

Supporting Information

Mechanistic Understanding of Domino Cyclization between Gem-Dialkylthio Vinylallenes and Benzylamine towards Economic Synthesis: A Computational Study

Haiyan Yuan, Yiying Zheng, Zhongxue Fang, Xihe Bi, and Jingping Zhang*

Faculty of Chemistry, Northeast Normal University, Changchun 130024, China

jpzhang@nenu.edu.cn

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Table S1. Relative energies of the BnNH₂ attack carbonyl carbon of **Re'** for the domino cyclization of pyrroles with various methods, calculating with 6-31G** basis set in the gas phase, ΔE (ΔG) values are in kcal/mol.

	B3LYP	PBE1PBE
Re'+BnNH₂+2H₂O	0.0	0.0
Com1W'	-22.0	-23.5
	(-13.7)	(-12.8)
TS1W'	-10.0	-18.9
	(8.2)	(-1.3)
Int1W'	-18.8	-27.7
	(-4.0)	(-11.3)
TS2W'	4.5	-8.7
	(20.0)	(8.3)
Int2W'	1.4	-14.3
	(17.2)	(3.1)
TS3W'	-0.4	-16.1
	(15.3)	(1.8)
Int3W'	-46.1	-61.5
	(-30.5)	(-44.3)
TS4W'	-31.4	-42.0
	(-16.3)	(-25.0)
Int4W'	-64.3	-75.7
	(-52.8)	(-62.0)

We employed the most favored mechanism of the BnNH₂ attacking to the carbonyl carbon of **Re'** of the formation of pyrroles to investigate the effect of the various methods on this mechanism, as shown in Table S1. The calculated results indicate PBE1PBE functional qualitatively gives the same prediction with the B3LYP method, and the ΔE and ΔG values of the rate-determining step **TS2W'** for PBE1PBE are 13.2 kcal/mol and 11.7 kcal/mol lower than that for B3LYP method.

Table S2. Energy and free energy of intermediates and transition states of the trace water-catalyzed the BnNH₂ attack carbonyl carbon of **Re'** at the B3LYP (PBE1PBE)/6-311+G** level, ΔE (ΔG) values are in kcal/mol.

	B3LYP	PBE1PBE
Re'+BnNH₂+2H₂O	0.0	0.0
Com1W'	-11.4	-15.2
	(-1.7)	(-4.3)
TS1W'	5.3	-6.6
	(22.5)	(11.2)
Int1W'	-4.1	-15.9
	(12.0)	(0.8)
TS2W'	19.6	3.2
	(36.1)	(20.3)

Int2W'	17.2 (34.1)	-2.0 (15.5)
TS3W'	14.8 (32.2)	-4.3 (13.9)
Int3W'	-29.9 (-12.7)	-48.8 (-31.4)
TS4W'	-19.9 (-3.5)	-33.7 (-16.5)
Int4W'	-51.2 (-37.9)	-65.7 (-51.7)

To further study basis set effects, we calculated the frequencies for a larger basis set, B3LYP (PBE1PBE)/6-311+G**. Table S2 shows that the prediction trend of the two methods with 6-311+G** basis set is similar, the rate-determining step is the intramolecular cyclization transition state **TS2W'**. PBE1PBE functional is better than B3LYP, because the ΔE values of the nucleophilic attack transition state **TS1W'** and the transition state **TS2W'** at the PBE1PBE level are 11.9 kcal/mol and 16.4 kcal/mol lower than that for B3LYP functional. Thus, the PBE1PBE is kinetic and thermodynamic favor. Thus, we use PBE1PBE/6-311+G** method to calculate the DMSO-assisted, trace water-catalyzed, and solvent-free conditions reaction mechanism of the domino cyclization of pyrroles.

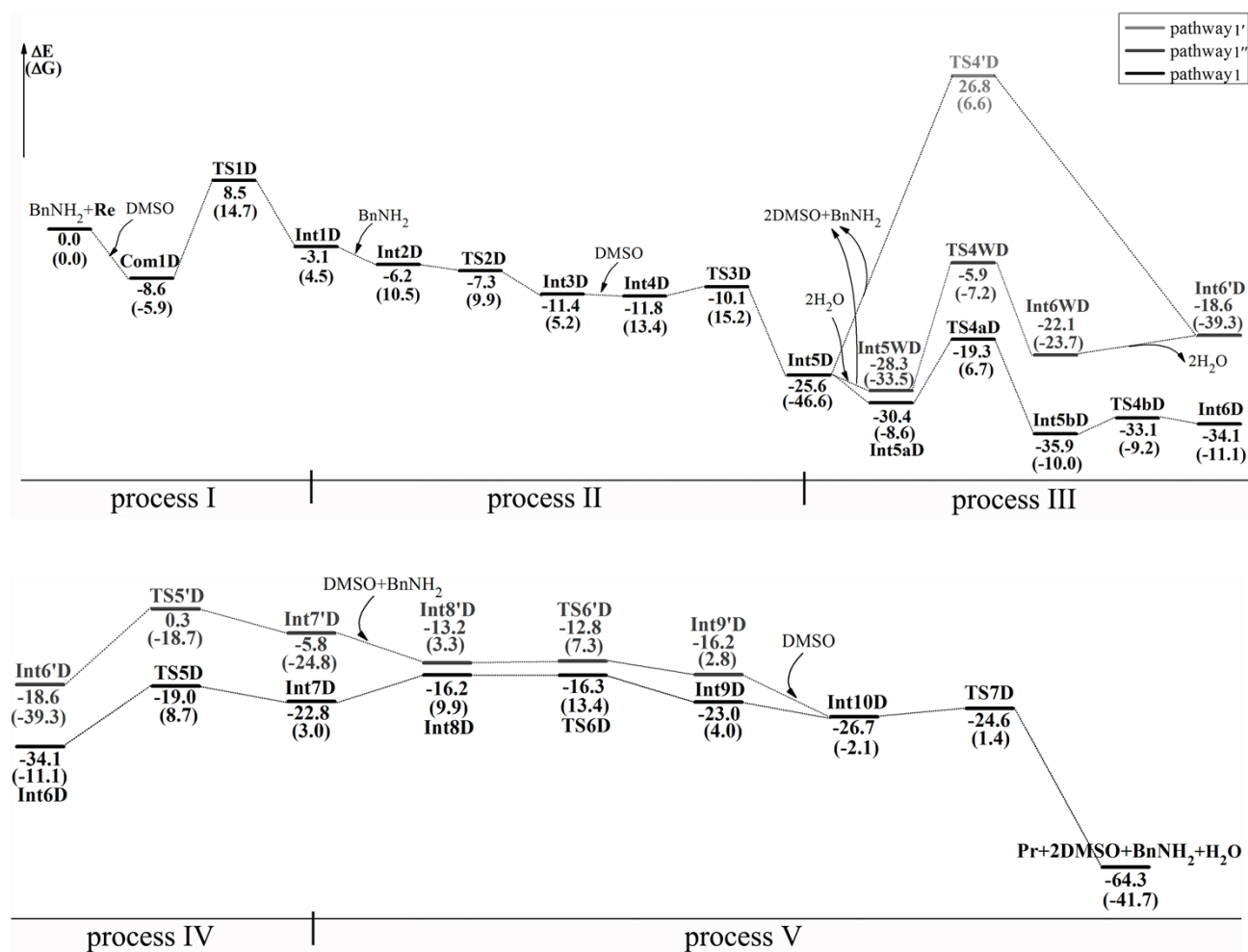
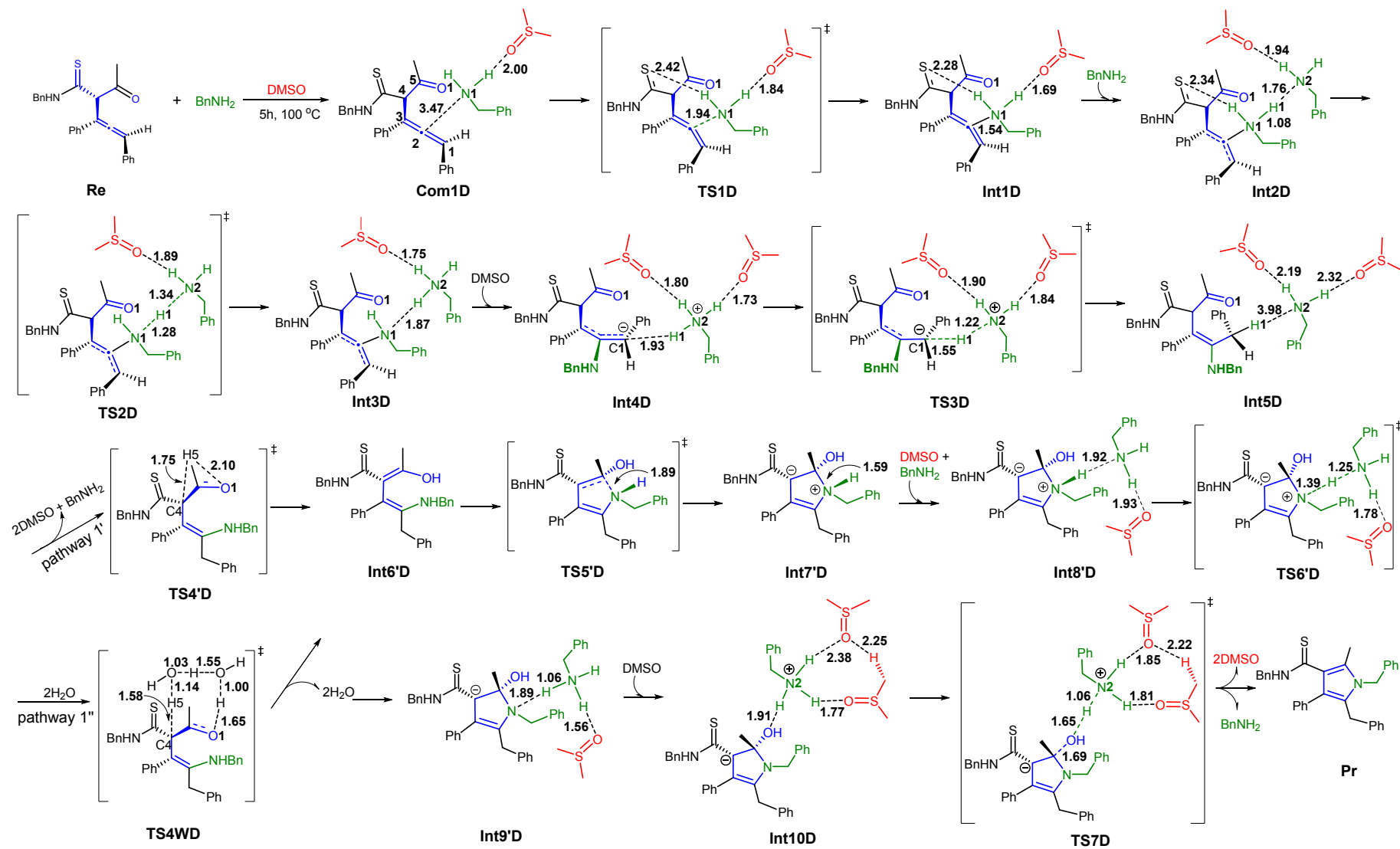


