0.40441800
C	-0.95503600	0.44135900	-1.14017500
H	0.08043000	1.47489900	0.36686500

O	-1.15114500	-0.34223800	-2.11911600
C	2.59704900	0.99726400	0.10584600
C	2.30871400	1.48712500	1.38735400
C	3.88920600	1.18470400	-0.39352800
C	3.27252000	2.16457400	2.12947800
C	4.85440600	1.85420600	0.35201600
H	4.13746500	0.81054500	-1.37951100
C	4.55142000	2.35484400	1.61406600
H	3.01649000	2.53904200	3.11648300
H	5.84861100	1.98473500	-0.06312400
H	1.33560500	1.31247100	1.83430000
H	5.30440400	2.88250200	2.19136100
Br	1.86660100	0.39796900	-2.64232000
C	-3.57646300	-3.23238200	2.56169300
C	-4.74917600	-3.10124100	1.82133700
C	-4.73752500	-2.30782400	0.67614900
C	-2.38431000	-1.79973700	1.01723000
C	-2.40254800	-2.58589500	2.16513700
H	-3.57675500	-3.84499200	3.45807600
H	-5.65761600	-3.60874500	2.13311900
H	-1.46096500	-1.30608400	0.72362000
H	-1.48694700	-2.68445300	2.74019200
C	-3.56358400	-1.66919600	0.29052600
C	-3.76234600	-0.85804900	-0.96669800
C	-5.29343400	-0.99037500	-1.29604100



H	-3.11286400	-1.18292400	-1.78128100
C	-5.85938200	-2.02893800	-0.29248200
H	-5.40995000	-1.33014100	-2.32518100
H	-6.76069500	-1.63148400	0.18776200
H	-6.16052200	-2.93910400	-0.82043800
N	-3.41814500	0.55341800	-0.70983300
O	-5.99884800	0.24394200	-1.26669000
C	-4.30784600	1.44985100	-0.19373100
C	-5.73987600	1.03206200	-0.12746100
H	-5.92518600	0.47742200	0.80491100
H	-6.39429300	1.90359700	-0.15837100
N	-3.72747600	2.56582200	0.13879600
C	-2.20317800	1.12725300	-0.66560400
N	-2.41013300	2.34855100	-0.16115900
C	-1.39958800	3.31230600	0.18261300
C	-1.13922800	3.49398100	1.54651600
C	-0.63513000	3.89940000	-0.82641300
C	-0.07562900	4.32236500	1.88987500
C	0.41833400	4.72134700	-0.42436300
C	0.72079000	4.93324400	0.91857900
H	0.15672000	4.46949200	2.94197600
H	1.04046600	5.17856000	-1.18981600
C	-1.92332000	2.74879500	2.59483100
H	-1.48823200	2.91378000	3.58176100
H	-2.96914500	3.06537400	2.61546900

H	-1.90803700	1.67009900	2.39427700
C	-0.83080800	3.58182900	-2.28380800
H	-0.18327100	2.73971800	-2.55925400
H	-1.86236800	3.30851700	-2.51668000
H	-0.55365900	4.43977200	-2.89975400
C	1.92627100	5.74251400	1.31639900
H	2.80115300	5.08702400	1.39329500
H	2.14974900	6.51395600	0.57613900
H	1.78080200	6.22390600	2.28632200
N	0.62429500	-2.06337500	-1.01724500
C	0.17258200	-3.28723800	-0.64271400
O	-0.81308600	-3.83467400	-1.08870600
O	0.97163100	-3.84488300	0.30341300
C	0.49669700	-5.08973500	0.80053200
H	1.22069200	-5.40593700	1.55097800
H	-0.49413200	-4.96997600	1.24571600
H	0.43293300	-5.82467900	-0.00445300
C	5.71131800	-2.70260700	-0.38114000
C	5.08757100	-2.60878000	-1.62124500
C	3.75397500	-2.19261100	-1.71845200
C	3.07435000	-1.87253800	-0.55912000
C	3.70228000	-2.01190000	0.68149800
C	5.02278900	-2.41139700	0.80055700
H	6.74783100	-3.02003700	-0.32444500
H	5.63843800	-2.86119500	-2.52085300

H	3.25929500	-2.10349400	-2.67894400
H	5.50182600	-2.50308800	1.76966300
C	1.67094400	-1.34680200	-0.33757000
C	1.55396400	-1.43444200	1.22081200
O	0.56442100	-1.21965800	1.89239600
N	2.80114900	-1.71410600	1.71002600
C	3.12020600	-1.72077900	3.11495500
H	3.47664500	-2.70694000	3.42949700
H	3.88878600	-0.97072800	3.32981300
H	2.20628900	-1.47404400	3.65593100

**IM3(RS)**

H	0.14919200	-1.36163200	-1.89042700
C	1.40517000	0.33629800	-0.49324200
C	-0.00633700	0.55153800	-0.05590800
C	-1.13064200	0.29956000	-0.79412700
H	-0.12450400	1.17660600	0.81647400
O	-1.33418100	-0.31839300	-1.88592500
C	2.38531100	1.11175100	0.39734700
C	2.16683500	1.15703400	1.78026200
C	3.53696500	1.72386300	-0.10728200
C	3.05620600	1.81235000	2.62656200
C	4.43068700	2.37179100	0.74107700
H	3.73327900	1.69217500	-1.17243500
C	4.19254700	2.42720900	2.11097500
H	2.86016900	1.82995900	3.69417900

H	5.31601500	2.83966900	0.32131900
H	1.30728800	0.65373300	2.21105300
H	4.88807600	2.93806600	2.76994300
Br	1.53523100	1.06094000	-2.37555300
C	-2.70962400	-4.14867400	1.51303400
C	-3.84681700	-3.41744200	1.86045700
C	-4.21581400	-2.34042500	1.06521100
C	-2.32918100	-2.73564300	-0.42057000
C	-1.97173600	-3.82485300	0.37423700
H	-2.41452900	-4.99891700	2.12020100
H	-4.44455900	-3.70166600	2.72149000
H	-1.76261600	-2.49221500	-1.31252300
H	-1.11475100	-4.42218900	0.07929400
C	-3.43946600	-1.98706200	-0.04465400
C	-4.08506600	-0.82954800	-0.76933800
C	-5.55327400	-0.95730300	-0.29869100
H	-3.94618000	-0.84872100	-1.85066100
C	-5.44386900	-1.46699700	1.15636100
H	-6.01501100	-1.73730800	-0.90862400
H	-5.28579500	-0.63942700	1.86006200
H	-6.34220600	-2.00164100	1.47306800
N	-3.61689800	0.50597000	-0.30642600
O	-6.33459000	0.19695300	-0.52005100
C	-4.44537300	1.52509900	0.08700200
C	-5.92594600	1.33100200	0.20379700

H	-6.20333300	1.25957400	1.26446700
H	-6.43918700	2.19443900	-0.22351000
N	-3.77603500	2.61113100	0.35078200
C	-2.36270900	0.99206800	-0.27982200
N	-2.48097100	2.26496600	0.10935900
C	-1.38990400	3.20328700	0.18529300
C	-0.90352100	3.54751200	1.44645300
C	-0.75460000	3.54588500	-1.01011400
C	0.30093100	4.24489900	1.49331400
C	0.46285400	4.21398500	-0.90522900
C	1.00957200	4.55688000	0.33169200
H	0.72224800	4.50428800	2.46143500
H	1.01032900	4.44393300	-1.81539300
C	-1.61030200	3.09521700	2.69641500
H	-1.06880700	3.42658400	3.58385700
H	-2.63039400	3.48655000	2.74218200
H	-1.67878300	2.00093600	2.73088200
C	-1.32571500	3.15453600	-2.34703300
H	-1.18729500	2.08703800	-2.54836100
H	-2.39528000	3.38296000	-2.39610600
H	-0.82074500	3.70497500	-3.14267400
C	2.33984100	5.25773400	0.40932900
H	2.82788300	5.06456800	1.36744900
H	3.00599500	4.90857300	-0.38336800
H	2.21752300	6.34046800	0.29785000

N	0.94704400	-1.86893400	-1.48389600
C	0.97609600	-3.20933000	-1.66550300
O	0.11454700	-3.86438400	-2.22234300
O	2.09867100	-3.75536500	-1.14034100
C	2.19076400	-5.16677800	-1.27807700
H	3.14167700	-5.44611600	-0.82605300
H	1.36461500	-5.66027900	-0.76027800
H	2.16611600	-5.45246300	-2.33136700
C	2.35399400	-2.69316200	3.38589400
C	1.03554700	-2.52045300	2.97539100
C	0.75208200	-2.03952300	1.68998900
C	1.80421400	-1.74720800	0.84612900
C	3.12395000	-1.95221900	1.25871000
C	3.42544900	-2.41470600	2.53021300
H	2.56045200	-3.05978100	4.38679700
H	0.22102000	-2.75992900	3.65107900
H	-0.26952500	-1.88572400	1.35616800
H	4.45208700	-2.56025800	2.84941300
C	1.81533000	-1.18181000	-0.56286100
C	3.32631700	-1.29566200	-0.93212000
O	3.83973200	-1.07653000	-2.00193700
N	4.00193400	-1.64002800	0.22349400
C	5.43666600	-1.74726200	0.29312200
H	5.83600000	-1.05567800	1.04221000
H	5.74039900	-2.76876400	0.54591000

H	5.82652700	-1.48588400	-0.69122400
<b>IM3(SR)</b>			
H	-0.16490700	-2.40322700	0.08321000
C	-1.39447800	-0.26312400	-0.60116900
C	-0.27238400	0.35946100	0.16178200
C	0.95795200	-0.21350100	0.33966400
H	-0.39410900	1.40612900	0.37719000
O	1.33532500	-1.41210200	0.16041500
C	-2.44231300	0.80519700	-0.94662400
C	-2.80435200	1.73403900	0.03779300
C	-3.10568400	0.85302700	-2.17629500
C	-3.78911500	2.68704900	-0.20235100
C	-4.09285000	1.80582500	-2.41454800
H	-2.84672900	0.13969300	-2.94950000
C	-4.43868300	2.72892200	-1.43225300
H	-4.04660400	3.39429400	0.58080500
H	-4.59154800	1.82311900	-3.37860700
H	-2.33042700	1.70332400	1.01402900
H	-5.20796800	3.47177500	-1.62144600
Br	-0.57380700	-0.96034800	-2.31740000
C	5.88633000	-2.03175700	-2.69059300
C	6.55198500	-2.04201300	-1.46866000
C	5.84261200	-1.71616700	-0.31573800
C	3.80849500	-1.39804600	-1.61019500
C	4.52619400	-1.71990600	-2.75902900

H	6.42656500	-2.28062200	-3.59853100
H	7.60525800	-2.30182400	-1.41516100
H	2.73919100	-1.20496400	-1.64458600
H	4.01827500	-1.74126100	-3.71763700
C	4.49248200	-1.38479900	-0.39553700
C	3.93802800	-1.04037100	0.97058200
C	5.18650500	-1.06591800	1.93130300
H	3.15285800	-1.72875100	1.27709200
C	6.33228900	-1.70244400	1.10940000
H	4.95010100	-1.65318400	2.81882000
H	7.25469400	-1.12969700	1.25350400
H	6.53179700	-2.72013600	1.46039400
N	3.33883500	0.31047300	0.95426300
O	5.54735300	0.20691400	2.44929700
C	4.12038500	1.42385900	1.07800600
C	5.54372700	1.23262600	1.48058800
H	6.16272700	0.97658700	0.60836700
H	5.93042000	2.14236300	1.94037000
N	3.43694600	2.51349600	0.89837600
C	2.08736900	0.72756300	0.66401900
N	2.17513000	2.06770000	0.62580900
C	1.16206500	3.03137400	0.28164000
C	0.82738500	3.19874600	-1.06513900
C	0.53091600	3.71369600	1.32177800
C	-0.19362200	4.10065800	-1.35241900



C	-0.48137600	4.60811100	0.97829600
C	-0.85774400	4.80934800	-0.34960700
H	-0.49470100	4.23503600	-2.38864500
H	-0.99582900	5.14777700	1.76931000
C	1.45242400	2.36879700	-2.15197000
H	2.49098600	2.10962900	-1.92805700
H	0.88421500	1.43758000	-2.27569600
H	1.43056500	2.90700400	-3.10159300
C	0.89816900	3.43804500	2.75515700
H	0.68842500	2.39253900	3.00931300
H	1.96216800	3.61602800	2.93435900
H	0.32042500	4.07238400	3.42892300
C	-1.97533400	5.75211700	-0.70895000
H	-2.41167300	6.20985100	0.18147800
H	-1.61712300	6.55210700	-1.36354700
H	-2.76594200	5.21380700	-1.24049300
N	-1.16418400	-2.58923200	0.22666400
C	-1.50551000	-3.81472400	0.69658800
O	-0.74003700	-4.73398900	0.89020900
O	-2.84139300	-3.89516900	0.93008200
C	-3.28145700	-5.17166500	1.37303300
H	-3.09419900	-5.92953400	0.60917600
H	-2.76142300	-5.45973500	2.28889400
H	-4.35093900	-5.06965900	1.55462700
C	-4.36214700	-0.09368200	3.40862700

C	-2.98749400	-0.18533400	3.60721700
C	-2.15623000	-0.65917100	2.58379400
C	-2.72747100	-1.02801200	1.38313400
C	-4.11275600	-0.96170800	1.20651300
C	-4.95185700	-0.48682200	2.20290400
H	-4.99503400	0.28051400	4.20738600
H	-2.55945000	0.11018800	4.55930900
H	-1.08094300	-0.73247200	2.71646200
H	-6.02470800	-0.42373800	2.05419800
C	-2.09231900	-1.50140700	0.08937700
C	-3.34942200	-1.87724100	-0.75491700
O	-3.37029900	-2.40102300	-1.84201800
N	-4.45513700	-1.42539800	-0.06114400
C	-5.79177100	-1.47562500	-0.59526500
H	-6.44209000	-2.09047300	0.03566600
H	-6.20926000	-0.46607700	-0.67322900
H	-5.72218600	-1.92068900	-1.58841500
<b>IM3(SS)</b>			
H	-0.17068600	-1.84353800	0.88724500
C	1.64574700	-0.10223500	0.79565000
C	0.41273600	0.63559900	0.39654100
C	-0.87377200	0.26750300	0.68227000
H	0.56704700	1.51851700	-0.19923900
O	-1.34759200	-0.66820000	1.40491600
C	2.91653300	0.72216100	0.54626800

C	2.99361600	1.54495200	-0.58728000
C	4.05219700	0.61413600	1.35357200
C	4.15533700	2.25128800	-0.88514100
C	5.21573800	1.31597300	1.05161400
H	4.02276000	-0.02082100	2.23082800
C	5.27361300	2.14340400	-0.06477300
H	4.18061400	2.88260000	-1.76873900
H	6.08042100	1.21216300	1.69927400
H	2.15767100	1.61414700	-1.27589000
H	6.18029300	2.69394000	-0.29534600
Br	1.50730000	-0.52604100	2.75960000
C	-6.65311200	-1.38359500	2.49487800
C	-6.77687400	-1.85849900	1.19145700
C	-5.70686500	-1.70007500	0.31529800
C	-4.39674100	-0.61785600	2.05296400
C	-5.47216700	-0.77283200	2.92355700
H	-7.48085100	-1.49539800	3.18823100
H	-7.69291100	-2.34235700	0.86480800
H	-3.45221600	-0.18372900	2.36887800
H	-5.38976100	-0.42413400	3.94792300
C	-4.53946500	-1.07699400	0.74768900
C	-3.52082000	-1.00321000	-0.36607800
C	-4.29851200	-1.47132400	-1.64878200
H	-2.65321200	-1.64014000	-0.17945500
C	-5.58211000	-2.15195800	-1.11824500

H	-3.66980300	-2.15855200	-2.21585400
H	-6.43597900	-1.87477500	-1.74478600
H	-5.48029000	-3.24105400	-1.17102900
N	-3.03776100	0.37554500	-0.54520900
O	-4.60006000	-0.42510400	-2.56728300
C	-3.75174000	1.29404600	-1.26119100
C	-4.96967700	0.79890400	-1.96746100
H	-5.80717500	0.67844900	-1.26545100
H	-5.25632700	1.49263800	-2.75812000
N	-3.14593100	2.44408100	-1.30821000
C	-1.91974100	0.98669700	-0.11326200
N	-2.00753000	2.23856000	-0.57678000
C	-1.02389500	3.27468000	-0.43370500
C	-0.89411500	3.90909000	0.79916000
C	-0.17224000	3.51129500	-1.51822000
C	0.13844500	4.83813100	0.93039400
C	0.84080500	4.44636600	-1.33478300
C	1.01558600	5.11037800	-0.11709300
H	0.27112100	5.34166400	1.88435700
H	1.52927300	4.64346200	-2.15360000
C	-1.78052100	3.54518100	1.95937600
H	-2.82753300	3.46058900	1.65512300
H	-1.47080200	2.58090800	2.37985600
H	-1.70808200	4.29586000	2.74800100
C	-0.29436300	2.70203500	-2.78190900

H	-0.08301600	1.64263700	-2.58060200
H	-1.30113600	2.76857100	-3.20295800
H	0.41930300	3.05252600	-3.52963800
C	2.16750400	6.06393400	0.06092500
H	3.11067900	5.50930900	0.10235300
H	2.23203600	6.76628900	-0.77442600
H	2.07257000	6.63626900	0.98571500
N	0.52741900	-2.23976000	0.23906500
C	-0.01671100	-3.00936100	-0.73625900
O	-1.20110000	-3.27593300	-0.84599300
O	0.92801200	-3.48612600	-1.57847300
C	0.41694500	-4.10442700	-2.75239600
H	-0.23419400	-4.94079000	-2.49290900
H	-0.14579800	-3.37968400	-3.34650100
H	1.28739000	-4.45322600	-3.30684200
C	5.58149500	-3.31948700	0.49088100
C	4.69713000	-3.49908700	1.54993800
C	3.40630800	-2.96002600	1.49795600
C	3.03144700	-2.24539600	0.37656700
C	3.91805300	-2.10602300	-0.69503100
C	5.20339200	-2.62062100	-0.65988900
H	6.58172100	-3.73696700	0.55079600
H	5.00941600	-4.06167600	2.42316200
H	2.71146000	-3.07765700	2.32147500
H	5.88852300	-2.49283700	-1.49126800

C	1.75620800	-1.50131800	0.04995900
C	1.99269500	-1.12303700	-1.45134100
O	1.19466200	-0.60864300	-2.20834800
N	3.29839700	-1.41423000	-1.74246100
C	3.93210400	-1.05637500	-2.98557500
H	4.75038300	-0.35133700	-2.80287000
H	4.32324800	-1.94489100	-3.49148800
H	3.17365000	-0.58495500	-3.61141200

**TS4(RR)**

H	0.96770000	-0.95382500	-2.21704300
C	1.23813100	0.15481000	0.13209600
C	-0.11602300	0.39052000	0.18886000
C	-1.19469200	0.02010400	-0.67076600
H	-0.38385200	1.16348400	0.89775700
O	-1.27551300	-0.68568300	-1.66568100
C	2.01801000	0.93735400	1.14895500
C	1.74800700	0.69859700	2.50209100
C	2.97012100	1.89741500	0.79508800
C	2.42823700	1.40313700	3.49163700
C	3.64277800	2.59903800	1.79084500
H	3.13834500	2.09763900	-0.25805600
C	3.37781400	2.35688500	3.13715000
H	2.21362300	1.20571200	4.53732200
H	4.37790900	3.34662900	1.50836100
H	1.00741900	-0.05215100	2.76912900

H	3.90983200	2.90852100	3.90605100
Br	1.68772700	1.48602000	-2.35661400
C	-3.24942400	-3.86071200	2.48973800
C	-4.52022900	-3.34940000	2.23106300
C	-4.69013900	-2.50329000	1.14314500
C	-2.33765400	-2.70582700	0.56267700
C	-2.16998900	-3.53984500	1.66772600
H	-3.10039000	-4.51970900	3.33935700
H	-5.36176600	-3.60719900	2.86722800
H	-1.48474400	-2.48445000	-0.06985800
H	-1.17885700	-3.92485700	1.87620200
C	-3.60604300	-2.18525000	0.31777000
C	-4.05236600	-1.26004700	-0.79325400
C	-5.59875700	-1.40488800	-0.76043300
H	-3.60928100	-1.47837100	-1.76505200
C	-5.95194500	-1.82133300	0.68225600
H	-5.84943600	-2.22428900	-1.43728300
H	-6.16875500	-0.95179600	1.31416300
H	-6.83440400	-2.46477400	0.70898800
N	-3.72940300	0.16319100	-0.50314700
O	-6.29003100	-0.28361000	-1.27274600
C	-4.64711400	1.16520800	-0.35315500
C	-6.10986300	0.90311800	-0.53919600
H	-6.61777100	0.87326200	0.43301300
H	-6.54454500	1.71573500	-1.12363300

N	-4.06791700	2.30593500	-0.09475700
C	-2.51727100	0.72166400	-0.34241100
N	-2.74188700	2.00890100	-0.08757800
C	-1.71417600	3.01071500	0.05914000
C	-1.35594100	3.39647500	1.35370800
C	-1.01572600	3.37913100	-1.08941400
C	-0.20842400	4.17117500	1.48170300
C	0.13400200	4.14547000	-0.90227500
C	0.55605600	4.53281600	0.36770600
H	0.12197900	4.46315600	2.47523800
H	0.74099800	4.38388000	-1.77025000
C	-2.12758000	2.90541900	2.54982600
H	-1.74548000	3.36215900	3.46382000
H	-3.19250900	3.13850200	2.46312600
H	-2.03485200	1.81731200	2.65665400
C	-1.43960100	2.91046000	-2.45494800
H	-1.02878000	1.91603500	-2.65942400
H	-2.52937600	2.89499400	-2.55346400
H	-1.02921000	3.57243400	-3.21877300
C	1.82431800	5.32791600	0.52828800
H	2.59530000	4.95235900	-0.14990600
H	1.65522300	6.38345100	0.29149100
H	2.20439900	5.26228100	1.55009100
N	1.31607000	-1.64194400	-1.55397400
C	1.57794900	-2.87809500	-2.05974500



O	1.21129200	-3.28730000	-3.13732200
O	2.29611600	-3.62416100	-1.18193300
C	2.58319200	-4.94074000	-1.63584400
H	3.17045100	-5.40572000	-0.84484300
H	1.65979600	-5.49787700	-1.80713300
H	3.15190300	-4.90823100	-2.56704600
C	6.18832200	-1.14313800	0.04781000
C	5.69211600	-0.50853500	-1.08597200
C	4.31389600	-0.43711900	-1.32464200
C	3.45638000	-1.01058900	-0.40471800
C	3.97113700	-1.67307900	0.71218600
C	5.32904200	-1.74612200	0.97137500
H	7.25955000	-1.18179200	0.21857600
H	6.37919900	-0.05863200	-1.79452400
H	3.90975700	0.07978100	-2.18861800
H	5.71245800	-2.25677600	1.84844100
C	1.93560200	-1.10917200	-0.37592700
C	1.72048400	-2.07277500	0.85959700
O	0.65959400	-2.51714600	1.24165100
N	2.93171300	-2.24011700	1.46356300
C	3.11850400	-3.02602700	2.65717100
H	3.75199500	-3.89543200	2.45318300
H	3.58245100	-2.41847000	3.44041600
H	2.13470400	-3.36088200	2.98586100

**TS4(RS)**

H	0.01263500	-2.55984900	-1.25902100
C	1.55167200	-0.38055700	-0.60075200
C	0.74210200	0.59654200	0.09611500
C	-0.47190600	0.37410300	0.72998400
H	0.88927600	1.59856000	-0.29357600
O	-0.91648500	-0.56704400	1.42315000
C	2.94345300	0.13441100	-0.93285900
C	3.63231400	0.79305000	0.09275900
C	3.60506500	-0.10429800	-2.14234300
C	4.95426500	1.19340100	-0.08049100
C	4.92482200	0.30092700	-2.31297800
H	3.07942100	-0.60493800	-2.94689600
C	5.60620000	0.94750200	-1.28413800
H	5.47194800	1.69494200	0.73092400
H	5.42004300	0.11216400	-3.26021000
H	3.12656600	0.96838200	1.03753200
H	6.63600200	1.26162800	-1.42324000
Br	0.47091200	-0.47161500	-2.53861700
C	-6.26603900	-2.01682100	1.68948700
C	-6.21924600	-2.14344300	0.30242600
C	-5.11840400	-1.63606800	-0.38059100
C	-4.11790000	-0.89870700	1.70846800
C	-5.22388500	-1.40331500	2.38846600
H	-7.12168700	-2.40294800	2.23435200
H	-7.02936100	-2.62820500	-0.23421900

H	-3.28163800	-0.43773700	2.22735700
H	-5.27659000	-1.32315900	3.46943900
C	-4.09063200	-1.01758300	0.32473900
C	-3.01366000	-0.54522000	-0.61872500
C	-3.65311200	-0.66188700	-2.04117100
H	-2.12193700	-1.17051400	-0.54570000
C	-4.80128600	-1.67699000	-1.85633300
H	-2.89856200	-0.99842700	-2.75383000
H	-5.64237300	-1.41868600	-2.50563700
H	-4.45460700	-2.67833700	-2.13440000
N	-2.62738400	0.83947400	-0.35290600
O	-4.11851300	0.57520200	-2.58087200
C	-3.34808000	1.89687000	-0.82783300
C	-4.54331900	1.55478400	-1.65573500
H	-5.36248200	1.19547800	-1.01769300
H	-4.87639600	2.42490800	-2.22128100
N	-2.76013900	3.02825100	-0.56865000
C	-1.52908000	1.33194300	0.24009200
N	-1.62411400	2.65453200	0.10629800
C	-0.62377900	3.61458200	0.47192900
C	-0.46287000	3.93656700	1.81770900
C	0.17537100	4.13482000	-0.55278700
C	0.54410500	4.84773000	2.13621700
C	1.16470700	5.03936000	-0.17972700
C	1.35951800	5.40819200	1.15440800

H	0.69472000	5.12111700	3.17724500
H	1.80914300	5.45808100	-0.94864800
C	-1.32918500	3.30587100	2.87607700
H	-1.16804600	3.78959000	3.84061700
H	-2.38935100	3.39076500	2.62006100
H	-1.10074300	2.24024400	2.98926200
C	-0.01240000	3.69914200	-1.98335900
H	0.09127100	2.61148700	-2.09490100
H	-1.00695400	3.97149000	-2.34727700
H	0.73329400	4.17277000	-2.62346400
C	2.43484400	6.40044300	1.51374700
H	3.38706300	6.12854300	1.05063900
H	2.17184200	7.40186300	1.15946800
H	2.58208700	6.45321300	2.59415700
N	0.32712300	-2.57147400	-0.29600600
C	-0.62283700	-3.02616400	0.56716500
O	-1.76080600	-3.27457300	0.20847600
O	-0.16814200	-3.23476600	1.80659100
C	-1.19614300	-3.43083200	2.77059600
H	-0.68633000	-3.50486400	3.73083400
H	-1.87934900	-2.57808300	2.75878100
H	-1.75472000	-4.34448800	2.55876100
C	4.12353300	-1.86695600	3.30837200
C	2.83934600	-1.36270300	3.50212900
C	1.90856500	-1.35875600	2.45948300

C	2.27931100	-1.88579000	1.23323300
C	3.57418500	-2.38588900	1.05371400
C	4.51407200	-2.38772000	2.07446100
H	4.83558700	-1.85606900	4.12767300
H	2.55824600	-0.96662300	4.47208800
H	0.90288800	-0.97472700	2.59309700
H	5.51553500	-2.77242900	1.91482400
C	1.58369600	-1.88467600	-0.11872200
C	2.61785400	-2.64785000	-1.00267000
O	2.44424000	-3.01225600	-2.14278900
N	3.75235100	-2.83654100	-0.25525900
C	4.97920400	-3.36566800	-0.79719000
H	5.76636600	-2.60496000	-0.76270300
H	5.30091900	-4.25069400	-0.24012600
H	4.78049900	-3.63928800	-1.83371300