Figure S1. DFT computed energy surface for the DMSO-catalyzed domino reaction of pyrroles in the solvent phase, relative energies and free energies are given in kcal/mol.



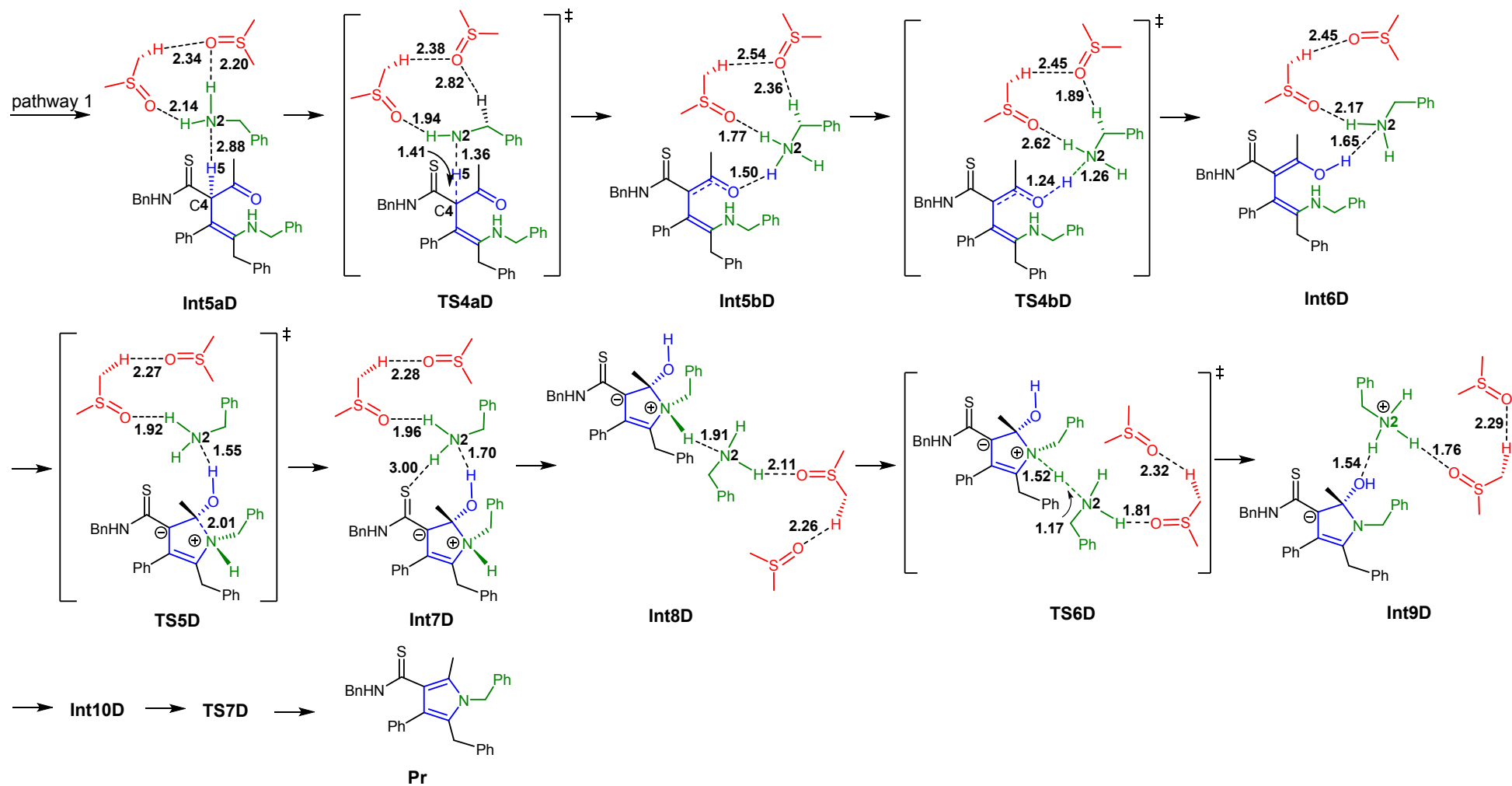


Figure S2. Structures of the DMSO-assisted domino cyclization of pyrroles, bond distances are in Å.

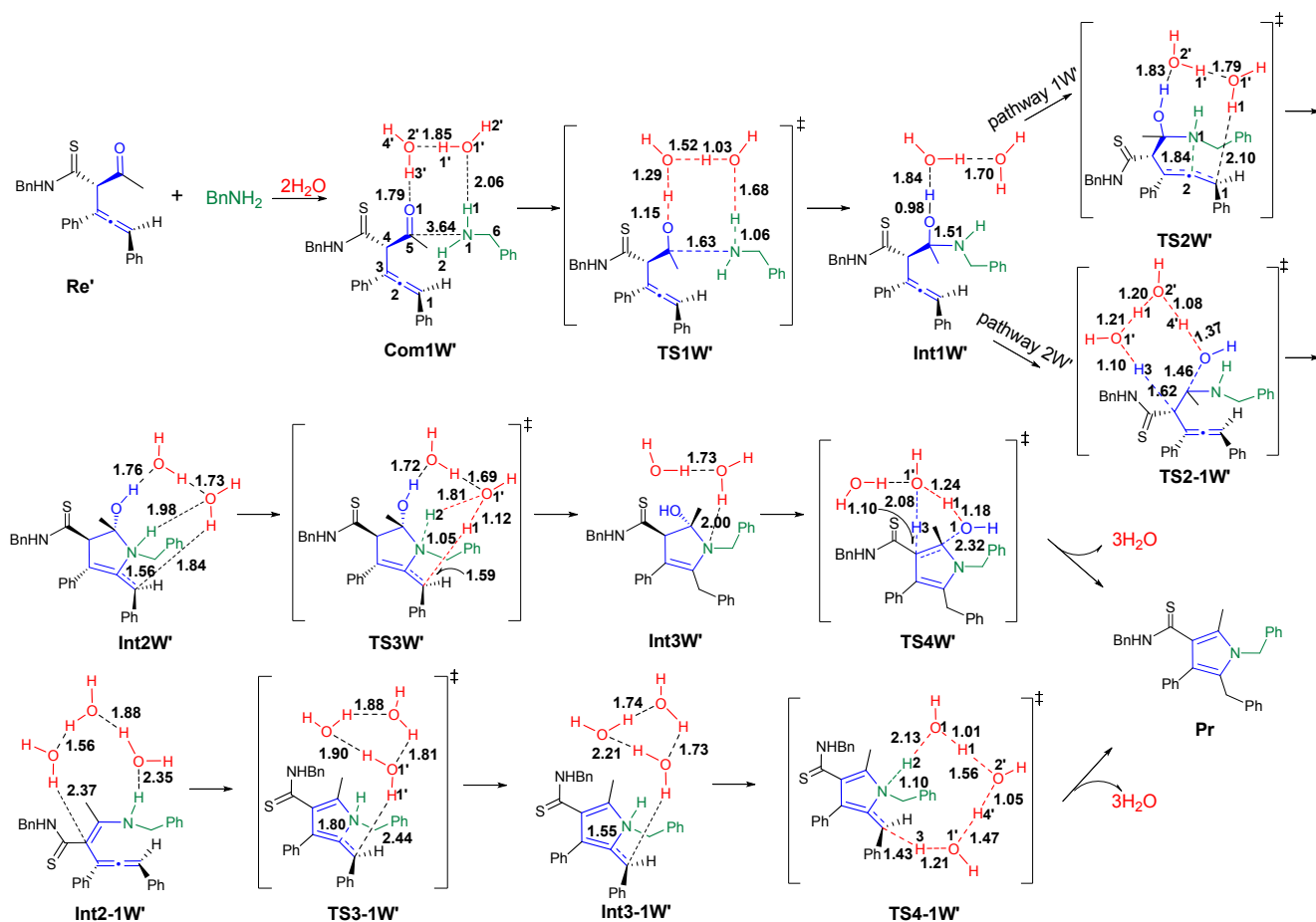
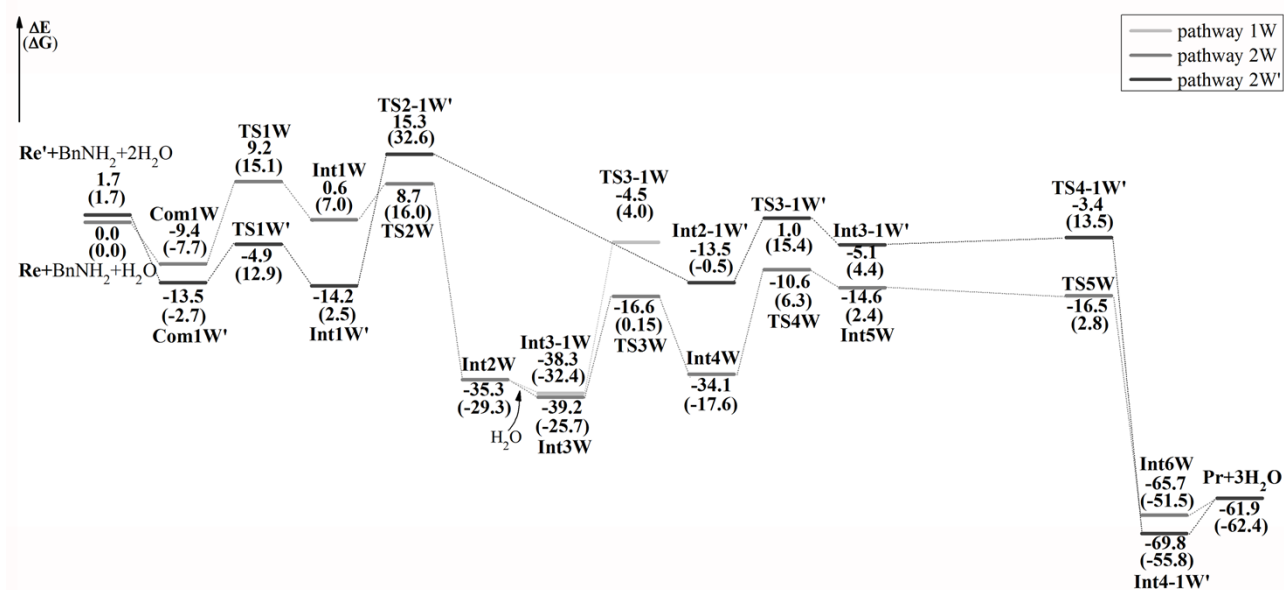


Figure S3. DFT computed energy surface for the water-catalyzed domino reaction of pyrroles and the corresponding geometry structures of reactants, intermediates, and transition states for pathways 1W' and 2W'. Distances are in Å and relative energies and free energies are given in kcal/mol.

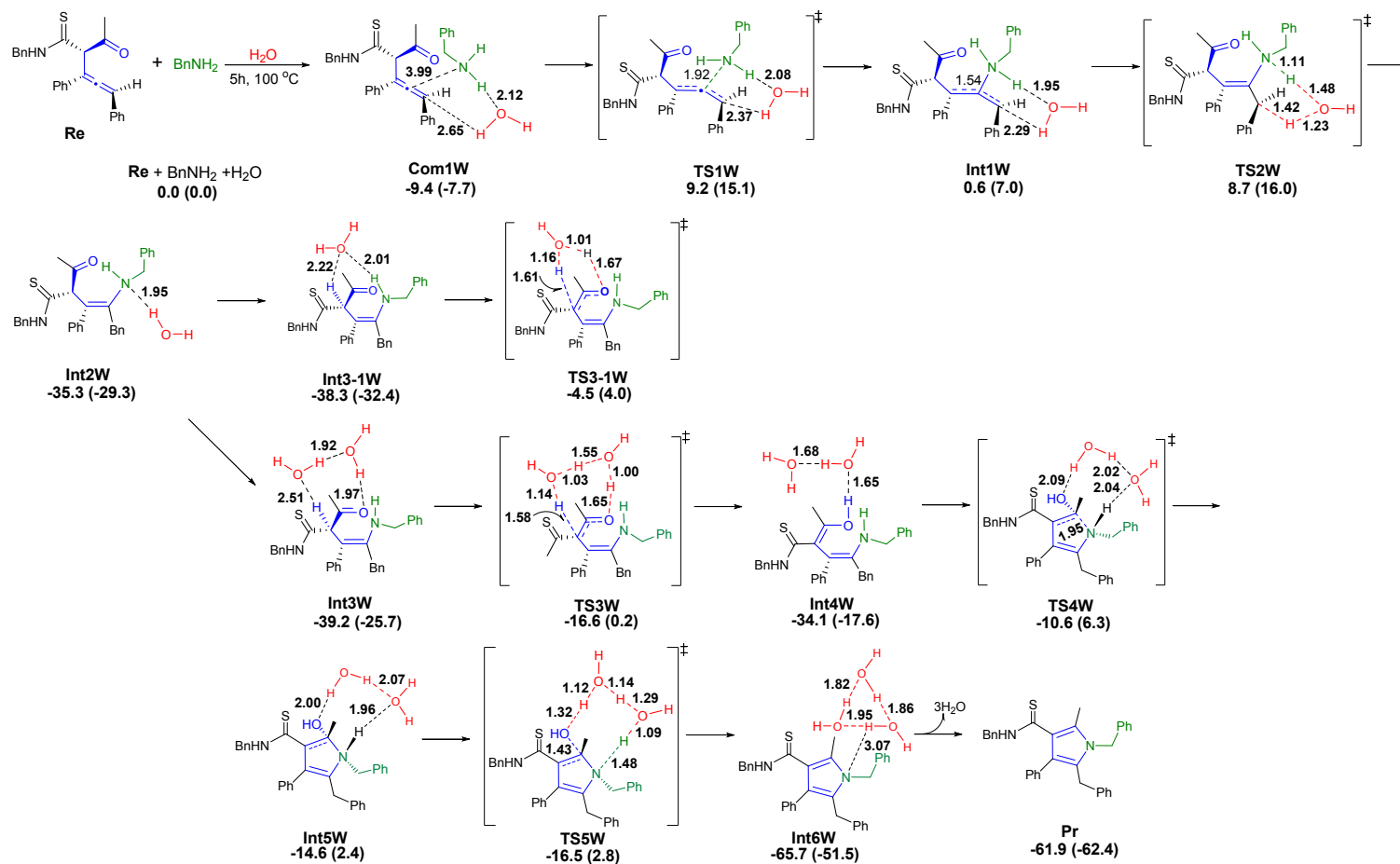


Figure S4. Structures of pathways 1W and 2W for the domino cyclization of pyrroles under trace water-catalyzed condition, bond distances are in Å.

S1. The effect of water cluster on the keto-enol tautomerization step

It was thought that water molecules could form clusters in the reaction system and that water could act as a reactive medium by supplying the protons via a hydrogen bonding network. Thus, we calculate single water, two water, and three water molecules catalyzed the deprotonation and the [1,3]-H shift processes, namely, keto-enol tautomerization. Our calculation results suggested that the two-water cluster as catalyst is more favorable in reducing energy barrier of the keto-enol tautomerization than one water molecule, and similar with the results of three cluster.

Table S3. Single water and two water molecules catalyzed deprotonation of the nitrogen of BnNH₂ in the mechanism of BnNH₂ attack the allenic carbon of **Re**, $\Delta\Delta E^\ddagger$ ($\Delta\Delta G^\ddagger$) values are in kcal/mol.

TSs	single water	two water molecules
	8.5	8.6
	(9.0)	(10.3)

Table S3 shows that the $\Delta\Delta E^\ddagger$ and $\Delta\Delta G^\ddagger$ values of single water catalyzed deprotonation process are 0.1 kcal/mol and 1.3 kcal/mol lower than that assisted by two water molecule.

Table S4. Single water, two water molecules and three water cluster catalyzed the [1,3]-H shift processes in the domino cyclization of pyrroles, $\Delta\Delta E^\ddagger$ ($\Delta\Delta G^\ddagger$) values are in kcal/mol.

TSs	single water	two water molecules	three water molecules
	36.3	23.0	23.6
	(25.6)	(26.8)	(28.8)

Table S4 suggests that the $\Delta\Delta E^\ddagger$ in two water molecules catalyzed [1,3]-H shift process is lower by 13.3 kcal/mol and 0.6 kcal/mol compared to that in single water and three water molecules catalyzed. Thereby, in the following water-catalyst mechanism and considering entropic disadvantages, we employed a two-water cluster as catalyst to calculate the reaction system.

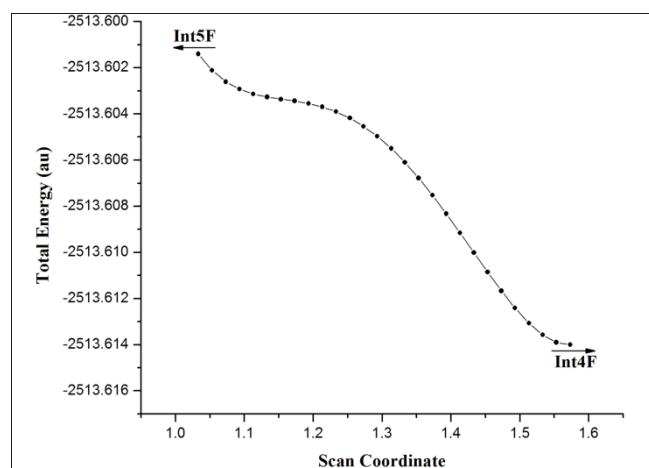


Figure S5. The potential energy surface scans for N2-H4 bond from **Int5F** to **Int4F**.