**TS4(SR)**

H	-1.65064200	1.49181900	-0.13198500
C	-1.28637700	-0.88739600	0.72755900
C	0.06611100	-0.68611500	0.68205800
C	0.83725000	0.00569500	-0.30839000
H	0.59466700	-0.91667400	1.60416000
O	0.67886000	0.10621900	-1.51496000
C	-1.79581100	-1.85461300	1.74700200
C	-1.43501600	-3.19606100	1.57309400
C	-2.64807900	-1.49738300	2.79884700

C	-1.92755100	-4.17567100	2.43096100
C	-3.12706900	-2.48262900	3.65587300
H	-2.89575300	-0.44967300	2.93762500
C	-2.77500700	-3.81915900	3.47494300
H	-1.65094000	-5.21407700	2.27866000
H	-3.77831700	-2.19928700	4.47647600
H	-0.79384600	-3.46650100	0.73826500
H	-3.15766700	-4.57940200	4.14892500
Br	-1.51042500	1.66850400	2.21561900
C	5.81132100	-2.46836900	-2.86187000
C	6.27106400	-2.72991800	-1.57368100
C	5.48874500	-2.34147900	-0.48940500
C	3.79890000	-1.44020300	-1.99086700
C	4.58721400	-1.82791800	-3.07075800
H	6.41367600	-2.76137000	-3.71551300
H	7.22643500	-3.22186000	-1.41851600
H	2.84664500	-0.93676300	-2.14758300
H	4.24858900	-1.62973500	-4.08190700
C	4.26840200	-1.70961400	-0.70846400
C	3.59602700	-1.36389300	0.60156000
C	4.68531400	-1.65844000	1.69924800
H	2.68346300	-1.94224700	0.77350200
C	5.76206900	-2.50903700	0.98401200
H	4.23673400	-2.19221000	2.53736900
H	6.75842800	-2.17110200	1.28518600

H	5.67563700	-3.55932800	1.28127600
N	3.22880400	0.05217000	0.63024000
O	5.22033200	-0.48456100	2.28716400
C	4.15522100	1.03122500	0.87048700
C	5.47994600	0.58083200	1.39410900
H	6.13814500	0.27426300	0.56847400
H	5.95880400	1.38139600	1.95744800
N	3.66115700	2.21171000	0.64305200
C	2.10944900	0.66673900	0.21964300
N	2.38643400	1.96570800	0.22258700
C	1.43821900	3.01524800	-0.06558800
C	1.06330600	3.24367300	-1.39312400
C	0.87125100	3.66922700	1.02994800
C	0.00149700	4.11869700	-1.59531900
C	-0.17820500	4.54338600	0.76332300
C	-0.64929200	4.74689600	-0.53234800
H	-0.35611900	4.28264900	-2.60830600
H	-0.68317100	5.01594200	1.60033000
C	1.75381800	2.61728900	-2.57735200
H	2.60893700	2.00148700	-2.28949100
H	1.05855100	1.98212900	-3.12909600
H	2.11404200	3.40378800	-3.24630400
C	1.34703400	3.39947400	2.43077200
H	1.24006900	2.33662200	2.66619000
H	2.39006000	3.70559700	2.56040200

H	0.72152300	3.93537000	3.14493900
C	-1.87523800	5.57605400	-0.79413900
H	-2.16869000	6.14710400	0.08868900
H	-1.71585900	6.26996300	-1.62429500
H	-2.69423600	4.90483900	-1.07027100
N	-1.96938400	0.85038700	-0.87204700
C	-2.76625200	1.46038000	-1.79950800
O	-2.70842100	2.63172000	-2.10854200
O	-3.62796800	0.58662000	-2.36905300
C	-4.48349000	1.15987800	-3.35030900
H	-5.10553000	1.93930000	-2.90587900
H	-3.89735200	1.59617400	-4.16164000
H	-5.09898500	0.34102900	-3.72012600
C	-2.78644600	-4.03268600	-2.64743300
C	-1.63312300	-3.30102800	-2.91166400
C	-1.37999200	-2.10107400	-2.23534300
C	-2.30659900	-1.64724700	-1.31641000
C	-3.47335400	-2.38484000	-1.07121800
C	-3.72992800	-3.58369500	-1.71945600
H	-2.96375800	-4.96633900	-3.17199400
H	-0.92219600	-3.66242900	-3.64702100
H	-0.48625700	-1.52042900	-2.42773700
H	-4.63296900	-4.14907500	-1.51569100
C	-2.28465200	-0.45731400	-0.35489100
C	-3.74460400	-0.51061300	0.21416400



O	-4.30819100	0.35076600	0.83712800
N	-4.28038500	-1.73054300	-0.14658100
C	-5.58515000	-2.17177500	0.27747000
H	-6.25445500	-2.29659500	-0.58032900
H	-5.50797300	-3.11996300	0.81887400
H	-5.98361100	-1.40333200	0.94036100

**TS4(SS)**

H	-0.86146900	-1.38191600	-1.88023000
C	-1.60568300	0.13171600	0.08961700
C	-0.31183600	0.58163700	0.31975500
C	0.94573900	0.01291700	-0.00173800
H	-0.26590100	1.58263700	0.73062900
O	1.29396600	-1.05237700	-0.50638100
C	-2.65738600	0.93297000	0.81349500
C	-2.51871400	1.01495300	2.20631400
C	-3.76456200	1.53415700	0.20850600
C	-3.47148000	1.67280900	2.97931700
C	-4.70768800	2.19888100	0.98493100
H	-3.85904700	1.49058700	-0.86951600
C	-4.57023600	2.26829600	2.36922400
H	-3.34967300	1.71987100	4.05703400
H	-5.55914800	2.66580800	0.49998100
H	-1.66321500	0.53889100	2.67920000
H	-5.31408100	2.78544000	2.96723300
Br	-1.91972900	0.81912700	-2.44358600

C	6.36359600	-2.38592500	-2.09555900
C	6.72865600	-2.40561500	-0.75183600
C	5.83018200	-1.92057800	0.19397400
C	4.21074900	-1.41737300	-1.54812800
C	5.11509100	-1.89966900	-2.49033700
H	7.05502400	-2.75785000	-2.84477000
H	7.69734800	-2.79083900	-0.44789100
H	3.22418500	-1.06584800	-1.83346600
H	4.84240400	-1.90619800	-3.54015200
C	4.59161100	-1.42815400	-0.20955900
C	3.79130900	-0.94416400	0.98119300
C	4.81353700	-0.97197500	2.17841900
H	2.91177000	-1.56296400	1.16907600
C	5.97962000	-1.86146600	1.69301700
H	4.33457200	-1.37404900	3.07161000
H	6.93149200	-1.43783400	2.02765300
H	5.89969900	-2.86277500	2.12949300
N	3.31854900	0.43063000	0.77046000
O	5.25998200	0.31762200	2.57731300
C	4.15440000	1.50101900	0.91665600
C	5.49270600	1.22694000	1.51931700
H	6.18542700	0.82068000	0.76953100
H	5.91135500	2.13909300	1.94397500
N	3.55813300	2.61654300	0.60713300
C	2.13301800	0.90677600	0.35780400

N	2.30130700	2.22622300	0.25035600
C	1.30883000	3.15332800	-0.22603500
C	0.85871300	3.01059500	-1.53964100
C	0.73117300	4.02335200	0.70373100
C	-0.25958900	3.75670600	-1.90459500
C	-0.37635800	4.75195300	0.28117600
C	-0.90128600	4.60446800	-1.00492500
H	-0.67607000	3.61225200	-2.89701300
H	-0.86832500	5.41541100	0.98748000
C	1.46351500	2.03219600	-2.50990300
H	2.50896500	1.80472600	-2.28339700
H	0.87097100	1.10985200	-2.50977800
H	1.41400800	2.43743100	-3.52254200
C	1.23736800	4.10082400	2.11979100
H	1.20845000	3.11596800	2.60066000
H	2.27179700	4.45219900	2.15732800
H	0.61691600	4.77862500	2.70763500
C	-2.17273000	5.29639800	-1.41581000
H	-2.93400200	4.54436700	-1.64622000
H	-2.55357600	5.94323600	-0.62311100
H	-2.02235800	5.90081900	-2.31458100
N	-1.20875800	-1.97832900	-1.13944600
C	-1.00541600	-3.30954100	-1.27824000
O	-0.35872000	-3.83295800	-2.15841800
O	-1.63818100	-4.00544200	-0.29862300

C	-1.43750200	-5.41070300	-0.36238600
H	-1.80646700	-5.80764800	-1.31019100
H	-0.37655300	-5.65214300	-0.26977100
H	-1.99938600	-5.82900200	0.47205900
C	-6.15426400	-2.20960100	0.11220200
C	-5.69393400	-1.72193000	-1.10710900
C	-4.34111100	-1.40906800	-1.28621200
C	-3.47806900	-1.59164000	-0.22340000
C	-3.94665300	-2.11007100	0.98498300
C	-5.28215700	-2.41881700	1.18504000
H	-7.20749200	-2.44170000	0.23513200
H	-6.38984600	-1.57970400	-1.92688700
H	-3.96423300	-1.00546800	-2.22049100
H	-5.63776300	-2.81323700	2.13112100
C	-1.98204300	-1.34960200	-0.11007300
C	-1.67976300	-1.94977900	1.32226200
O	-0.59835500	-2.03484900	1.85777000
N	-2.88717600	-2.26605900	1.88728900
C	-3.01646500	-2.79799100	3.21973600
H	-3.66256400	-2.15347900	3.82461300
H	-3.43837200	-3.80819500	3.19524500
H	-2.01758600	-2.83086700	3.65514200
<b>IM4(RR)</b>			
H	1.10473800	-0.76794800	-2.23139600
C	1.22204500	0.10481800	0.24122600

C	-0.11451900	0.37396400	0.22870400
C	-1.19174100	0.00296300	-0.65516500
H	-0.40310500	1.13980900	0.93814900
O	-1.26460100	-0.71713800	-1.63253600
C	1.98231900	0.86432100	1.28503900
C	1.78972600	0.52922200	2.62868400
C	2.83279000	1.91942800	0.94307300
C	2.45840400	1.23239400	3.62775600
C	3.49507200	2.61600100	1.94916700
H	2.93003700	2.18691800	-0.10609000
C	3.31420000	2.27595900	3.28855000
H	2.30749600	0.96467200	4.66896000
H	4.15532500	3.43551900	1.68128300
H	1.11772700	-0.28860400	2.88021800
H	3.83774800	2.82376300	4.06601900
Br	1.70795900	1.62929300	-2.38474000
C	-3.24854200	-3.90115200	2.46620700
C	-4.51609200	-3.37675800	2.21851000
C	-4.68570200	-2.52364400	1.13619100
C	-2.33994600	-2.74574300	0.53855800
C	-2.17215000	-3.58665400	1.63789400
H	-3.10027200	-4.56731500	3.31049000
H	-5.35629500	-3.63153400	2.85772800
H	-1.48820500	-2.53199400	-0.09781000
H	-1.18322200	-3.98395700	1.83430900

C	-3.60439200	-2.21096800	0.30508400
C	-4.05167000	-1.28161700	-0.80246300
C	-5.59802600	-1.42569000	-0.76363600
H	-3.61243900	-1.49720600	-1.77679700
C	-5.94459800	-1.83141300	0.68364300
H	-5.85096100	-2.25064600	-1.43315700
H	-6.14543200	-0.95584400	1.31273500
H	-6.83389300	-2.46481200	0.72088100
N	-3.72873500	0.14231900	-0.50906300
O	-6.28999400	-0.30772900	-1.28091600
C	-4.64969000	1.14062300	-0.35489100
C	-6.11185000	0.87977800	-0.54849800
H	-6.62466500	0.85210500	0.42139400
H	-6.54223800	1.69259500	-1.13622100
N	-4.07429500	2.28067600	-0.08363500
C	-2.51933800	0.70469800	-0.33762500
N	-2.74856500	1.98785800	-0.07204900
C	-1.72640800	2.99425400	0.08501000
C	-1.36390600	3.35997400	1.38495700
C	-1.04357000	3.39265100	-1.06187300
C	-0.22468900	4.14420000	1.51863500
C	0.09431800	4.17585000	-0.86946600
C	0.52262800	4.54134700	0.40418100
H	0.11400800	4.41717600	2.51490700
H	0.69067300	4.43852000	-1.73777600

C	-2.12353400	2.83981900	2.57640500
H	-1.74097800	3.28412800	3.49637000
H	-3.19134300	3.06416700	2.49987800
H	-2.01983600	1.75084800	2.66525500
C	-1.46246600	2.93697800	-2.43286300
H	-0.98413800	1.97945400	-2.66764600
H	-2.55022500	2.85338500	-2.51843300
H	-1.10681400	3.64396900	-3.18384000
C	1.78279600	5.34784600	0.56882400
H	2.55406000	4.98784700	-0.11800000
H	1.60225700	6.40402100	0.34369000
H	2.16679200	5.27602300	1.58884200
N	1.37092400	-1.52326200	-1.59905000
C	1.64913300	-2.71634600	-2.19423700
O	1.32393400	-3.03207100	-3.31524500
O	2.32738000	-3.54048900	-1.35441600
C	2.61175700	-4.82201100	-1.90076400
H	3.17273700	-5.35413900	-1.13309400
H	1.68676900	-5.35265700	-2.13678000
H	3.20415800	-4.72599400	-2.81271600
C	6.19689500	-1.13144200	0.11993900
C	5.70796700	-0.38245600	-0.94530100
C	4.33249800	-0.29454900	-1.19239800
C	3.47046000	-0.96742700	-0.34673600
C	3.97662800	-1.73713900	0.70218500

C	5.33227600	-1.83156700	0.96641300
H	7.26669300	-1.18328700	0.29651300
H	6.39955600	0.14345500	-1.59483700
H	3.93170000	0.30282100	-2.00645200
H	5.70921500	-2.43099600	1.78859900
C	1.95137900	-1.09204500	-0.35996100
C	1.72659900	-2.16450900	0.78138600
O	0.66229800	-2.64314900	1.10978800
N	2.93136600	-2.38192900	1.38112800
C	3.11364400	-3.30208800	2.47568500
H	3.72915200	-4.15351000	2.16671200
H	3.59635700	-2.79661800	3.31759600
H	2.12708700	-3.65562300	2.77552400