Table S5. Solvent Effects on the trace water-catalyzed mechanism of BnNH₂ attack to the carbonyl carbon of **Re'** for pathway 1W' at the PBE1PBE/6-311+G** level, ΔE (ΔG) values are in kcal/mol.

	PBE1PBE (gas)	PBE1PBE (solvent)	$\Delta E_{TS_{gas}} - \Delta E_{TS_{solvent}}$ ($\Delta G_{TS_{gas}} - \Delta G_{TS_{solvent}}$)
Re'+BnNH₂+2H₂O	0.0	0.0	
Com1W'	-13.5 (-2.7)	-6.6 (3.6)	-6.9 (6.3)
TS1W'	-4.9 (12.9)	2.1 (19.6)	-7.0 (-6.7)
Int1W'	-14.2 (2.5)	-5.2 (11.4)	-9.0 (-8.9)
TS2W'	4.8 (21.9)	11.2 (28.0)	-6.4 (-6.1)
Int2W'	-0.3 (17.2)	5.9 (23.1)	6.2 (-5.9)
TS3W'	-2.6 (15.6)	4.3 (22.4)	-6.9 (-6.8)
Int3W'	-47.2 (-29.7)	-39.8 (-22.6)	-7.4 (-7.1)
TS4W'	-32.0 (-14.9)	-24.4 (-7.6)	-7.6 (-7.3)
Int4W'	-64.1 (-50.0)	-57.0 (-43.4)	-7.1 (-6.6)

From Table S5, obviously the energy values of TSs in gas phase are much lower than those in solvent phase.

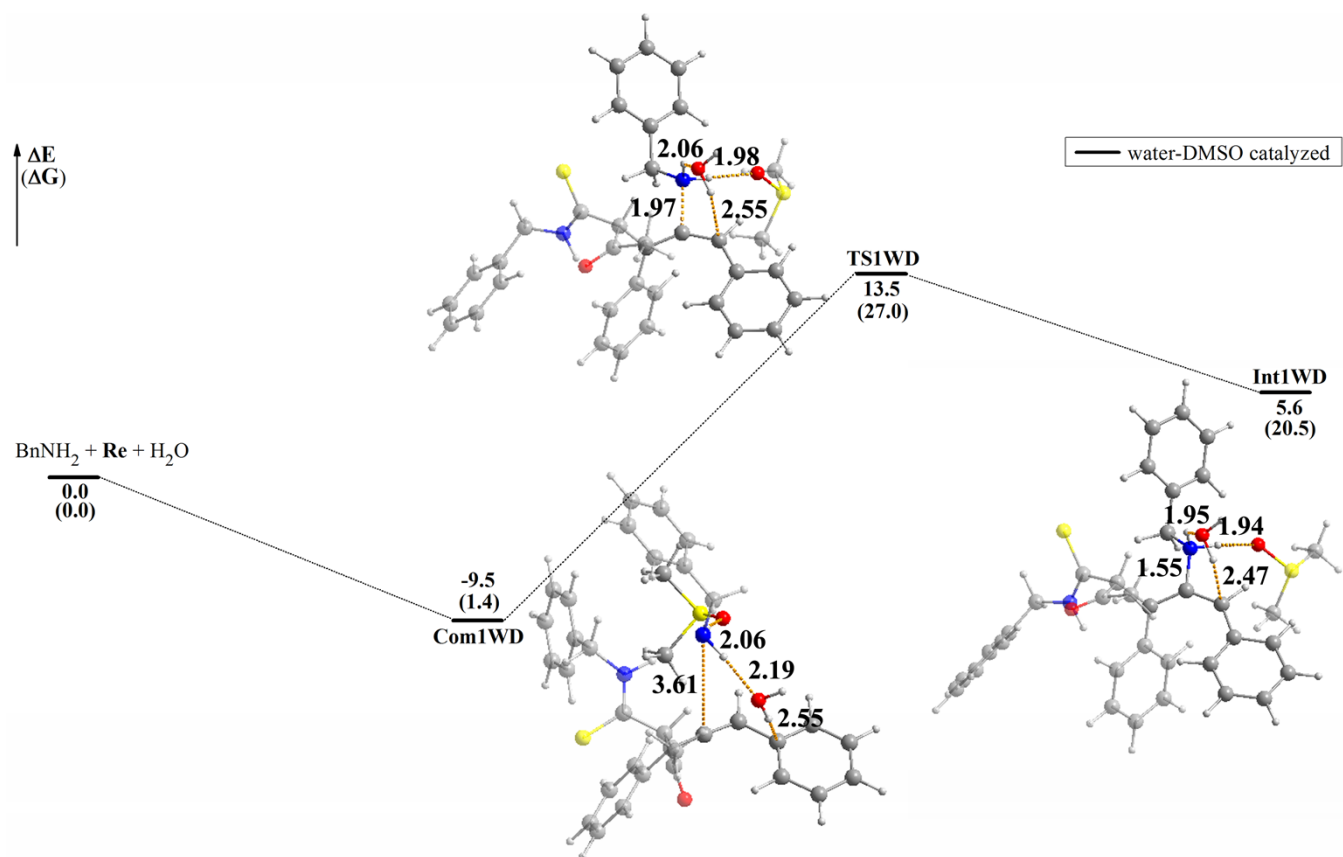


Figure S6. DFT computed energy profile of nucleophilic addition catalyzed by water-DMSO in solvent and the corresponding optimized structures, values and distances are in kcal/mol and Å.

S2. The PBE1PBE/6-31G** optimized coordinates for the formation of pyrroles.

Re

C	-5.31220300	-2.08444700	-2.04228500
C	-4.70987500	-0.82671600	-2.10882900
C	-3.95820700	-0.33889400	-1.03439300
C	-3.81413400	-1.13494500	0.11189300
C	-4.40874100	-2.39433600	0.17533700
C	-5.16062300	-2.87169000	-0.90078900
H	-5.89515300	-2.44884800	-2.88307400
H	-4.82608600	-0.21739100	-3.00148400
H	-3.23721400	-0.76609400	0.95569000
H	-4.28782400	-3.00049100	1.06822400
H	-5.62642900	-3.85137400	-0.84858200
C	-3.31777900	1.02939300	-1.09850100
H	-3.67646900	1.68140100	-0.29372800
H	-3.56625600	1.53500900	-2.03913700

N	-1.86327300	0.92953900	-0.96438900
H	-1.46187100	0.00325600	-1.05022700
C	-1.05035100	1.94330500	-0.63813200
S	-1.57806400	3.51303000	-0.41581800
C	0.42978000	1.53481200	-0.54799800
C	1.32526100	2.64979700	0.06297900
O	1.63029000	2.64387500	1.23744700
C	1.89316400	3.65596400	-0.91438200
H	2.66306500	3.16027100	-1.52079800
H	1.11902000	4.03019700	-1.58774200
H	2.34924300	4.48064700	-0.36554400
H	0.75612500	1.43128600	-1.59125900
C	0.67418600	0.16327600	0.11533100
C	-0.02370600	-0.24972500	1.37091000
C	-0.54785800	0.68734200	2.27594800
C	-0.18244400	-1.61758800	1.65790600
C	-1.20932000	0.26380600	3.42938600
H	-0.41158900	1.74596300	2.09668500
C	-0.83504700	-2.03643600	2.81406600
H	0.20995800	-2.35345300	0.96247900
C	-1.35711600	-1.09580200	3.70530400
H	-1.60262300	1.00570400	4.11808400
H	-0.94211000	-3.09856900	3.01521800
H	-1.87136500	-1.42002000	4.60526400
C	1.53334500	-0.63725500	-0.48485000
C	2.43150800	-1.39204700	-1.07749500
H	2.09139000	-2.11988400	-1.81682900
C	3.88820900	-1.35548500	-0.83688000
C	4.47026500	-0.46126800	0.07896600
C	4.72203100	-2.23677300	-1.54212200
C	5.84706600	-0.45446300	0.27819200
H	3.83534500	0.22539500	0.63176400
C	6.10173400	-2.22812400	-1.34036800
H	4.28233400	-2.93225600	-2.25261500
C	6.66926100	-1.33707600	-0.42958300
H	6.28232500	0.24127800	0.98962000
H	6.73191700	-2.91750500	-1.89474100
H	7.74345500	-1.32852400	-0.27067600

BnNH₂

C	-1.40538900	-1.33729600	0.05678300
C	-0.04147300	-1.06901100	0.17240300
C	0.42991700	0.24981300	0.13832200
C	-0.49310100	1.29007200	-0.01993100
C	-1.85889400	1.02438300	-0.13022100
C	-2.31951300	-0.29214500	-0.09251000
H	-1.75611900	-2.36543100	0.08333800
H	0.67642200	-1.87563700	0.27957500
H	-0.13877400	2.31780200	-0.05920000
H	-2.56062800	1.84459700	-0.25363300
H	-3.38134200	-0.50247700	-0.18345600
C	1.90821400	0.55195200	0.30118800
H	2.15593000	0.56159100	1.37191600
H	2.09831600	1.57653500	-0.06312900
N	2.74718100	-0.47611800	-0.32311300
H	2.62962400	-0.44780100	-1.33348900
H	3.72773000	-0.28295400	-0.13634300

DMSO

S	0.00001800	0.24190600	-0.43927200
O	0.00023500	1.50801500	0.38625300
C	-1.36362400	-0.82129200	0.18049100
H	-2.29822400	-0.31192500	-0.06126500
H	-1.33188800	-1.79445700	-0.31679000
H	-1.27562400	-0.93148800	1.26432200
C	1.36340000	-0.82164700	0.18047400
H	1.33125300	-1.79492900	-0.31654800
H	2.29814200	-0.31266500	-0.06153800
H	1.27550900	-0.93152300	1.26434700

Com1D

C	4.42551000	-1.60630300	1.78260200
C	3.91417000	-1.51850300	0.48454900
C	2.63016300	-1.99121700	0.18946800
C	1.85633300	-2.54021800	1.22267800
C	2.36354500	-2.62103700	2.51993300
C	3.65146800	-2.15822100	2.80428100
H	5.42926000	-1.24618300	1.99164600

H	4.51891800	-1.08072500	-0.30547700
H	0.85883300	-2.91078200	1.00798200
H	1.75266600	-3.05562300	3.30609500
H	4.04937400	-2.23327000	3.81249700
C	2.10618400	-1.94944800	-1.23530400
H	2.03105000	-2.96271500	-1.64238900
H	2.79563000	-1.37444700	-1.86200700
N	0.78411400	-1.34320000	-1.34428700
H	0.75529900	-0.30658200	-1.25142900
C	-0.34426300	-2.00736700	-1.61973000
S	-0.46063000	-3.65471800	-1.92228100
C	-1.58445900	-1.09682700	-1.60537400
C	-2.71923900	-1.56929600	-2.54242800
O	-3.84468100	-1.77247700	-2.13219600
C	-2.39836300	-1.60216000	-4.02476300
H	-2.34753700	-0.56954400	-4.39482800
H	-1.43970700	-2.08358400	-4.22444900
H	-3.19838900	-2.12240600	-4.55272100
H	-1.26896100	-0.13640100	-2.03519900
C	-2.05333500	-0.77827700	-0.17008000
C	-2.28729000	-1.83305800	0.86532800
C	-2.89963700	-3.06203700	0.57129300
C	-1.90398300	-1.58112400	2.19395300
C	-3.12114900	-3.99981400	1.57964200
H	-3.21965200	-3.27430500	-0.43874900
C	-2.13021000	-2.51787100	3.20012400
H	-1.42418000	-0.63691900	2.42993000
C	-2.74032600	-3.73571400	2.89544600
H	-3.59912600	-4.94270200	1.33064700
H	-1.82688700	-2.29772500	4.22010400
H	-2.91546900	-4.47136100	3.67522000
C	-2.20154300	0.49214600	0.14190500
C	-2.37946200	1.76452400	0.43176600
H	-1.54264700	2.32189500	0.86015200
C	-3.63033000	2.52410500	0.23158600
C	-4.77622700	1.93562100	-0.33261900
C	-3.68276800	3.87426500	0.61129700
C	-5.93740100	2.68189700	-0.50657400
H	-4.74501600	0.89225400	-0.63431500

C	-4.84820000	4.61970600	0.43562300
H	-2.80145500	4.33879000	1.04667600
C	-5.98015800	4.02635600	-0.12335400
H	-6.81478300	2.21355300	-0.94335700
H	-4.87074000	5.66355100	0.73561900
H	-6.88899100	4.60480600	-0.26084400
S	1.72565900	2.63659500	2.85478300
O	1.26872700	2.90131600	1.42228500
C	3.46069500	2.06260100	2.77957300
H	4.05870900	2.90311100	2.42283600
H	3.78535400	1.78058800	3.78460100
H	3.54791800	1.21721800	2.09298400
C	0.99249300	1.04598600	3.37557800
H	1.37074300	0.78447600	4.36723800
H	-0.08725200	1.19783500	3.42227800
H	1.23354800	0.26414400	2.65153700
C	5.20254100	2.20916200	-1.15207000
C	3.84616500	2.53061500	-1.20257300
C	3.02331200	2.00533100	-2.20881100
C	3.59186900	1.15515000	-3.16465000
C	4.95045200	0.83292000	-3.11912100
C	5.75966200	1.35926200	-2.11104900
H	5.82995300	2.62974400	-0.37090800
H	3.41174400	3.18917400	-0.45455400
H	2.96771400	0.74788300	-3.95630600
H	5.37616100	0.17782500	-3.87379800
H	6.81783900	1.11667900	-2.07778200
C	1.55051900	2.35304700	-2.24245600
H	1.14004900	2.10620200	-3.22758100
H	1.43830600	3.44013600	-2.11135400
N	0.79044000	1.59672600	-1.22300800
H	1.11006900	1.87793400	-0.29001200
H	-0.18349100	1.89685100	-1.25367200

TS1D

C	-6.67089300	-1.02580400	0.86881800
C	-5.32260600	-1.29623800	0.64032800
C	-4.93374900	-2.11240100	-0.43195400
C	-5.91931500	-2.65176700	-1.26520600

C	-7.27032600	-2.38641800	-1.03365600
C	-7.64833900	-1.57189200	0.03336300
H	-6.95998700	-0.39206500	1.70219000
H	-4.56473300	-0.86873900	1.29174300
H	-5.62724800	-3.28408600	-2.09975000
H	-8.02449800	-2.81331200	-1.68829800
H	-8.69861000	-1.36277400	0.21430000
C	-3.47195000	-2.41528800	-0.67156800
H	-3.35111900	-3.15816000	-1.46910500
H	-3.00058100	-2.84345500	0.21998000
N	-2.73005100	-1.20351700	-1.02325400
H	-3.24892200	-0.37288900	-1.31911500
C	-1.40781100	-1.12127100	-1.09208900
S	-0.39112600	-2.44730100	-0.81087400
C	-0.80833200	0.24542200	-1.45065000
C	-1.68229400	1.20786800	-2.26416600
O	-2.90827000	1.23696800	-2.19744100
C	-0.93923900	2.15470700	-3.18193600
H	-0.01620800	2.52132100	-2.72834800
H	-0.67093600	1.61048400	-4.09722900
H	-1.58807900	2.98890700	-3.45228800
H	0.04781800	0.01789400	-2.09111800
C	-0.22063900	1.01179100	-0.24407900
C	-0.97604800	1.25504500	1.00312000
C	-2.37827600	1.41987100	1.04063700
C	-0.29257400	1.35155600	2.23930900
C	-3.05122200	1.65693700	2.24106100
H	-2.95216500	1.40172700	0.12339200
C	-0.96795900	1.59947700	3.42987300
H	0.78513300	1.22288900	2.25476300
C	-2.35814900	1.74809600	3.44691100
H	-4.13007800	1.79136800	2.22161400
H	-0.40199500	1.67319300	4.35545000
H	-2.88450400	1.93897600	4.37730600
C	1.10745900	1.34921400	-0.31509000
C	1.97640400	2.36498100	-0.19822600
H	3.02600000	2.13380900	-0.02942900
C	1.67601200	3.80100500	-0.26867200
C	0.37122800	4.33303200	-0.28141400

C	2.75566400	4.70478300	-0.32656700
C	0.16474000	5.70709800	-0.37794700
H	-0.47624700	3.66362600	-0.19798000
C	2.54578200	6.07814500	-0.41451300
H	3.77102800	4.31613600	-0.30625200
C	1.24633400	6.58836900	-0.44579100
H	-0.85082100	6.09341300	-0.38470000
H	3.39769900	6.75108800	-0.45899300
H	1.07877600	7.65943100	-0.51117800
S	2.82929700	-1.83445600	3.01900600
O	3.14066800	-0.62009400	2.14426400
C	3.30118200	-3.32446200	2.06778500
H	4.37986100	-3.27879900	1.91118000
H	3.04309900	-4.21369500	2.64891800
H	2.79131500	-3.32973100	1.10199600
C	1.02283100	-2.10813000	2.98023800
H	0.79272200	-2.99057800	3.58380400
H	0.55293300	-1.22452000	3.41545300
H	0.67259000	-2.23611900	1.95215900
C	6.21306700	-2.50415000	-0.66213500
C	5.38971900	-1.38457400	-0.79267400
C	4.17062800	-1.46980100	-1.47748900
C	3.79111600	-2.70230200	-2.02826800
C	4.61082000	-3.82318600	-1.89706400
C	5.82575800	-3.72665300	-1.21436300
H	7.15968400	-2.41917300	-0.13596200
H	5.69407300	-0.43648500	-0.35712800
H	2.84536000	-2.78300900	-2.55852600
H	4.30476500	-4.76949900	-2.33368200
H	6.46846700	-4.59697500	-1.11865500
C	3.25876900	-0.26466800	-1.58864900
H	2.75888900	-0.25095500	-2.56273800
H	3.83909700	0.65987000	-1.51204000
N	2.21345000	-0.23024400	-0.54665900
H	1.52602700	-0.98402300	-0.68081400
H	2.61092000	-0.35599500	0.40012000