**IM4(RS)**

H	0.29660900	-1.09804600	-1.17105800
C	1.98585600	0.26884500	0.07928400
C	0.90851100	0.98454600	0.44098700
C	-0.38451600	0.47014100	0.91656400
H	0.94793900	2.06232400	0.29193400
O	-0.57511400	-0.39976900	1.74061200
C	3.16882200	1.01075900	-0.43700300
C	4.39975600	0.97367000	0.22285800
C	3.03177800	1.70838100	-1.64066800
C	5.48794700	1.65718700	-0.31138000
C	4.12717000	2.38554200	-2.16710700



H	2.07486500	1.66326500	-2.15845000
C	5.35193300	2.36378100	-1.50430300
H	6.44168500	1.64080400	0.20686100
H	4.02554900	2.91929700	-3.10657900
H	4.49651400	0.42288300	1.15535000
H	6.20412000	2.89175400	-1.92090400
Br	-0.58031000	0.58286000	-2.43957100
C	-5.55720400	-3.32297100	1.98776200
C	-5.42848100	-3.48823100	0.60891800
C	-4.49207700	-2.72249000	-0.07635400
C	-3.80989200	-1.64876000	1.99606900
C	-4.75555600	-2.41291800	2.67790600
H	-6.29187400	-3.90818900	2.53189900
H	-6.05585300	-4.19882500	0.07889700
H	-3.16691800	-0.94563600	2.51885800
H	-4.86905100	-2.30115800	3.75138300
C	-3.69968000	-1.81303200	0.62209100
C	-2.75922400	-1.11662100	-0.33279100
C	-3.37005800	-1.39009500	-1.74124700
H	-1.75404900	-1.54014100	-0.29162500
C	-4.13337100	-2.71257800	-1.54366200
H	-2.57020300	-1.44388200	-2.47965600
H	-4.99351400	-2.76396600	-2.21575400
H	-3.46196900	-3.54839800	-1.77082400
N	-2.67387500	0.31616400	-0.07795200

O	-4.24181000	-0.35584600	-2.20260900
C	-3.62929300	1.17128900	-0.53698300
C	-4.77723500	0.54529600	-1.26005000
H	-5.44890700	0.05309300	-0.54264900
H	-5.32994800	1.30724900	-1.81012100
N	-3.28710100	2.41550700	-0.34666900
C	-1.64618400	1.06657500	0.32504100
N	-2.04756900	2.32829100	0.22009000
C	-1.32468000	3.49071200	0.65416800
C	-1.11676000	3.65958000	2.02602200
C	-0.85301800	4.38364500	-0.31599600
C	-0.35977900	4.76095400	2.42457500
C	-0.10470200	5.46518100	0.14219600
C	0.16186800	5.66300400	1.49883700
H	-0.18087500	4.91808100	3.48509900
H	0.28530800	6.17187700	-0.58600900
C	-1.69587800	2.71137400	3.04708400
H	-1.74418300	3.19897000	4.02222100
H	-2.70825300	2.40045500	2.77237900
H	-1.09024700	1.80639900	3.16105800
C	-1.14727600	4.18414500	-1.77640900
H	-0.97380900	3.14547200	-2.07948700
H	-2.19577600	4.41609900	-1.98689000
H	-0.51948100	4.84085200	-2.38085300
C	1.00966600	6.82549300	1.94459100

H	0.75766700	7.73189200	1.38867700
H	0.88001000	7.02717600	3.00985200
H	2.06947300	6.61568000	1.76886300
N	0.73473700	-1.72148500	-0.46997000
C	0.40656200	-3.03241500	-0.66360600
O	-0.65854500	-3.40193500	-1.12137300
O	1.37806900	-3.87135200	-0.26149700
C	1.05601400	-5.25464700	-0.37870300
H	1.92455700	-5.79107500	0.00022300
H	0.16959000	-5.49147500	0.21294900
H	0.86637500	-5.51351000	-1.42202700
C	4.14798300	-2.93802600	3.29158200
C	2.88267000	-2.43501500	3.57181300
C	2.09893100	-1.87289400	2.55593200
C	2.59880400	-1.84557300	1.26901300
C	3.87308000	-2.36354900	0.99733700
C	4.66788900	-2.90827800	1.99346800
H	4.74732800	-3.36304800	4.09063500
H	2.49966400	-2.47310200	4.58583900
H	1.11381800	-1.47074900	2.76091800
H	5.65412800	-3.30310600	1.77291700
C	2.03430800	-1.26410900	-0.01971100
C	3.12787200	-1.68049800	-1.05687200
O	3.05789700	-1.54501500	-2.25269800
N	4.17092600	-2.24702400	-0.35983100

C	5.38275400	-2.70652000	-0.99046200
H	6.24791900	-2.15591000	-0.60638000
H	5.52928300	-3.77738600	-0.81675800
H	5.27770500	-2.52022700	-2.05969200

**IM4(SR)**

H	1.06684800	0.41686200	-1.35910500
C	1.05256800	-1.53080700	0.29792300
C	-0.11125600	-1.00652000	0.69830600
C	-0.42046700	0.42485000	0.90941600
H	-0.92366900	-1.69834300	0.91096600
O	0.19650800	1.15487800	1.64900900
C	1.15019100	-3.01245000	0.16014600
C	1.82631700	-3.79365600	1.09995300
C	0.57437500	-3.60250900	-0.96930200
C	1.91540800	-5.17066200	0.91343300
C	0.66877300	-4.97968400	-1.14462000
H	0.08184300	-2.95891000	-1.69686800
C	1.33711500	-5.76329400	-0.20670700
H	2.43381400	-5.78078700	1.64647900
H	0.22572800	-5.43957200	-2.02214200
H	2.27521600	-3.32236600	1.97070700
H	1.40968600	-6.83709800	-0.34907400
Br	-0.91278100	-0.36484100	-2.42154800
C	-5.77983100	-2.54634500	2.76370300
C	-6.06773900	-2.65783900	1.40480200

C	-5.19897100	-2.08490600	0.48136600
C	-3.76373600	-1.30266000	2.27725600
C	-4.63745500	-1.87314900	3.19980000
H	-6.45502400	-2.98224200	3.49294900
H	-6.96203800	-3.17712200	1.07315300
H	-2.87767400	-0.76783100	2.61353700
H	-4.43137000	-1.79136100	4.26173100
C	-4.05709000	-1.41993400	0.92339600
C	-3.26064900	-0.90248800	-0.24803500
C	-4.21527000	-1.05068700	-1.48794100
H	-2.35519200	-1.46709800	-0.48168300
C	-5.28265400	-2.07051400	-1.02532300
H	-3.61721700	-1.39057900	-2.33416300
H	-6.26543000	-1.77608600	-1.40486700
H	-5.05871000	-3.06225100	-1.43330300
N	-2.84433700	0.48697000	-0.05627700
O	-4.80700800	0.15972300	-1.93387600
C	-3.67152000	1.50665400	-0.41578200
C	-5.01587000	1.14540200	-0.94951300
H	-5.67031500	0.79275700	-0.13853700
H	-5.46944100	2.01184500	-1.43082900
N	-3.07377400	2.66051700	-0.32718600
C	-1.65875500	1.03826700	0.26216900
N	-1.82828500	2.35564100	0.12084300
C	-0.86016800	3.41711800	0.29101600

C	-0.73376500	3.99229400	1.55991100
C	-0.14317900	3.83340400	-0.82740800
C	0.20998900	4.99907100	1.70581500
C	0.81318400	4.83224900	-0.61452300
C	1.00752100	5.41416100	0.63253100
H	0.33666900	5.46528800	2.68012000
H	1.41997300	5.14498200	-1.45948500
C	-1.58623600	3.52815600	2.70881000
H	-2.64605000	3.51426400	2.43535100
H	-1.29887900	2.51654100	3.01222400
H	-1.46528200	4.19017300	3.56790900
C	-0.42432900	3.32001900	-2.21186700
H	0.44654800	3.47688000	-2.84738200
H	-0.66703500	2.25451200	-2.24388100
H	-1.27833600	3.86511300	-2.63058000
C	2.06284600	6.46965600	0.83941400
H	2.43299200	6.85119000	-0.11416800
H	1.67196500	7.31096300	1.41843200
H	2.91530400	6.05968700	1.39067800
N	1.86683000	0.53040400	-0.71908300
C	2.77129800	1.45354600	-1.18265700
O	2.48644700	2.42463000	-1.84730500
O	4.02959600	1.16655400	-0.78895100
C	5.00457700	2.12528300	-1.18343600
H	5.05136000	2.19727000	-2.27180300

H	4.76039500	3.10805500	-0.77416500
H	5.95012900	1.76621600	-0.77964800
C	5.15768400	-1.10393000	3.00998300
C	4.07855200	-0.26768000	3.27547600
C	3.08522500	-0.05914400	2.30948900
C	3.21366500	-0.68035600	1.08359100
C	4.30745300	-1.51690000	0.82475200
C	5.28930500	-1.74791400	1.77521700
H	5.91394100	-1.26373600	3.77210100
H	3.99974500	0.22134100	4.24049600
H	2.22860600	0.57608000	2.50614700
H	6.13033900	-2.40082600	1.56674800
C	2.28452900	-0.72241100	-0.12170600
C	3.12917000	-1.55575100	-1.13823900
O	2.86488200	-1.73756300	-2.30062500
N	4.23576700	-2.02970700	-0.46966600
C	5.21707000	-2.89303200	-1.07700800
H	6.20303300	-2.41678300	-1.08442600
H	5.27821900	-3.84291400	-0.53583500
H	4.89259600	-3.07670700	-2.10166600

**IM4(SS)**

H	0.18128900	-1.55803700	0.17090600
C	-1.72959100	-0.16704000	-1.15810500
C	-0.64829200	0.36033900	-1.76109900
C	0.81235300	0.42315200	-1.50325100

H	-0.83367100	0.79130200	-2.74362700
O	1.60416100	0.40511100	-2.42071900
C	-3.05003100	0.09883000	-1.81252800
C	-3.78655500	-0.89940300	-2.45605900
C	-3.55779300	1.40194000	-1.75072700
C	-5.01584100	-0.59268500	-3.03226300
C	-4.79103800	1.69945700	-2.32194400
H	-2.98302900	2.16518300	-1.23028100
C	-5.52200300	0.70255400	-2.96317200
H	-5.57731800	-1.37122000	-3.53842000
H	-5.18098300	2.71102600	-2.26544800
H	-3.39363200	-1.90911800	-2.51206400
H	-6.48286900	0.93473700	-3.41167400
Br	1.16923600	-2.86773800	-1.19281700
C	7.29066700	0.55118500	-1.64674400
C	7.13602400	-0.55330500	-0.80899300
C	5.85828800	-0.90733000	-0.39198200
C	4.89882700	0.92639600	-1.66777100
C	6.18323200	1.28339800	-2.07607400
H	8.28407400	0.84267700	-1.97261500
H	8.00167500	-1.12380200	-0.48528300
H	4.02310000	1.46607800	-2.01854200
H	6.32294800	2.13160200	-2.73837400
C	4.75832500	-0.16111100	-0.81659300
C	3.49342900	-0.76020800	-0.25112800



C	3.98303600	-1.66566800	0.91103800
H	2.94646400	-1.36828300	-0.98119000
C	5.40796700	-2.05960200	0.47822900
H	3.29666200	-2.50797200	1.01997900
H	6.03854400	-2.23344800	1.35376100
H	5.37561900	-2.98576600	-0.10725300
N	2.58484200	0.25519900	0.27597500
O	4.00334000	-1.01324900	2.18085900
C	2.91609300	0.92377000	1.41734800
C	4.07712400	0.39284200	2.19647400
H	5.01864100	0.77088900	1.77317200
H	3.99470600	0.71496000	3.23517200
N	2.08152000	1.89106000	1.65936500
C	1.43918400	0.78120200	-0.16986100
N	1.16525200	1.79972900	0.64997100
C	0.14891400	2.80747600	0.51701800
C	0.09517800	3.56767500	-0.66011300
C	-0.69477800	3.04099100	1.60781200
C	-0.92140600	4.51600500	-0.76154800
C	-1.67710000	4.01555000	1.45507600
C	-1.82540000	4.74089600	0.27525400
H	-0.98565400	5.11305500	-1.66812800
H	-2.36224000	4.19164100	2.28037100
C	1.10886100	3.46714900	-1.77424300
H	1.29773200	4.46490800	-2.17592300

H	2.06381300	3.06014200	-1.43260500
H	0.75847900	2.84346900	-2.60163100
C	-0.56338400	2.30378100	2.91224900
H	-0.12452000	1.31488200	2.77988300
H	0.08947800	2.85944000	3.59286300
H	-1.54871100	2.18825500	3.36530400
C	-2.94246800	5.73982500	0.12282600
H	-3.15187000	6.24609500	1.06805500
H	-2.70200600	6.49582100	-0.62801700
H	-3.86331000	5.23775900	-0.19267600
N	-0.48400200	-0.98721900	0.74735400
C	-0.21144300	-1.09198500	2.08324300
O	0.91736400	-1.09453300	2.53350100
O	-1.31828200	-1.15059300	2.84886300
C	-1.07234300	-1.16308100	4.25252000
H	-2.05324100	-1.21529000	4.72260100
H	-0.46688700	-2.02965000	4.52290000
H	-0.54842700	-0.25447700	4.55901500
C	-4.44944900	-4.27037800	0.06709400
C	-3.19919500	-4.46082100	-0.51269000
C	-2.24709800	-3.43362200	-0.52266900
C	-2.57920700	-2.22487300	0.06260800
C	-3.83369900	-2.05362400	0.65515800
C	-4.78970400	-3.05503400	0.66814400
H	-5.17515600	-5.07767600	0.05889200