Int1D

C	-6.60555600	-0.28874100	0.87627100
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C	-5.29097600	-0.73214300	0.74192900
C	-4.99999400	-1.86528300	-0.03179000
C	-6.04798500	-2.54242400	-0.66367400
C	-7.36574900	-2.10233000	-0.52447000
C	-7.64673300	-0.97385000	0.24512600
H	-6.81831200	0.59041200	1.47749200
H	-4.48416800	-0.19287400	1.23126800
H	-5.83198400	-3.41994000	-1.26788300
H	-8.16936500	-2.63884600	-1.02039400
H	-8.67067000	-0.62815000	0.35256900
C	-3.57594400	-2.35842500	-0.16001000
H	-3.53661000	-3.28300200	-0.74897300
H	-3.14511300	-2.59615600	0.81819600
N	-2.71554400	-1.34910600	-0.77982600
H	-3.13997900	-0.64085300	-1.38693700
C	-1.39392000	-1.31929100	-0.70329800
S	-0.48907700	-2.52169700	0.09029200
C	-0.66311100	-0.15137000	-1.38429500
C	-1.39505500	0.59360800	-2.50711100
O	-2.61792600	0.63010900	-2.62508400
C	-0.51452400	1.30377100	-3.51656900
H	0.45609900	1.58280300	-3.10473700
H	-0.35734400	0.62832900	-4.36832200
H	-1.03266900	2.18921000	-3.88969500
H	0.17126900	-0.62683200	-1.90799900
C	-0.03485100	0.87067500	-0.41599600
C	-0.85344400	1.68913900	0.48015900
C	-2.26618500	1.78773100	0.37478400
C	-0.27586700	2.41445800	1.55979600
C	-3.02929100	2.51648900	1.28554900
H	-2.78609900	1.31367000	-0.44379400
C	-1.04500700	3.13322000	2.46790000
H	0.80028500	2.41033800	1.68056000
C	-2.43566900	3.19380000	2.35043700
H	-4.10669300	2.56248700	1.14315300
H	-0.54401400	3.66561400	3.27319100
H	-3.03280900	3.76672200	3.05321300
C	1.38985800	0.90997500	-0.38924800
C	2.32195100	1.91356500	-0.26734700

H	3.32133100	1.60210000	0.03399100
C	2.21034300	3.34590700	-0.48957400
C	1.04439300	4.01252700	-0.93014500
C	3.36816400	4.13554100	-0.29272300
C	1.05533200	5.38292200	-1.18236100
H	0.13135200	3.45189900	-1.07804100
C	3.37002500	5.50419900	-0.53257400
H	4.27993100	3.65128400	0.04998600
C	2.20997200	6.14133200	-0.98362500
H	0.14349600	5.86452400	-1.52569800
H	4.27905000	6.07712000	-0.36916000
H	2.20596600	7.21132000	-1.16979600
S	2.72439500	-1.14010300	3.32884700
O	3.35731200	-0.61693800	2.03084800
C	2.38076100	-2.91621600	3.06847100
H	3.34176300	-3.40393400	2.89734000
H	1.91103500	-3.32119300	3.96856500
H	1.73060200	-3.04744900	2.20061900
C	0.99216400	-0.56967800	3.37304100
H	0.52817900	-0.95518900	4.28500200
H	1.00391400	0.52082300	3.39569300
H	0.45128900	-0.91327200	2.48744100
C	5.34060600	-3.55203800	-0.34469800
C	4.73350400	-2.30453900	-0.48232100
C	3.65887800	-2.13248700	-1.36729600
C	3.20585800	-3.23196300	-2.10664000
C	3.81504100	-4.47983800	-1.97120200
C	4.88479900	-4.64169500	-1.09047500
H	6.17580300	-3.67159600	0.33931800
H	5.08267400	-1.46505800	0.11154100
H	2.37125300	-3.11114300	-2.79214000
H	3.45439600	-5.32236900	-2.55351400
H	5.36284900	-5.61131200	-0.98647700
C	3.00097500	-0.78222700	-1.52175900
H	2.41716600	-0.73139100	-2.44447400
H	3.73340200	0.02568600	-1.55053900
N	2.06502600	-0.46927900	-0.38432900
H	1.33261400	-1.20783500	-0.30815100
H	2.58697000	-0.53972200	0.52874700

Int2D

C	7.27893000	-1.05610000	-1.34573200
C	5.94046300	-1.26585200	-1.01654700
C	5.59188400	-2.18102300	-0.01247600
C	6.60613200	-2.88013700	0.65020500
C	7.94668300	-2.67506900	0.31717400
C	8.28543500	-1.76166300	-0.68108300
H	7.53672200	-0.34357900	-2.12474300
H	5.16032700	-0.71170500	-1.53310200
H	6.34542100	-3.59016600	1.43189700
H	8.72371900	-3.22588800	0.84047800
H	9.32808100	-1.59857300	-0.94042300
C	4.13899500	-2.41829700	0.33458600
H	4.03879400	-3.22672100	1.06982800
H	3.56176900	-2.72527500	-0.54487000
N	3.51360500	-1.20418200	0.86314800
H	4.11295500	-0.45714000	1.22564700
C	2.20992600	-1.02382500	1.01617900
S	1.06730100	-2.23420700	0.66959500
C	1.73183500	0.34220400	1.52637900
C	2.71050400	1.17780600	2.36095500
O	3.93337600	1.07531100	2.29320800
C	2.08206000	2.17380400	3.31733600
H	1.11044200	2.53158200	2.97035100
H	1.94725700	1.68105900	4.29104600
H	2.76149300	3.01697300	3.46290600
H	0.92991900	0.10699800	2.23354700
C	1.10114800	1.23788000	0.44166200
C	1.85356100	1.69211100	-0.72966200
C	3.27043100	1.67480800	-0.81468300
C	1.18270200	2.14792800	-1.89779300
C	3.94751200	2.04965900	-1.97519300
H	3.86431100	1.39686500	0.04422400
C	1.86314200	2.51797700	-3.05128300
H	0.10007200	2.21358200	-1.88884400
C	3.25864400	2.46927700	-3.11281100
H	5.03579100	2.02719900	-1.97431000
H	1.29195400	2.85389600	-3.91443000

H	3.79016700	2.76677500	-4.01243800
C	-0.29104100	1.50910900	0.59140900
C	-1.06793400	2.62697800	0.39769300
H	-2.14341500	2.45893700	0.33710200
C	-0.70518800	4.03110500	0.28424300
C	0.61048900	4.54258200	0.35666100
C	-1.75187900	4.97109800	0.12859800
C	0.84993400	5.91438900	0.30039500
H	1.44468200	3.86176400	0.45872600
C	-1.50736000	6.33747900	0.05963400
H	-2.77721400	4.60879400	0.07044900
C	-0.19887700	6.82276500	0.14726700
H	1.87419700	6.27435800	0.36286500
H	-2.33931400	7.02744600	-0.06112300
H	-0.00164400	7.88991200	0.08982800
S	-2.25305300	-4.24757100	-2.20459800
O	-2.82042400	-2.86732400	-2.52527400
C	-2.12231600	-4.37568700	-0.38588900
H	-3.13643700	-4.32585100	0.01649900
H	-1.66492900	-5.33517000	-0.12564800
H	-1.52884400	-3.54706500	0.00962600
C	-0.45826800	-4.18830900	-2.55334900
H	-0.01272500	-5.15487300	-2.29869100
H	-0.34897900	-4.00262800	-3.62453900
H	0.01422600	-3.38633700	-1.97817800
C	-4.78357000	-2.25627900	2.14475000
C	-4.06698200	-1.07952000	1.92248500
C	-2.75806500	-0.94334900	2.40334900
C	-2.18022800	-2.00720300	3.11103900
C	-2.89618900	-3.18282200	3.33572600
C	-4.20152100	-3.30904400	2.85377900
H	-5.79794700	-2.34214800	1.76615700
H	-4.53219400	-0.26369000	1.37589600
H	-1.16374100	-1.91616600	3.48582900
H	-2.43746900	-3.99566700	3.89215100
H	-4.76433300	-4.22070800	3.03728600
C	-1.98334500	0.33224900	2.16973500
H	-1.29664500	0.53753800	2.99652900
H	-2.65046400	1.18980300	2.07576300

N	-1.15110700	0.28304100	0.91651100
H	-0.53825300	-0.55791100	0.92874500
H	-1.75617700	0.13064100	0.03868800
C	-6.47614200	1.40801300	-0.29676000
C	-5.23059300	1.57165600	-0.90922100
C	-4.63852600	0.52450000	-1.62639600
C	-5.32086400	-0.69770800	-1.72211400
C	-6.56448100	-0.86303100	-1.11127800
C	-7.14671600	0.18809100	-0.39686100
H	-6.92289200	2.23413100	0.25049600
H	-4.71731400	2.52863500	-0.83990800
H	-4.86865200	-1.52352100	-2.26608900
H	-7.08532000	-1.81327700	-1.20031800
H	-8.11915600	0.05933400	0.07139600
C	-3.29110200	0.70627300	-2.29387700
H	-2.99199400	1.75769400	-2.23671100
H	-3.37671200	0.44910500	-3.36071800
N	-2.23331200	-0.09899800	-1.63728300
H	-2.40698600	-1.09546700	-1.82387000
H	-1.34378600	0.11308300	-2.09443800

TS2D

C	6.98295100	-0.87845800	-0.80699400
C	5.65836600	-1.11467100	-0.44247400
C	5.35590600	-1.74482200	0.77364000
C	6.40499100	-2.13509400	1.61231500
C	7.73287100	-1.90480300	1.24618400
C	8.02426400	-1.27478600	0.03637000
H	7.20369800	-0.38620600	-1.75038800
H	4.84975900	-0.80479300	-1.10072500
H	6.18124000	-2.62217300	2.55870200
H	8.53706300	-2.21416500	1.90840200
H	9.05665400	-1.09142200	-0.24891600
C	3.91743500	-2.00820300	1.15998800
H	3.86270400	-2.60058800	2.08232600
H	3.39660500	-2.58848800	0.39030600
N	3.17797800	-0.75906400	1.34152800
H	3.70098100	0.10837100	1.50381500
C	1.85503100	-0.64075600	1.31678400

S	0.80933100	-1.95749800	1.10678300
C	1.26450800	0.76469700	1.53575100
C	2.19152300	1.85646100	2.07404600
O	3.40584100	1.88808700	1.86841600
C	1.53574400	2.94532300	2.90295900
H	0.47918500	3.08284500	2.66558100
H	1.62338200	2.66467900	3.96291600
H	2.07425400	3.88597700	2.76457900
H	0.51754600	0.61847700	2.32450400
C	0.51285800	1.40405500	0.35448400
C	1.12821700	1.61206900	-0.94197100
C	2.51109400	1.37532500	-1.19969300
C	0.37167700	2.01891000	-2.08531800
C	3.05598900	1.46709900	-2.47671400
H	3.17723200	1.14772200	-0.38057100
C	0.92661000	2.09776700	-3.36038200
H	-0.66471800	2.31185000	-1.95538000
C	2.27451900	1.80762400	-3.58537800
H	4.12247200	1.28553500	-2.60149200
H	0.29338900	2.41487300	-4.18717700
H	2.70888700	1.88550100	-4.57798500
C	-0.89587000	1.63698200	0.57930300
C	-1.69014900	2.72904000	0.34919400
H	-2.76504700	2.56568500	0.41848700
C	-1.35378200	4.12266800	0.07217200
C	-0.04713300	4.63277700	-0.09425300
C	-2.42131900	5.04651300	-0.00943800
C	0.16784600	5.99444300	-0.30208300
H	0.79819100	3.95922500	-0.05712400
C	-2.20370900	6.40189400	-0.23013900
H	-3.44014000	4.68274600	0.11275500
C	-0.90144600	6.88860400	-0.37598600
H	1.18637600	6.35602600	-0.42189500
H	-3.05114800	7.08106900	-0.28640400
H	-0.72504400	7.94655400	-0.55144500
S	0.03870700	-3.37380000	-3.25553300
O	-1.30276500	-2.82356400	-2.76573400
C	0.66325800	-4.49484600	-1.95372100
H	-0.05193100	-5.31688200	-1.87232200

H	1.63913800	-4.88510300	-2.25944100
H	0.73774500	-3.95888100	-1.00275200
C	1.28971400	-2.05935100	-3.03707100
H	2.26709200	-2.45758200	-3.32688000
H	1.02675400	-1.22774000	-3.69501700
H	1.30378500	-1.71907800	-1.99776200
C	-3.91279100	-2.99062900	2.95194700
C	-3.75810700	-1.81568800	2.21609300
C	-2.98949600	-0.75782300	2.71916100
C	-2.38496200	-0.89877300	3.97558200
C	-2.53944000	-2.07252900	4.71305400
C	-3.30396800	-3.12243200	4.20140400
H	-4.51337900	-3.80163400	2.54876700
H	-4.24127300	-1.71852500	1.24774000
H	-1.79452700	-0.07996800	4.38157300
H	-2.06645000	-2.16538100	5.68700100
H	-3.42728700	-4.03704600	4.77526700
C	-2.79923400	0.50951400	1.91917600
H	-2.61549800	1.36582400	2.57657900
H	-3.70163700	0.72630700	1.33891400
N	-1.64634600	0.40394800	0.96694200
H	-0.98028600	-0.31819500	1.28071800
H	-1.94999900	-0.05251900	-0.19031800
C	-6.59602600	-0.81883900	-0.61964800
C	-5.48588700	-0.13327600	-1.11928800
C	-4.42062100	-0.82673000	-1.70666200
C	-4.48427300	-2.22623600	-1.79001300
C	-5.59035700	-2.91102900	-1.28610800
C	-6.64907800	-2.21061200	-0.70075300
H	-7.41599200	-0.26548700	-0.16978900
H	-5.45144300	0.95273400	-1.06069200
H	-3.66461700	-2.77490100	-2.24833300
H	-5.62943100	-3.99488500	-1.35736200
H	-7.51139000	-2.74713000	-0.31404500
C	-3.22473000	-0.08028700	-2.25568000
H	-3.39662100	0.99908500	-2.20789500
H	-3.06234200	-0.34932600	-3.30674600
N	-1.98029100	-0.36938100	-1.49159200
H	-1.69884200	-1.34927600	-1.65877100

H	-1.21563400	0.19578400	-1.87994200
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Int3D

C	6.89019700	-0.61746800	-0.73745500
C	5.58816300	-0.87941200	-0.31505900
C	5.35119900	-1.49640800	0.92196800
C	6.44321900	-1.84750100	1.72211200
C	7.74864300	-1.59208500	1.29749200
C	7.97464300	-0.97502500	0.06756400
H	7.05990600	-0.13431400	-1.69530400
H	4.74609500	-0.59998700	-0.94300800
H	6.27079400	-2.32255100	2.68455300
H	8.58627400	-1.87006100	1.93050000
H	8.98896200	-0.77075500	-0.26234700
C	3.93776100	-1.79678400	1.36946400
H	3.94191000	-2.31396900	2.33711700
H	3.42912400	-2.46485300	0.66689000
N	3.13450800	-0.58026100	1.47220900
H	3.60783900	0.31976500	1.61588300
C	1.81170500	-0.51690300	1.36214800
S	0.83253700	-1.87634900	1.09259600
C	1.15805800	0.86375800	1.55030900
C	2.04275200	2.01698800	2.02506500
O	3.25470100	2.08823200	1.80657600
C	1.34929300	3.11586600	2.80565200
H	0.29205500	3.21075900	2.55533700
H	1.43628700	2.87656800	3.87477600
H	1.86204000	4.06441500	2.63574600
H	0.44137000	0.70395700	2.36332000
C	0.34113100	1.41884200	0.37288600
C	0.91474800	1.58091000	-0.93724900
C	2.30116100	1.35928100	-1.22123900
C	0.12619100	1.92230800	-2.08803100
C	2.81274700	1.39962500	-2.51123900
H	2.99276000	1.19856600	-0.40735400
C	0.65474200	1.94433100	-3.37927000
H	-0.90002700	2.24142300	-1.94426300
C	1.99925200	1.66187500	-3.62260200
H	3.88040300	1.24022900	-2.65145800

H	0.00016900	2.21776200	-4.20452700
H	2.41147100	1.70196300	-4.62588100
C	-1.08179500	1.61188800	0.63958700
C	-1.88656900	2.69316700	0.36262400
H	-2.95425800	2.53199000	0.50068400
C	-1.57873800	4.06599400	-0.02534800
C	-0.28559300	4.59666100	-0.23518800
C	-2.66619200	4.95891900	-0.17738400
C	-0.10315900	5.94135300	-0.55260200
H	0.57648900	3.95135300	-0.13923900
C	-2.48099300	6.29682600	-0.50668600
H	-3.67576200	4.58380300	-0.02206300
C	-1.19207100	6.80263300	-0.69583500
H	0.90652500	6.31571500	-0.70089100
H	-3.34464100	6.94830900	-0.61339000
H	-1.04099800	7.84659600	-0.95477900
S	0.44763100	-3.44916900	-3.14473600
O	-0.92147800	-2.88260700	-2.73598700
C	1.00418200	-4.51689700	-1.77434400
H	0.28290800	-5.33230600	-1.69631900
H	1.98976900	-4.91967700	-2.02342600
H	1.03787900	-3.94219400	-0.84475000
C	1.67073700	-2.11561700	-2.92448200
H	2.66182000	-2.51433700	-3.15746900
H	1.42672300	-1.31261900	-3.62269900
H	1.63455200	-1.73956300	-1.89912000
C	-3.98242700	-2.92608400	3.11907200
C	-3.82253000	-1.74337600	2.39732100
C	-3.06837000	-0.68430500	2.91977000
C	-2.47902200	-0.83646200	4.18127300
C	-2.63862200	-2.01760700	4.90646100
C	-3.39076600	-3.06638800	4.37579400
H	-4.57250900	-3.73669100	2.70097700
H	-4.29272100	-1.63723200	1.42336100
H	-1.89662200	-0.01961200	4.60075300
H	-2.17864600	-2.11734800	5.88540800
H	-3.51785400	-3.98607800	4.93955800
C	-2.86768200	0.58600500	2.12472500
H	-2.68678800	1.43670400	2.79669900

H	-3.78638900	0.81269200	1.57128300
N	-1.74407100	0.44733600	1.17491400
H	-1.07992900	-0.27139400	1.46446200
H	-1.86558600	-0.39556900	-0.48562800
C	-6.30198700	-1.13395500	-0.87863400
C	-5.17949800	-0.42322500	-1.30821800
C	-4.09487700	-1.09029800	-1.89018900
C	-4.14706800	-2.48406700	-2.03961300
C	-5.26592600	-3.19277100	-1.60344500
C	-6.34523100	-2.52093700	-1.02402900
H	-7.13851900	-0.60460200	-0.43248900
H	-5.14761300	0.65747100	-1.19515100
H	-3.30744400	-3.00765900	-2.48933600
H	-5.29820500	-4.27186400	-1.72171100
H	-7.21719300	-3.07601300	-0.69088500
C	-2.88736800	-0.31090800	-2.35450200
H	-3.07608400	0.76349200	-2.31123400
H	-2.60893900	-0.57704700	-3.37720900
N	-1.67948900	-0.57700800	-1.50675600
H	-1.32663000	-1.54361700	-1.68437800
H	-0.92008800	0.07472700	-1.77591500