H	-2.95500000	-5.41547600	-0.96582600
H	-1.26808900	-3.57370200	-0.97240100
H	-5.76206600	-2.90275600	1.12469800
C	-1.80588900	-0.91371400	0.17420200
C	-2.79880200	-0.04285800	1.01638800
O	-2.62178400	1.10238900	1.36766400
N	-3.94625300	-0.76334400	1.18390700
C	-5.13024400	-0.22769100	1.80864000
H	-5.97278000	-0.26177700	1.11078700
H	-5.38475000	-0.79533700	2.70924400
H	-4.91667500	0.80743000	2.07503600

**TS5(RR)**

H	2.75849600	1.72394600	-1.73957800
C	0.70735500	-0.75309000	0.92778000
C	-0.54729400	-0.28743800	0.73437900
C	-1.28250300	-0.05272900	-0.50560600
H	-1.13131000	-0.04723800	1.62232600
O	-1.20025900	-0.49532400	-1.62655100
C	1.16048300	-0.92227300	2.32892800
C	1.77087600	-2.11072400	2.74983100
C	0.96432300	0.10788600	3.25546400
C	2.15302300	-2.26905000	4.07568900
C	1.36461400	-0.04878300	4.57876900
H	0.53135000	1.04635100	2.91773200
C	1.95483100	-1.23861600	4.99308300

H	2.61407400	-3.19860600	4.39353400
H	1.22219900	0.76338400	5.28488000
H	1.92671800	-2.91690400	2.03921300
H	2.26755500	-1.36181800	6.02503700
Br	3.88068200	2.57754000	-1.43591200
C	-4.16177800	-3.91080000	1.35687800
C	-5.26706100	-3.06631400	1.24886500
C	-5.21447700	-2.01047200	0.34846100
C	-2.97479200	-2.66421400	-0.35202500
C	-3.03173200	-3.71326400	0.56458700
H	-4.18857500	-4.73883600	2.05824600
H	-6.15369600	-3.23682800	1.85230000
H	-2.08712600	-2.53981900	-0.96513800
H	-2.17916700	-4.37927500	0.64519100
C	-4.07127000	-1.81001800	-0.43376100
C	-4.27287000	-0.61134100	-1.33042800
C	-5.81340600	-0.45921700	-1.34069900
H	-3.82646700	-0.70053700	-2.32193700
C	-6.27027800	-0.97682700	0.04002800
H	-6.19308500	-1.13144200	-2.11338700
H	-6.25712600	-0.17803500	0.79266900
H	-7.28589600	-1.37751700	0.00862500
N	-3.72979600	0.63741500	-0.72988400
O	-6.25437400	0.82721800	-1.72238100
C	-4.43713500	1.78958000	-0.51445300

C	-5.89626200	1.86830600	-0.84596900
H	-6.48637400	1.84944700	0.07977900
H	-6.10030100	2.80964200	-1.35939400
N	-3.68110200	2.72233900	-0.00215800
C	-2.47631800	0.88108400	-0.32071900
N	-2.46083600	2.13094200	0.11387900
C	-1.26989800	2.83989300	0.50884600
C	-1.10376900	3.13556400	1.86651200
C	-0.31575100	3.11334500	-0.47326500
C	0.09933500	3.72110600	2.24303800
C	0.86298400	3.71934600	-0.03733800
C	1.09880700	4.00196500	1.30394500
H	0.27182200	3.94247900	3.29383500
H	1.63717800	3.92689200	-0.76874700
C	-2.16957900	2.78876000	2.87212300
H	-1.84339000	3.05165600	3.87968900
H	-3.10327000	3.31831100	2.66163500
H	-2.39188900	1.71489800	2.86151000
C	-0.47480200	2.76462100	-1.92824000
H	0.13733600	1.88585800	-2.17611800
H	-1.51392400	2.56842200	-2.20689900
H	-0.11336300	3.59194100	-2.54322000
C	2.41846000	4.59844300	1.71454200
H	2.63438500	4.40364500	2.76746200
H	3.21880000	4.17427600	1.10198900

H	2.41954800	5.68280900	1.56417500
N	1.49250700	0.00144200	-1.18709300
C	1.80215200	-0.20029400	-2.45609300
O	1.84116500	0.69997800	-3.30979300
O	2.12774000	-1.49163500	-2.82238000
C	2.45598300	-1.65188400	-4.19027700
H	2.68677600	-2.71043200	-4.32575500
H	1.61821300	-1.36414400	-4.83028500
H	3.31913200	-1.03803500	-4.45873200
C	5.70653900	-2.13940400	0.44385900
C	5.35577700	-0.81982000	0.71476600
C	4.03577200	-0.38794100	0.54754300
C	3.08904400	-1.29843300	0.12284600
C	3.45524900	-2.61539800	-0.15698200
C	4.75759000	-3.06437200	-0.00407300
H	6.73612700	-2.45907500	0.57127600
H	6.11315900	-0.11870000	1.04901500
H	3.75766200	0.64805600	0.71398000
H	5.03327300	-4.08982900	-0.22893300
C	1.63128200	-1.07764900	-0.24108500
C	1.21597800	-2.54375300	-0.67811900
O	0.11136700	-2.94625400	-0.97402000
N	2.33148600	-3.34613400	-0.56254400
C	2.37711400	-4.69277600	-1.07379400
H	3.02979600	-4.74741700	-1.95225000

H	2.74641800	-5.38632800	-0.31170300
H	1.36057000	-4.96699000	-1.35651700
<b>TS5(RS)</b>			
H	-0.21329200	-0.98294700	-1.58635600
C	2.02636100	0.25071500	0.63606000
C	0.95227500	0.81968500	1.17527700
C	-0.39293200	0.13742200	1.09388400
H	1.00800400	1.77532300	1.68734100
O	-0.99609000	-0.26820900	2.10078200
C	3.37809900	0.85612600	0.66468700
C	3.92617200	1.27999200	1.87896900
C	4.09338500	1.07188300	-0.51991300
C	5.16410500	1.91394100	1.91205200
C	5.32991800	1.70921300	-0.48324500
H	3.66930800	0.75981700	-1.47072800
C	5.86860100	2.13082900	0.73037700
H	5.58157700	2.23291800	2.86186500
H	5.87265800	1.87969200	-1.40788300
H	3.37640500	1.09264400	2.79679700
H	6.83557900	2.62355400	0.75566900
Br	-1.12335000	-0.96361900	-2.78513500
C	-6.62151800	0.54057100	2.82322100
C	-6.79141000	-0.35868900	1.77113400
C	-5.68772500	-0.70313800	0.99721900
C	-4.25561400	0.72782400	2.34482900

C	-5.36520300	1.07649000	3.11255500
H	-7.47670600	0.82382700	3.42878200
H	-7.77051400	-0.77852400	1.55920300
H	-3.26037900	1.10273300	2.56935100
H	-5.25279700	1.76392500	3.94468100
C	-4.44236100	-0.14857000	1.28435900
C	-3.40133800	-0.67306300	0.32655800
C	-4.22669400	-1.32884300	-0.82438400
H	-2.73451800	-1.39940900	0.78800900
C	-5.58210700	-1.66459200	-0.16495400
H	-3.69134600	-2.19935900	-1.20681000
H	-6.38921500	-1.57168200	-0.89678900
H	-5.57907600	-2.69877700	0.19800900
N	-2.57556300	0.40623100	-0.20746900
O	-4.41061400	-0.48843500	-1.96082500
C	-3.08222100	1.25362300	-1.14928000
C	-4.41340700	0.90286600	-1.72854400
H	-5.22280800	1.21180200	-1.05189200
H	-4.53757200	1.39855200	-2.69174500
N	-2.23177000	2.18841200	-1.45548900
C	-1.32162200	0.79298200	0.04832100
N	-1.13812700	1.89105300	-0.69377100
C	-0.08216300	2.86380700	-0.56822700
C	-0.16400200	3.74074100	0.51498000
C	0.96957500	2.86425300	-1.48324800



C	0.89656500	4.62360700	0.70559300
C	2.00539400	3.76590500	-1.24622200
C	1.99677300	4.63297100	-0.15283800
H	0.87001300	5.30494200	1.55219500
H	2.85805500	3.76881900	-1.92141100
C	-1.31202700	3.66334000	1.48782600
H	-1.31813400	4.53440400	2.14496500
H	-2.27492100	3.61486500	0.96968200
H	-1.23198200	2.76769700	2.11871500
C	1.01354600	1.88577900	-2.61911100
H	1.32263100	0.89238500	-2.27014000
H	0.03504700	1.76067200	-3.08796400
H	1.73233600	2.21208500	-3.37375200
C	3.17598000	5.53467900	0.10114100
H	3.44676100	6.09231800	-0.79955300
H	2.96780200	6.25091900	0.89855000
H	4.04653200	4.93928800	0.39524600
N	0.33591400	-1.25037900	-0.01660600
C	-0.22925700	-2.50239400	-0.00296200
O	-1.40783000	-2.73958500	0.17614300
O	0.65086600	-3.47485900	-0.32865100
C	0.09542600	-4.78377500	-0.40631600
H	0.92942100	-5.44353800	-0.64175000
H	-0.35845600	-5.06334600	0.54650400
H	-0.66336000	-4.82621400	-1.19064600

C	3.98955500	-3.79095700	2.66034900
C	2.91050100	-3.14345900	3.25558400
C	2.11441400	-2.26123900	2.51319300
C	2.42205000	-2.07359600	1.18284800
C	3.50137200	-2.72942300	0.59053600
C	4.30677700	-3.59556300	1.31063900
H	4.60129200	-4.46433600	3.25230400
H	2.68755600	-3.32163200	4.30202100
H	1.26310600	-1.74156800	2.95014800
H	5.14678700	-4.10518500	0.85026800
C	1.77550200	-1.16762300	0.14932900
C	2.55985800	-1.54027400	-1.13027200
O	2.33474500	-1.14122900	-2.25481000
N	3.57807900	-2.38534400	-0.76650300
C	4.51093200	-2.95133300	-1.70975400
H	5.53844100	-2.69356800	-1.43575400
H	4.40985900	-4.04093200	-1.74434300
H	4.27559500	-2.53304800	-2.68880400

**TS5(SS)**

H	0.62375600	-2.19516300	-0.11291500
C	-1.94138200	0.07399200	-1.04073200
C	-0.86934900	0.74639300	-1.44077700
C	0.49741600	0.27925900	-0.99975500
H	-0.92221500	1.49805500	-2.22234900
O	1.20151800	-0.35002000	-1.80837400

C	-3.33763300	0.32146400	-1.48256700
C	-4.01508400	-0.57659500	-2.31385000
C	-4.00483600	1.45591200	-1.00838500
C	-5.33640300	-0.33137400	-2.67643100
C	-5.32760400	1.69325900	-1.36995500
H	-3.47787700	2.12686000	-0.33603500
C	-5.99484000	0.80185200	-2.20604800
H	-5.85267700	-1.03031000	-3.32682100
H	-5.84205400	2.57051700	-0.98881300
H	-3.50473100	-1.46501600	-2.67330000
H	-7.02696700	0.98745500	-2.48675600
Br	1.54952700	-3.37834500	-0.11075900
C	6.69318200	0.32163600	-2.68282700
C	6.84418600	-0.29855900	-1.44349100
C	5.72754100	-0.44955000	-0.62815400
C	4.32023200	0.61623900	-2.29918800
C	5.44203600	0.77137400	-3.11016300
H	7.55737800	0.45120800	-3.32688600
H	7.81794000	-0.65483500	-1.12024200
H	3.33105000	0.92879600	-2.62132600
H	5.34293600	1.23804600	-4.08491100
C	4.48698200	0.01554100	-1.05779500
C	3.43020200	-0.26660300	-0.01778800
C	4.23215200	-0.66353400	1.26386000
H	2.77898300	-1.08215400	-0.32870600

C	5.60753500	-1.11325300	0.72278400
H	3.69625000	-1.45380200	1.79000300
H	6.39782300	-0.84006100	1.42769800
H	5.62354200	-2.20331200	0.60978600
N	2.59686400	0.90554100	0.24060200
O	4.37038500	0.38536200	2.21890800
C	3.03220000	1.89890000	1.06310800
C	4.36376400	1.70139900	1.70853000
H	5.17471500	1.87308800	0.98681600
H	4.47570500	2.38633300	2.54936600
N	2.11276400	2.80256700	1.24922100
C	1.32474500	1.17497700	-0.07407900
N	1.05524700	2.33619100	0.51952700
C	-0.16441700	3.09022400	0.45311100
C	-0.40646600	3.84724400	-0.69837800
C	-1.02243000	3.04994600	1.54860500
C	-1.60898800	4.54000300	-0.76023200
C	-2.21809300	3.76412900	1.43491900
C	-2.53005200	4.49651000	0.29239900
H	-1.83729500	5.12721800	-1.64650200
H	-2.92381400	3.72872400	2.26053900
C	0.61357300	3.91927900	-1.80521500
H	0.27906300	4.59945700	-2.59002200
H	1.57258600	4.28124100	-1.42108000
H	0.79867600	2.94153400	-2.26374800

C	-0.64992800	2.33017100	2.81422600
H	-0.10342700	1.40697200	2.60980000
H	-0.00137900	2.97015500	3.42207300
H	-1.54462400	2.07721500	3.38169400
C	-3.84679000	5.21749400	0.16460700
H	-4.43044100	5.14682400	1.08444000
H	-3.69570700	6.27610800	-0.06561500
H	-4.43872100	4.78727100	-0.65019600
N	-0.26598100	-0.84569200	0.34716300
C	0.16598600	-1.02300200	1.63152700
O	1.23818400	-0.62918900	2.06566800
O	-0.67169100	-1.78003000	2.36942800
C	-0.21588100	-2.05994500	3.68972200
H	-1.00598300	-2.64715200	4.15558000
H	0.71517300	-2.62904900	3.65042100
H	-0.04781700	-1.13278500	4.24180200
C	-3.57050400	-4.65667500	-0.90204700
C	-2.41113700	-4.37038000	-1.61809000
C	-1.69888000	-3.19088400	-1.37109600
C	-2.16478700	-2.33829300	-0.38966600
C	-3.32768900	-2.63482500	0.32403300
C	-4.05357800	-3.79057400	0.08464900
H	-4.11477200	-5.57229300	-1.11069300
H	-2.05889700	-5.06342400	-2.37406100
H	-0.79836500	-2.94535000	-1.92802600

H	-4.96125100	-4.01505500	0.63491500
C	-1.67422400	-0.97402500	0.03584300
C	-2.65354900	-0.61995200	1.19104100
O	-2.63442200	0.38742000	1.86670600
N	-3.60535300	-1.60653500	1.23468800
C	-4.74297000	-1.57285000	2.11955700
H	-5.67435900	-1.57342700	1.54454400
H	-4.73466400	-2.43546300	2.79341300
H	-4.67298000	-0.65313000	2.70069100

**IM5(RR)**

C	1.70801000	0.15640400	1.06927000
C	0.48332800	0.63816300	1.25104100
C	-0.61915500	-0.22148600	0.62965300
H	0.23938700	1.45574200	1.92033000
O	-1.36914000	-0.85030400	1.45719800
C	2.95604300	0.60705800	1.72598100
C	3.13882300	0.37357100	3.09206300
C	3.95933300	1.26111200	1.00170800
C	4.30298500	0.79859900	3.72728300
C	5.12074800	1.68488100	1.63975200
H	3.81624600	1.43927700	-0.06068900
C	5.29383900	1.45586800	3.00348800
H	4.43677600	0.61319100	4.78842600
H	5.89500000	2.19153700	1.07096500
H	2.36220500	-0.15403600	3.63845400

H	6.20143200	1.78610800	3.49920000
C	-6.47976700	0.13533500	2.92320100
C	-6.85179900	-0.50726000	1.74446600
C	-5.87044500	-0.79797700	0.80140500
C	-4.15691100	0.16850800	2.22924800
C	-5.14386200	0.46376600	3.16651300
H	-7.23504100	0.37231000	3.66631300
H	-7.88911600	-0.77569900	1.56553800
H	-3.10108900	0.35587200	2.40543900
H	-4.87201100	0.94277400	4.10181500
C	-4.54517700	-0.44477900	1.04276500
C	-3.66076700	-0.85362400	-0.11229500
C	-4.66167100	-1.27400300	-1.24448100
H	-2.97512800	-1.65414400	0.15637300
C	-6.00327400	-1.52059800	-0.51690200
H	-4.28486200	-2.16108700	-1.75417800
H	-6.83328300	-1.16880800	-1.13753600
H	-6.15349000	-2.59319300	-0.35067100
N	-2.83395800	0.26970200	-0.57382000
O	-4.81006300	-0.30931800	-2.28343100
C	-3.37548400	1.25528300	-1.34641400
C	-4.76068600	1.03562900	-1.85628100
H	-5.50578800	1.25015900	-1.07725000
H	-4.94854300	1.67253200	-2.72112100
N	-2.50961900	2.18862400	-1.61519700

C	-1.54845000	0.58919900	-0.34627600
N	-1.38007200	1.75721500	-0.97426800
C	-0.17220300	2.52667800	-1.03017600
C	0.05570000	3.48450000	-0.04008700
C	0.72344400	2.25475200	-2.05970300
C	1.29198200	4.12178200	-0.04853900
C	1.94544000	2.92830700	-2.03217800
C	2.25582700	3.83606500	-1.01900000
H	1.51456600	4.85145800	0.72616300
H	2.67550200	2.73077800	-2.81431300
C	-1.00536400	3.81415200	0.97533800
H	-0.59801300	4.44136500	1.77007400
H	-1.83120900	4.35244000	0.49954400
H	-1.43106500	2.91457700	1.43094500
C	0.34910300	1.28007500	-3.14547800
H	0.18003700	0.27954200	-2.73064900
H	-0.57652900	1.59487600	-3.63647500
H	1.13574700	1.21431400	-3.89986900
C	3.61215000	4.48674500	-0.94950900
H	4.19168500	4.05298200	-0.12688400
H	4.17319500	4.33959400	-1.87485800
H	3.52795900	5.56071200	-0.76362400
N	0.31231600	-1.08180900	-0.29782800
C	-0.23762000	-2.15299900	-0.93079400
O	-1.38177400	-2.20329600	-1.34814300



O	0.64627800	-3.16011000	-1.09771600
C	0.14024600	-4.28511800	-1.80746100
H	0.97194800	-4.98417800	-1.88330400
H	-0.69228000	-4.73621200	-1.26399600
H	-0.20361500	-3.98871800	-2.80065900
C	5.05201000	-1.85952800	-2.28151500
C	4.21996600	-0.82055400	-2.68429000
C	3.07907200	-0.50176700	-1.93718500
C	2.78777300	-1.23073800	-0.80329100
C	3.63829100	-2.27045400	-0.40847900
C	4.77426200	-2.60306600	-1.13087700
H	5.93484100	-2.09961600	-2.86557800
H	4.45600300	-0.25376400	-3.57887700
H	2.43584300	0.31894100	-2.22766300
H	5.42484900	-3.41157300	-0.81449100
C	1.67249600	-1.10198900	0.21219100
C	1.97407200	-2.30362600	1.16831800
O	1.32514600	-2.64849300	2.12370400
N	3.16601700	-2.86723900	0.75781800
C	3.76731600	-4.00238200	1.41070200
H	3.79125500	-4.86960500	0.74189300
H	4.78775800	-3.76798000	1.72955100
H	3.15470900	-4.23265900	2.28278800

**IM5(RS)**

C	1.78887900	0.11529200	0.89085800
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C	0.56152000	0.50832500	1.22013500
C	-0.53244500	-0.23449400	0.44723500
H	0.32007900	1.15633700	2.05581300
O	-1.18124900	-1.11859700	1.13971400
C	3.05619500	0.45973400	1.57098900
C	3.21525700	0.17651200	2.93057200
C	4.10160700	1.08235700	0.87632400
C	4.39424200	0.51364200	3.58891300
C	5.27935000	1.41670000	1.53797500
H	3.97314600	1.32254200	-0.17615000
C	5.42877400	1.13413100	2.89416600
H	4.50719300	0.28563100	4.64412500
H	6.08150700	1.90553200	0.99267000
H	2.40865100	-0.32415900	3.45800000
H	6.34901100	1.39530100	3.40715300
C	-6.17277300	-0.64174600	3.21465400
C	-6.64379400	-0.97308200	1.94641500
C	-5.74584300	-0.99758100	0.88292800
C	-3.91677800	-0.38945500	2.36414000
C	-4.82032400	-0.35907300	3.42310100
H	-6.86238400	-0.61209500	4.05258200
H	-7.69315300	-1.20669100	1.79065700
H	-2.85015800	-0.22650000	2.49429300
H	-4.47067300	-0.12333800	4.42324500
C	-4.40437700	-0.69295200	1.09714800

C	-3.61779100	-0.77453500	-0.19005600
C	-4.70619200	-0.94323500	-1.30987700
H	-2.89514400	-1.58910300	-0.18352400
C	-5.99272700	-1.36317500	-0.55975200
H	-4.37275300	-1.69293400	-2.02763200
H	-6.85953900	-0.86278000	-1.00280800
H	-6.15625300	-2.44194200	-0.65945200
N	-2.84598900	0.45208000	-0.42250400
O	-4.92654800	0.21970300	-2.10078200
C	-3.42956800	1.56681100	-0.94997500
C	-4.84719700	1.44171900	-1.39676900
H	-5.53530500	1.47002000	-0.53966100
H	-5.09615100	2.24710100	-2.08814100
N	-2.57105600	2.53382700	-1.10313100
C	-1.54782800	0.73042600	-0.23245500
N	-1.40531000	1.99166400	-0.64199700
C	-0.16357400	2.70879200	-0.68697500
C	0.14590800	3.54286100	0.39470400
C	0.70196500	2.46449000	-1.74729500
C	1.41679900	4.09646600	0.42564400
C	1.97546100	3.03842000	-1.66203400
C	2.35110400	3.83277100	-0.58439700
H	1.69842100	4.73133900	1.26235600
H	2.69136800	2.82590300	-2.45110900
C	-0.87043400	3.80621800	1.47373600

H	-0.44095800	4.42224400	2.26555600
H	-1.74374500	4.32397700	1.06534100
H	-1.23338200	2.87526000	1.92340900
C	0.31171900	1.64281200	-2.94652100
H	-0.63416600	1.11457900	-2.80910400
H	0.20798600	2.29578100	-3.81918400
H	1.09458100	0.91039300	-3.15013900
C	3.74349400	4.39879000	-0.48288200
H	4.34503500	4.12680800	-1.35304200
H	3.72159500	5.49020900	-0.40840600
H	4.24445900	4.01491000	0.41192000
N	0.36159500	-0.76632200	-0.69345300
C	-0.18148500	-1.51158700	-1.68454600
O	-1.35789100	-1.49208700	-2.00986500
O	0.74953600	-2.24836700	-2.32928500
C	0.25160300	-2.99489300	-3.43496800
H	1.11412800	-3.51025700	-3.85485800
H	-0.49967900	-3.71371800	-3.10218500
H	-0.19673500	-2.32892600	-4.17516600
C	3.19601400	-4.68105000	1.13347200
C	1.98064900	-4.27109600	1.67592200
C	1.39953800	-3.05635300	1.29087300
C	2.06591800	-2.29370700	0.35337100
C	3.27598700	-2.71487100	-0.19500000
C	3.87037700	-3.90800800	0.18105500

H	3.63291000	-5.62282500	1.45098000
H	1.48089600	-4.89933900	2.40568100
H	0.44593700	-2.70024900	1.67852100
H	4.81446800	-4.23383900	-0.24315300
C	1.71949400	-0.93369000	-0.21998200
C	2.82214500	-0.74705000	-1.29287700
O	2.93541900	0.16345200	-2.09025700
N	3.71690100	-1.77444600	-1.13923400
C	4.91085100	-1.90819800	-1.93577900
H	5.79812100	-1.92378600	-1.29545000
H	4.87897700	-2.82913800	-2.52708500
H	4.95427300	-1.04731800	-2.60317300

**IM5(SR)**

C	-1.72069200	-0.28717000	1.31549200
C	-0.46078500	-0.12468400	1.70966700
C	0.55504900	-0.48941800	0.62542400
H	-0.14242900	0.10204400	2.72180600
O	1.21340200	-1.58603500	0.83042500
C	-2.93940900	-0.20146700	2.14738000
C	-3.08707900	-1.04969600	3.24858000
C	-3.94402600	0.73062100	1.85785400
C	-4.21902800	-0.96828700	4.05275900
C	-5.07336600	0.81043000	2.66773700
H	-3.82229600	1.39655200	1.00664100
C	-5.21393400	-0.03816200	3.76337400

H	-4.32680900	-1.63563800	4.90195900
H	-5.84543900	1.54032500	2.44460600
H	-2.31107000	-1.78137800	3.45307000
H	-6.09815400	0.02440500	4.38985500
C	6.17157000	-2.51606400	-1.38219000
C	6.67467600	-1.89829100	-0.23995400
C	5.79083000	-1.22843700	0.60138000
C	3.91399900	-1.81803400	-0.83043500
C	4.80523700	-2.47922200	-1.67158500
H	6.84873900	-3.03805700	-2.05151400
H	7.73562300	-1.93916500	-0.01026500
H	2.84535400	-1.79003600	-1.02129000
H	4.43141700	-2.97576700	-2.56128100
C	4.43412500	-1.18449500	0.29324500
C	3.65901300	-0.42260100	1.34085100
C	4.76253700	0.19329800	2.28193400
H	2.95937900	-1.07395700	1.86432900
C	6.07863700	-0.52939400	1.90536100
H	4.49356400	0.02246900	3.32531400
H	6.89373100	0.19970400	1.84545000
H	6.35271000	-1.25144400	2.68207400
N	2.83902200	0.65099600	0.74613000
O	4.89334200	1.60518100	2.18902800
C	3.39078000	1.86517000	0.44584400
C	4.80032700	2.10365800	0.86924900

H	5.50768600	1.60527600	0.19125200
H	5.01110100	3.17284600	0.89274200
N	2.50870200	2.68426400	-0.04036400
C	1.53877200	0.70453100	0.39775700
N	1.35711700	1.94674800	-0.06288600
C	0.14390400	2.59161900	-0.50098000
C	-0.01803800	2.80525100	-1.87565000
C	-0.75112400	3.07869700	0.45220200
C	-1.17610900	3.45185900	-2.28780400
C	-1.89849400	3.71814200	-0.01940200
C	-2.14052300	3.88502900	-1.37738300
H	-1.33675500	3.61088900	-3.35129700
H	-2.62021100	4.09087500	0.70480700
C	1.05085700	2.41545900	-2.86205200
H	1.91772200	3.07612600	-2.75586300
H	1.39493500	1.38931700	-2.71227300
H	0.67326400	2.51233100	-3.88215900
C	-0.51081500	3.01741600	1.93893700
H	-1.31136200	2.46103600	2.43519100
H	0.43927200	2.54529600	2.19506500
H	-0.50051700	4.03197200	2.34791100
C	-3.44028600	4.46535100	-1.86143200
H	-3.86637800	5.16215800	-1.13553900
H	-3.31817000	4.98669100	-2.81398900
H	-4.15815900	3.65202900	-2.01244900

N	-0.40615800	-0.48410800	-0.56823600
C	0.05917500	-0.82751600	-1.79133200
O	1.22527700	-0.74562600	-2.14118400
O	-0.93259100	-1.22181000	-2.61803300
C	-0.51570300	-1.49908000	-3.95051100
H	-0.09786100	-0.60231500	-4.41442000
H	0.23944500	-2.28727500	-3.95865900
H	-1.41195600	-1.82050000	-4.47895400
C	-3.43331100	-4.66625400	-0.39302900
C	-2.18272300	-4.58145000	0.21338500
C	-1.53528800	-3.34565900	0.34314700
C	-2.17466600	-2.22940700	-0.15590700
C	-3.42154500	-2.32166500	-0.77299600
C	-4.07927000	-3.53378500	-0.90277800
H	-3.92084200	-5.63234700	-0.48020900
H	-1.70668100	-5.48151800	0.58774000
H	-0.54963200	-3.23309400	0.79317700
H	-5.05052500	-3.60759400	-1.38091000
C	-1.75432000	-0.77355100	-0.13049200
C	-2.86378700	-0.09989900	-0.97428700
O	-2.92034300	1.06070100	-1.31830000
N	-3.82430000	-1.05387200	-1.21695600
C	-5.02749700	-0.78975200	-1.96425100
H	-5.04380500	-1.37450700	-2.89013800
H	-5.91149500	-1.03742700	-1.36868000



H	-5.03278000	0.27363900	-2.20506300
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**IM5(SS)**

C	1.78880400	0.11522400	0.89101600
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C	0.56143000	0.50827900	1.22020900
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C	-0.53248500	-0.23449400	0.44717700
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H	0.31996100	1.15625000	2.05591000
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O	-1.18127200	-1.11869800	1.13954200
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C	3.05609900	0.45963500	1.57121100
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C	3.21515200	0.17624700	2.93075800
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C	4.10150300	1.08238400	0.87664100
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C	4.39411800	0.51332800	3.58916100
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C	5.27922000	1.41668400	1.53835400
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H	3.97305000	1.32269900	-0.17580300
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C	5.42863800	1.13394000	2.89450900
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H	4.50705800	0.28518400	4.64434400
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H	6.08136800	1.90561400	0.99312500
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H	2.40855200	-0.32450700	3.45811500
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H	6.34886100	1.39507900	3.40753600
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C	-6.17254000	-0.64205100	3.21482600
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C	-6.64367300	-0.97321600	1.94658500
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C	-5.74581100	-0.99760700	0.88302000
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C	-3.91661400	-0.38970000	2.36415000
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C	-4.82007100	-0.35942100	3.42318900
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H	-6.86208100	-0.61250500	4.05281400
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H	-7.69304900	-1.20678500	1.79088400
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H	-2.84997900	-0.22679100	2.49423500
H	-4.47032600	-0.12380700	4.42332900
C	-4.40432100	-0.69304300	1.09716100
C	-3.61783400	-0.77451400	-0.19011500
C	-4.70632700	-0.94312300	-1.30986800
H	-2.89518400	-1.58907600	-0.18371600
C	-5.99283600	-1.36303100	-0.55967900
H	-4.37298100	-1.69283100	-2.02765900
H	-6.85964300	-0.86251900	-1.00261300
H	-6.15646000	-2.44177200	-0.65947600
N	-2.84603100	0.45212000	-0.42251500
O	-4.92669000	0.21984100	-2.10074500
C	-3.42956400	1.56685600	-0.95001400
C	-4.84722400	1.44184700	-1.39671900
H	-5.53527000	1.47016300	-0.53956200
H	-5.09618300	2.24725700	-2.08805700
N	-2.57100400	2.53382000	-1.10324400
C	-1.54785200	0.73041500	-0.23251700
N	-1.40527100	1.99160600	-0.64214100
C	-0.16354600	2.70875100	-0.68704500
C	0.14577100	3.54290800	0.39461200
C	0.70211800	2.46436600	-1.74724200
C	1.41663900	4.09657100	0.42563900
C	1.97557700	3.03836300	-1.66188900
C	2.35108200	3.83277500	-0.58424200

H	1.69815000	4.73152800	1.26232400
H	2.69159600	2.82576500	-2.45084100
C	-0.87065900	3.80628100	1.47355700
H	-0.44123700	4.42231800	2.26540000
H	-1.74394400	4.32402800	1.06509900
H	-1.23363600	2.87533600	1.92323300
C	0.31207900	1.64228500	-2.94626400
H	-0.63360800	1.11372600	-2.80853100
H	0.20797400	2.29497800	-3.81908600
H	1.09515000	0.91006400	-3.14978000
C	3.74346600	4.39878900	-0.48259900
H	4.34531400	4.12615200	-1.35234500
H	3.72160600	5.49026000	-0.40892500
H	4.24411000	4.01552900	0.41265100
N	0.36164000	-0.76617800	-0.69352200
C	-0.18137800	-1.51130500	-1.68474700
O	-1.35776500	-1.49176900	-2.01013000
O	0.74971000	-2.24789600	-2.32959600
C	0.25187700	-2.99414600	-3.43550700
H	1.11437800	-3.50967000	-3.85524200
H	-0.49967100	-3.71280900	-3.10299900
H	-0.19610200	-2.32797600	-4.17574900
C	3.19580300	-4.68130600	1.13298000
C	1.98039400	-4.27142900	1.67539200
C	1.39935500	-3.05659100	1.29053400

C	2.06584400	-2.29377100	0.35325000
C	3.27594700	-2.71487100	-0.19509800
C	3.87027600	-3.90809000	0.18078300
H	3.63265000	-5.62315200	1.45034300
H	1.48054800	-4.89981400	2.40496300
H	0.44573200	-2.70053200	1.67816500
H	4.81440200	-4.23385800	-0.24339400
C	1.71948900	-0.93365500	-0.21993800
C	2.82222700	-0.74687400	-1.29268600
O	2.93556700	0.16376100	-2.08990300
N	3.71696800	-1.77429700	-1.13914000
C	4.91094600	-1.90794600	-1.93566600
H	5.79822700	-1.92330900	-1.29534500
H	4.87921600	-2.82895700	-2.52686600
H	4.95421300	-1.04713800	-2.60316400

**TS6(RR)**

C	1.69609200	-0.00497200	1.21364500
C	0.46263900	0.35391500	1.55475100
C	-0.58965800	-0.55600800	0.97770400
H	0.20127200	1.14555800	2.24519400
O	-1.50435900	-1.03970100	1.65326600
C	2.96614400	0.55861800	1.72009700
C	3.23199500	0.49845000	3.09198200
C	3.90598400	1.14919800	0.86581400
C	4.41223800	1.02768700	3.60580600

C	5.08586700	1.67472900	1.38453800
H	3.70247600	1.20720700	-0.19976800
C	5.34125400	1.61719400	2.75310500
H	4.60821800	0.97288600	4.67189700
H	5.81018800	2.12792300	0.71411000
H	2.50924700	0.01584200	3.74324700
H	6.26415400	2.02630200	3.15198500
C	-6.59249200	0.32459100	2.79448300
C	-6.93979100	-0.34771900	1.62470600
C	-5.93696600	-0.68016500	0.71909200
C	-4.25318000	0.30729200	2.16272300
C	-5.25985100	0.64377500	3.06449900
H	-7.36484100	0.59605300	3.50756400
H	-7.97584200	-0.60474900	1.42289400
H	-3.20414000	0.49839000	2.36956500
H	-5.00704400	1.15089200	3.99017700
C	-4.61286500	-0.34023700	0.98617500
C	-3.70309400	-0.79072400	-0.13444700
C	-4.68347900	-1.20870100	-1.28451100
H	-3.06313400	-1.61922300	0.16473200
C	-6.04467800	-1.43006500	-0.58618100
H	-4.31184300	-2.10857300	-1.77633000
H	-6.85656100	-1.08398500	-1.23331900
H	-6.20698600	-2.49784500	-0.40091400
N	-2.82864900	0.29516300	-0.58815100

O	-4.79156100	-0.25090800	-2.33355700
C	-3.33984000	1.29240600	-1.37517600
C	-4.71659300	1.09846600	-1.91703700
H	-5.47758400	1.33737200	-1.16074800
H	-4.87032200	1.72899100	-2.79337500
N	-2.45155300	2.20588000	-1.62347200
C	-1.53223200	0.57084300	-0.31400200
N	-1.34845200	1.74221900	-0.94557200
C	-0.13352900	2.49928000	-0.95996000
C	0.21713300	3.24392900	0.17088500
C	0.66022600	2.45158100	-2.10576000
C	1.46667800	3.85675800	0.17218600
C	1.89806900	3.09455700	-2.06347300
C	2.32595700	3.77765200	-0.92611100
H	1.77990200	4.41100700	1.05412800
H	2.54608100	3.04702500	-2.93573800
C	-0.73961600	3.43881400	1.31851700
H	-0.19747400	3.67415900	2.23732600
H	-1.41111800	4.27580800	1.10038300
H	-1.36391700	2.56101100	1.49774300
C	0.17516600	1.74248100	-3.34347800
H	-0.23528800	0.75518400	-3.10779900
H	-0.62772900	2.31478100	-3.81743600
H	0.98655200	1.62000200	-4.06467300
C	3.68158900	4.43157500	-0.87150800

H	4.22408200	4.11008000	0.02272900
H	4.28139400	4.17629900	-1.74794500
H	3.58997900	5.52134700	-0.82896000
N	0.24611800	-1.41116500	0.08206500
C	-0.27930100	-2.47389600	-0.58650800
O	-1.44214100	-2.60108000	-0.91153600
O	0.67851600	-3.37693700	-0.89350600
C	0.21814900	-4.49114200	-1.65139100
H	1.10001800	-5.09987900	-1.84549000
H	-0.52388800	-5.05691200	-1.08466800
H	-0.23053600	-4.15652600	-2.58898800
C	4.63069500	-1.48400100	-2.69694700
C	3.57093100	-0.61747600	-2.94710900
C	2.53400000	-0.48869800	-2.01516500
C	2.58413800	-1.22817500	-0.85447700
C	3.64539400	-2.10811600	-0.62020600
C	4.68466000	-2.24920500	-1.52702900
H	5.43140900	-1.57603400	-3.42393600
H	3.54741900	-0.04129700	-3.86641300
H	1.70345000	0.18547800	-2.18162700
H	5.50843400	-2.92975100	-1.33937000
C	1.66178800	-1.25533900	0.33903500
C	2.27491700	-2.40973700	1.19299200
O	1.82554100	-2.86034000	2.21756600
N	3.46476100	-2.76993300	0.59508600

C	4.32770700	-3.80393300	1.11047400
H	4.39575200	-4.63914300	0.40530000
H	5.33123100	-3.41001700	1.29810600
H	3.88998900	-4.15196500	2.04648000

**TS6(RS)**

C	1.76256700	0.08627800	0.91963100
C	0.51730500	0.27295000	1.35725400
C	-0.43238200	-0.71187400	0.74586900
H	0.19901900	0.97894000	2.11462600
O	-1.30104800	-1.33207500	1.34543100
C	2.99329500	0.74675200	1.40095300
C	3.23198700	0.81762500	2.77746900
C	3.92626000	1.30713800	0.51865000
C	4.37542500	1.43901200	3.26762000
C	5.07144300	1.92350200	1.01331100
H	3.73257700	1.29782400	-0.55008700
C	5.29996300	1.99179200	2.38564000
H	4.54886200	1.48286100	4.33803900
H	5.78456400	2.36122300	0.32123100
H	2.51763700	0.36400600	3.45813200
H	6.19642200	2.47139000	2.76567600
C	-6.30328900	-0.60355900	3.12277600
C	-6.74439100	-1.04171100	1.87569400
C	-5.84117700	-1.07439400	0.81801100
C	-4.06783300	-0.25316600	2.25625400



C	-4.97552300	-0.21557700	3.31220600
H	-6.99803200	-0.56532700	3.95609200
H	-7.77716900	-1.34610700	1.73139100
H	-3.02271800	0.00888100	2.38966000
H	-4.64743700	0.11364700	4.29301700
C	-4.51998000	-0.67747200	1.01218100
C	-3.72998200	-0.78931000	-0.27490700
C	-4.82913300	-0.98623500	-1.37347500
H	-3.03028500	-1.62705200	-0.25601700
C	-6.05994700	-1.51840600	-0.60779900
H	-4.47775900	-1.68375600	-2.13562500
H	-6.97845000	-1.13131300	-1.05840800
H	-6.09893300	-2.61240000	-0.66662800
N	-2.95323800	0.41207600	-0.55380100
O	-5.14425700	0.20104200	-2.09628500
C	-3.57337900	1.54400700	-1.01181100
C	-5.01336300	1.41822900	-1.38267900
H	-5.65420000	1.43915800	-0.49028500
H	-5.30670100	2.22570600	-2.05413800
N	-2.72693400	2.51746000	-1.16392600
C	-1.62820600	0.65140900	-0.40075500
N	-1.54097600	1.93803000	-0.76818200
C	-0.31180400	2.66995800	-0.78515100
C	-0.00504700	3.48981200	0.30309200
C	0.56295700	2.45448300	-1.84753600

C	1.24908100	4.09234900	0.32066600
C	1.80932000	3.07805400	-1.78660400
C	2.16715300	3.89294700	-0.71350500
H	1.52240800	4.72226400	1.16412800
H	2.51967000	2.90399400	-2.59131100
C	-1.00730300	3.69465600	1.40714400
H	-0.56412900	4.24643500	2.23836900
H	-1.87600700	4.25102600	1.04212400
H	-1.38320000	2.73705100	1.78339200
C	0.15178700	1.58257800	-3.00186300
H	0.00507300	0.55281900	-2.66467500
H	-0.78848100	1.93999100	-3.43333200
H	0.92440900	1.57233500	-3.77091900
C	3.51578500	4.56358000	-0.66982000
H	3.92553700	4.55294200	0.34376600
H	4.22711500	4.06033300	-1.33033800
H	3.44328500	5.60765700	-0.99242900
N	0.38603200	-1.31824100	-0.30295900
C	-0.11556700	-2.17784400	-1.23307700
O	-1.28919200	-2.33131700	-1.49345300
O	0.88507200	-2.82269500	-1.87140300
C	0.45664000	-3.68026300	-2.92579600
H	1.36528300	-4.12006400	-3.33374200
H	-0.20702600	-4.45586000	-2.53928000
H	-0.07135000	-3.10915400	-3.69211600

C	4.24079300	-4.25806400	1.39078200
C	3.06898500	-4.01982500	2.10388400
C	2.19333700	-3.00341300	1.70518500
C	2.52034200	-2.26210700	0.59001100
C	3.69017900	-2.51189400	-0.12477100
C	4.57506400	-3.50689100	0.25795700
H	4.91285800	-5.04584600	1.71583800
H	2.83463900	-4.62408800	2.97334400
H	1.26737700	-2.80173400	2.23873800
H	5.48761000	-3.70123800	-0.29567800
C	1.79504800	-1.09767000	-0.05135500
C	2.65712000	-0.83591300	-1.31349600
O	2.44071500	-0.03372400	-2.19562400
N	3.76668700	-1.64129300	-1.22086800
C	4.82104800	-1.64863700	-2.20429900
H	5.77906000	-1.39360500	-1.74037100
H	4.90161300	-2.63334200	-2.67605900
H	4.56805900	-0.90299300	-2.95853900

**TS6(SR)**

C	-1.67334600	-0.52667800	1.39675700
C	-0.39870300	-0.64599800	1.76223100
C	0.46545900	-1.09026400	0.61646000
H	0.01021100	-0.49299200	2.75391400
O	1.31464100	-1.97633500	0.67262500
C	-2.83415400	-0.14911200	2.23019900

C	-3.21744600	-0.94734000	3.31097100
C	-3.54636000	1.02481400	1.95258500
C	-4.29853300	-0.57896200	4.10630600
C	-4.62429200	1.38934600	2.75275700
H	-3.23818300	1.65263500	1.11966100
C	-5.00340300	0.58891500	3.82805600
H	-4.59184700	-1.20607500	4.94204900
H	-5.16726400	2.30440900	2.53804600
H	-2.66828400	-1.86226800	3.51260000
H	-5.84663700	0.87552100	4.44838500
C	6.29286200	-2.42372100	-1.46965700
C	6.74904600	-1.95586300	-0.23894200
C	5.84198800	-1.34411500	0.62121200
C	4.03608100	-1.68534700	-0.97219200
C	4.95025200	-2.29144700	-1.83117700
H	6.99004900	-2.89570200	-2.15533200
H	7.79381500	-2.06089400	0.03955200
H	2.98560600	-1.58588400	-1.23349600
H	4.61218900	-2.66566300	-2.79214900
C	4.50772900	-1.21243300	0.24719700
C	3.70596000	-0.51388800	1.32236100
C	4.79160500	0.02742100	2.32211800
H	3.01648800	-1.20625000	1.80614700
C	6.07458500	-0.77381200	1.99815200
H	4.46835700	-0.12684700	3.35327100

H	6.94677400	-0.11576300	2.06358900
H	6.21711400	-1.57543200	2.73156500
N	2.90875100	0.58614500	0.77684100
O	5.01021100	1.42843800	2.23476800
C	3.51160800	1.78146100	0.48897100
C	4.92637100	1.96232900	0.92531600
H	5.62116600	1.46103900	0.23669400
H	5.17465600	3.02241900	0.98069900
N	2.66708900	2.62340500	-0.01857900
C	1.59871600	0.64546000	0.41767300
N	1.49664100	1.89546100	-0.05653900
C	0.32158400	2.55699100	-0.54994600
C	0.18492700	2.71424100	-1.93034200
C	-0.56573700	3.12222800	0.36847500
C	-0.91374200	3.43610900	-2.38916500
C	-1.64763200	3.83698700	-0.14030900
C	-1.84383600	3.98926500	-1.51153500
H	-1.04810600	3.56464800	-3.46081900
H	-2.35413300	4.28577900	0.55529100
C	1.21729700	2.15758300	-2.87403000
H	2.17420800	2.67186100	-2.73902700
H	1.39106600	1.09198100	-2.69483200
H	0.89915400	2.29224100	-3.91028000
C	-0.34373300	2.98870500	1.85133500
H	-0.53065000	1.96273200	2.18338600

H	0.68676000	3.24267200	2.11836200
H	-1.01752800	3.64977500	2.40023700
C	-3.06938500	4.68827700	-2.03544900
H	-2.88264900	5.15339500	-3.00646300
H	-3.88009900	3.96258200	-2.16366400
H	-3.41873400	5.45941200	-1.34423500
N	-0.46017900	-0.98009800	-0.51791400
C	-0.08336200	-1.18092100	-1.80883600
O	1.05713700	-1.17302700	-2.22278400
O	-1.16376600	-1.35287900	-2.60046900
C	-0.86882800	-1.44194600	-3.99135400
H	-0.39769900	-0.52004300	-4.34035100
H	-0.19882600	-2.28106300	-4.18646400
H	-1.82760200	-1.59143500	-4.48525900
C	-4.35300200	-4.35678800	-0.39685300
C	-3.10830200	-4.57604900	0.18748500
C	-2.20131300	-3.51975300	0.33622400
C	-2.57242500	-2.27308900	-0.12101200
C	-3.81666500	-2.06292800	-0.71527700
C	-4.73245300	-3.09248200	-0.86183900
H	-5.04818200	-5.18398500	-0.49931000
H	-2.84113200	-5.56996500	0.52924000
H	-1.21953700	-3.66335300	0.78197700
H	-5.70200800	-2.93045100	-1.32111500
C	-1.83295800	-0.95240000	-0.06425500

C	-2.77049000	-0.02193900	-0.87193100
O	-2.55936000	1.12474100	-1.19212300
N	-3.92853400	-0.72569100	-1.11542800
C	-5.05172800	-0.17002900	-1.82735100
H	-5.22557900	-0.71414600	-2.76166000
H	-5.95559700	-0.21329400	-1.21213100
H	-4.81005200	0.86938800	-2.05121100

**TS6(SS)**

C	1.77593300	-1.16811800	0.51990600
C	0.62855200	-1.77818600	0.22786600
C	-0.09068100	-1.10693700	-0.91618100
H	0.26751200	-2.71334600	0.64100800
O	-0.48634000	-1.71706400	-1.90230000
C	2.84183400	-1.62812800	1.43584600
C	3.32543500	-0.81641500	2.46972700
C	3.38271000	-2.90665200	1.26468600
C	4.32981100	-1.28181900	3.31252100
C	4.38669600	-3.36822600	2.10936300
H	3.01629400	-3.52619900	0.45169900
C	4.86417100	-2.55545700	3.13393000
H	4.68992800	-0.64971900	4.11805200
H	4.80019400	-4.36084700	1.96305800
H	2.89058300	0.16506300	2.63293600
H	5.64870500	-2.91375000	3.79263400
C	-3.38439600	5.36354600	-0.90670900

C	-2.72284100	5.44089300	0.31886400
C	-2.07879500	4.30925900	0.80535600
C	-2.75217500	3.03531500	-1.15230700
C	-3.40206400	4.17241100	-1.63322000
H	-3.89942700	6.23661600	-1.29501800
H	-2.72395400	6.36530600	0.88906400
H	-2.74413400	2.10753700	-1.71553800
H	-3.92844000	4.12810400	-2.58106200
C	-2.09014400	3.12554900	0.06633700
C	-1.31726800	2.05048100	0.80624300
C	-1.25783400	2.58843200	2.26595800
H	-0.29749700	1.94271500	0.43708600
C	-1.31536700	4.11764700	2.09514400
H	-0.34016400	2.25445700	2.75235000
H	-1.78521800	4.58440100	2.96457800
H	-0.29675400	4.51392000	2.00427600
N	-1.96082700	0.74978200	0.77709100
O	-2.32417900	2.11523700	3.08871500
C	-3.10317900	0.56145800	1.51046000
C	-3.50005000	1.66357800	2.43743200
H	-4.00259200	2.47210700	1.89055200
H	-4.17030400	1.28203300	3.20820100
N	-3.57538700	-0.63438500	1.34032900
C	-1.66596900	-0.38826000	0.10181400
N	-2.67586600	-1.19367500	0.45968300



C	-2.88136600	-2.53787300	0.00500000
C	-3.29532100	-2.73655600	-1.31498400
C	-2.67316300	-3.58137000	0.90656600
C	-3.48702800	-4.05216400	-1.72729200
C	-2.87630800	-4.88132600	0.44348000
C	-3.27669300	-5.13227500	-0.86779400
H	-3.80714900	-4.23888000	-2.74951600
H	-2.71903300	-5.71382900	1.12503200
C	-3.51869200	-1.57077100	-2.23895000
H	-4.16990100	-0.82394400	-1.77269400
H	-2.56022600	-1.09768600	-2.47944200
H	-3.98856300	-1.90598900	-3.16561900
C	-2.26514700	-3.30643600	2.33032600
H	-1.44257200	-2.58541800	2.37811500
H	-3.09745900	-2.87637700	2.89486100
H	-1.94815200	-4.22679100	2.82437900
C	-3.46270000	-6.54384500	-1.36240300
H	-2.61405800	-6.85177100	-1.98154200
H	-3.54418900	-7.24867100	-0.53203200
H	-4.36355000	-6.63095400	-1.97548600
N	0.69086900	0.15207100	-1.04320800
C	0.31320100	1.13846100	-1.89714700
O	-0.75179200	1.19537400	-2.47248200
O	1.25769000	2.10719700	-1.96497100
C	0.87277100	3.23994900	-2.74290600

H	0.67676700	2.94371500	-3.77483400
H	-0.02797200	3.69856000	-2.32698600
H	1.71436600	3.92908100	-2.69477300
C	5.58770900	-0.15281800	-2.60395100
C	4.59346300	-1.05513100	-2.97351200
C	3.36074100	-1.06302900	-2.30968200
C	3.16450100	-0.15063500	-1.29493500
C	4.15956700	0.75789800	-0.93985900
C	5.38888500	0.77684300	-1.57651900
H	6.53955100	-0.16419800	-3.12500200
H	4.77689900	-1.75628300	-3.78017700
H	2.56195200	-1.74930400	-2.58099700
H	6.16518900	1.48174400	-1.29834600
C	1.97249600	0.05393100	-0.38667300
C	2.39504100	1.30822900	0.41990500
O	1.72922500	1.90317600	1.24865400
N	3.69130700	1.59079800	0.09064200
C	4.44761200	2.66428300	0.68766700
H	5.34340000	2.27134600	1.17805300
H	4.74344000	3.39473300	-0.07168400
H	3.80534700	3.14460100	1.42586700
<b>P(R)</b>			
C	0.68592500	-1.47453500	0.06198200
C	0.16590600	-2.66183600	0.38031000
C	-1.31553000	-2.58430800	0.43943100

H	0.69669200	-3.58861200	0.55126000
O	-2.10475700	-3.45786300	0.67206600
C	2.10912900	-1.10667600	-0.07953700
C	2.60571000	-0.58251600	-1.27914300
C	2.97601100	-1.29065700	1.00145900
C	3.95115000	-0.24734400	-1.38653400
C	4.31949600	-0.94886200	0.88988900
H	2.58351900	-1.68976900	1.93194500
C	4.80839500	-0.42427000	-0.30333700
H	4.33286400	0.14497300	-2.32359400
H	4.98413400	-1.09003200	1.73594500
H	1.94743100	-0.47863500	-2.13649600
H	5.85685100	-0.15826900	-0.39086300
N	-1.61931500	-1.22612900	0.15882900
C	-2.90829400	-0.72565800	0.02245200
O	-3.92565500	-1.33395000	0.20611000
O	-2.84246200	0.56947100	-0.34897200
C	-4.11453400	1.18994500	-0.53365200
H	-3.90001000	2.22248100	-0.80366000
H	-4.66781000	0.68792400	-1.32921400
H	-4.69531600	1.14493900	0.38922600
C	0.37063900	3.14654900	2.06828000
C	0.10762500	2.02359300	2.84720000
C	-0.17473400	0.79393700	2.24098400
C	-0.19697200	0.73033000	0.86368300

C	0.06493400	1.86345900	0.09013300
C	0.35513100	3.08687900	0.67087700
H	0.59219800	4.09221100	2.55232200
H	0.12376900	2.10149300	3.92855600
H	-0.38197700	-0.09197600	2.83522700
H	0.56131900	3.96541400	0.06889400
C	-0.42424700	-0.43839700	-0.06737600
C	-0.39070200	0.23968000	-1.46703100
O	-0.58898400	-0.30371600	-2.52792200
N	-0.02879400	1.54970900	-1.27104600
C	0.12440200	2.49483200	-2.35058300
H	-0.59779500	3.31156600	-2.25302800
H	1.13762100	2.90824400	-2.35708800
H	-0.05850400	1.95658400	-3.28108200

**P(S)**

C	-0.68605000	-1.47448300	0.06192800
C	-0.16611100	-2.66180500	0.38029900
C	1.31533000	-2.58437600	0.43940600
H	-0.69695500	-3.58854600	0.55126100
O	2.10449900	-3.45798100	0.67205000
C	-2.10923700	-1.10655900	-0.07959700
C	-2.60575500	-0.58221500	-1.27914600
C	-2.97618300	-1.29071500	1.00131700
C	-3.95118200	-0.24699400	-1.38654900
C	-4.31965700	-0.94887300	0.88973600

H	-2.58375900	-1.69000500	1.93175600
C	-4.80848600	-0.42406700	-0.30342100
H	-4.33283200	0.14549000	-2.32356900
H	-4.98432800	-1.09017900	1.73574000
H	-1.94745500	-0.47824200	-2.13647000
H	-5.85692900	-0.15801600	-0.39095200
N	1.61920600	-1.22622000	0.15878300
C	2.90823100	-0.72586300	0.02238200
O	3.92553700	-1.33427000	0.20596100
O	2.84251200	0.56929800	-0.34893900
C	4.11462800	1.18968100	-0.53361100
H	4.69552000	1.14437500	0.38918200
H	4.66775000	0.68780600	-1.32937300
H	3.90017900	2.22231000	-0.80332600
C	-0.37035100	3.14653000	2.06842200
C	-0.10749700	2.02350100	2.84729000
C	0.17472400	0.79383900	2.24101900
C	0.19699000	0.73029600	0.86371500
C	-0.06475600	1.86350000	0.09022200
C	-0.35481700	3.08692600	0.67101700
H	-0.59180000	4.09219400	2.55250700
H	-0.12365400	2.10134700	3.92865000
H	0.38185700	-0.09212400	2.83522700
H	-0.56088600	3.96551500	0.06907200
C	0.42418300	-0.43840400	-0.06740400

C	0.39070600	0.23975100	-1.46702500
O	0.58892100	-0.30361400	-2.52794500
N	0.02897600	1.54981800	-1.27097100
C	-0.12400400	2.49504800	-2.35044600
H	-1.13715400	2.90863300	-2.35698100
H	0.59832100	3.31165500	-2.25278300
H	0.05886500	1.95684500	-3.28097700