Int4D

C	7.45224700	-1.62766300	0.39937500
C	6.30578100	-0.90054700	0.71696700
C	6.29275500	0.49642100	0.59914400
C	7.45050800	1.14781900	0.15949200
C	8.60061600	0.42216300	-0.15555100
C	8.60343100	-0.96764000	-0.03653800
H	7.44943300	-2.70973200	0.49537300
H	5.41029800	-1.41560500	1.05465000
H	7.45052800	2.23068700	0.06492700
H	9.49205600	0.94243800	-0.49386000
H	9.49732000	-1.53420000	-0.28097400
C	5.04741300	1.28213700	0.94325500
H	5.27660800	2.34635400	1.07135000
H	4.61644600	0.94653800	1.89358200
N	4.02697500	1.13451300	-0.09351900
H	4.25527600	0.62844900	-0.95480100

C	2.80571000	1.65605900	-0.02746100
S	2.29641700	2.59289200	1.28904300
C	1.87637700	1.36437300	-1.20481500
C	2.52558000	0.97824900	-2.53848700
O	3.58726200	0.36073400	-2.63925500
C	1.76736500	1.38762000	-3.78319300
H	0.69641100	1.48478000	-3.60216900
H	2.14318800	2.37369100	-4.08880700
H	1.97283600	0.68360000	-4.59192700
H	1.31088600	2.27653400	-1.38772800
C	0.83238300	0.25612800	-0.92069900
C	1.27608600	-0.92497500	-0.14290900
C	2.38876800	-1.72608600	-0.48142400
C	0.62414500	-1.23517100	1.07052300
C	2.81629400	-2.76860400	0.34372400
H	2.92777000	-1.53408200	-1.40181400
C	1.03863300	-2.28315100	1.88879800
H	-0.18745000	-0.59219300	1.39145600
C	2.14753500	-3.05896200	1.53411200
H	3.67613600	-3.36323300	0.04436000
H	0.50210300	-2.48863900	2.81164100
H	2.48943000	-3.86397500	2.17932900
C	-0.49971500	0.45842400	-1.31380100
C	-1.52019400	-0.51776900	-1.55128400
H	-2.51238400	-0.07285600	-1.66193100
C	-1.42889600	-1.81710200	-2.19353000
C	-0.23146000	-2.43735400	-2.63706900
C	-2.63066200	-2.52627600	-2.47957100
C	-0.24502500	-3.65473800	-3.31503000
H	0.71092500	-1.93224900	-2.47797100
C	-2.63713500	-3.74331600	-3.15477400
H	-3.57980500	-2.06896600	-2.20411800
C	-1.43951100	-4.33222200	-3.57687000
H	0.69953400	-4.07687900	-3.65089000
H	-3.58751100	-4.22717400	-3.37224700
H	-1.44040700	-5.27896500	-4.10859600
S	-1.33974100	1.34133900	4.17306900
O	-2.04019600	0.58228800	3.04055000
C	-0.88142700	2.97665500	3.50835200

H	-1.80977100	3.48849800	3.24926200
H	-0.35901900	3.53365600	4.29088700
H	-0.24539600	2.86004400	2.62716600
C	0.35272100	0.67609800	4.32661400
H	0.86922800	1.23990600	5.10815100
H	0.26129900	-0.36934800	4.62575900
H	0.88365100	0.75954600	3.37522800
C	-0.80223400	6.33394600	-1.44298700
C	-0.49195100	5.04391200	-1.01284200
C	-1.49992300	4.08578700	-0.83704900
C	-2.82644600	4.45287000	-1.09805900
C	-3.14026300	5.74206600	-1.53281200
C	-2.12771000	6.68611600	-1.70760400
H	-0.00982300	7.06678200	-1.56803100
H	0.53807300	4.77557700	-0.79263400
H	-3.62003100	3.72309100	-0.95321100
H	-4.17459100	6.01037800	-1.73080500
H	-2.36955200	7.69102200	-2.04219900
C	-1.16000500	2.67694800	-0.40266100
H	-1.97231000	2.27746400	0.22743500
H	-0.25136500	2.68125600	0.20438400
N	-0.91725600	1.80711300	-1.57286500
H	-1.73794400	1.80333000	-2.16950900
H	-2.26298600	-1.02696500	0.15794500
C	-6.38310100	0.90883000	-0.99796000
C	-5.67853900	-0.22787200	-0.59834100
C	-4.90456800	-0.21689800	0.56816600
C	-4.84713700	0.95573200	1.33557400
C	-5.54830300	2.09244800	0.93350200
C	-6.31965700	2.07224800	-0.23157300
H	-6.97845400	0.88327200	-1.90567000
H	-5.73573800	-1.13336700	-1.19681900
H	-4.24063700	0.98170900	2.23667400
H	-5.49675600	2.99586400	1.53410000
H	-6.86877500	2.95782400	-0.53757700
C	-4.18949300	-1.47353000	1.00941900
H	-4.39871200	-2.29359500	0.32022800
H	-4.51748500	-1.78643200	2.00504000
N	-2.69950100	-1.34589800	1.07995500

H	-2.40983300	-0.67549500	1.81368900
H	-2.31823700	-2.29139500	1.31751600
S	-1.92494400	-5.29096300	1.30848700
O	-2.21661800	-3.91052700	1.91221900
C	-0.58755400	-5.10568000	0.08717700
H	0.30976900	-4.80738700	0.63076300
H	-0.43303700	-6.07322700	-0.39781400
H	-0.83999600	-4.34118100	-0.65035400
C	-3.26937600	-5.64729800	0.12398700
H	-3.09312500	-6.62869500	-0.32426400
H	-4.20060600	-5.66427400	0.69316100
H	-3.29466500	-4.87569000	-0.64976500

TS3D

C	-7.41100500	1.51957100	0.29443700
C	-6.26451400	0.80767400	0.64509300
C	-6.23181200	-0.58942400	0.53297900
C	-7.36961100	-1.25655800	0.06547400
C	-8.51958400	-0.54607800	-0.28255100
C	-8.54215900	0.84405400	-0.16908200
H	-7.42385700	2.60188300	0.38646800
H	-5.38496900	1.33556000	1.00419500
H	-7.35429200	-2.33969100	-0.02460700
H	-9.39550000	-1.07834300	-0.64198500
H	-9.43608000	1.39880600	-0.43903200
C	-4.98675100	-1.35978100	0.91077800
H	-5.20652300	-2.42575700	1.03940600
H	-4.58069400	-1.01402700	1.86851400
N	-3.94487200	-1.20821800	-0.10459900
H	-4.15653700	-0.69453100	-0.96411200
C	-2.73283900	-1.74888900	-0.02459900
S	-2.25526600	-2.71316600	1.28018400
C	-1.77578000	-1.45361500	-1.17972500
C	-2.40706100	-1.11144800	-2.53774700
O	-3.46264600	-0.49426400	-2.66666300
C	-1.63595900	-1.57368200	-3.75366900
H	-0.56080500	-1.59823300	-3.56848100
H	-1.95102200	-2.60275400	-3.97398400
H	-1.88461900	-0.94865900	-4.61315500

H	-1.18965400	-2.35674500	-1.33202200
C	-0.76673800	-0.31284100	-0.87949300
C	-1.28186600	0.86978900	-0.13347000
C	-2.33517700	1.68910300	-0.58596900
C	-0.76602500	1.13845300	1.15031000
C	-2.83980700	2.72480500	0.20344300
H	-2.77355700	1.51224500	-1.56112100
C	-1.25533400	2.18303300	1.93320200
H	0.00130200	0.48158100	1.54528600
C	-2.30402300	2.98100200	1.46722600
H	-3.65341200	3.33668100	-0.17801700
H	-0.82413800	2.36805200	2.91328600
H	-2.70170500	3.78365600	2.08276800
C	0.56643300	-0.47018100	-1.22589100
C	1.59626300	0.56611800	-1.32573200
H	2.57425000	0.10523500	-1.50131400
C	1.48256900	1.79749900	-2.13085100
C	0.29452600	2.29348300	-2.71196300
C	2.65884600	2.55014800	-2.38314500
C	0.28571200	3.45577400	-3.48455600
H	-0.62436400	1.73831800	-2.58261000
C	2.64834100	3.71031000	-3.15337300
H	3.60589000	2.17963800	-1.99561200
C	1.45513900	4.18408000	-3.70941900
H	-0.65185200	3.78853400	-3.92394500
H	3.58185300	4.23817100	-3.33723800
H	1.44276900	5.08542900	-4.31503400
S	1.20524100	-1.41855300	4.23723900
O	1.78922900	-0.63072200	3.06280300
C	0.82294100	-3.08886200	3.60944700
H	1.77275200	-3.55176500	3.33609200
H	0.34823500	-3.66491500	4.40838500
H	0.16707300	-3.01492900	2.73793700
C	-0.52040200	-0.86406500	4.46428400
H	-0.97227400	-1.45764600	5.26361400
H	-0.48243400	0.18533300	4.76169100
H	-1.07809500	-0.97931100	3.53145800
C	1.21228000	-6.31605400	-1.66698400
C	0.79333300	-5.07700800	-1.18263200

C	1.72168700	-4.06387900	-0.90779200
C	3.08110700	-4.32256200	-1.12669700
C	3.50393600	-5.56011900	-1.61554400
C	2.56963800	-6.56015100	-1.88782800
H	0.48026100	-7.09325500	-1.86852100
H	-0.26210700	-4.89347900	-0.99895800
H	3.81339500	-3.54938200	-0.90503000
H	4.56222500	-5.74487400	-1.77886300
H	2.89662100	-7.52534400	-2.26420700
C	1.26624600	-2.70937400	-0.41166300
H	2.01652900	-2.29411800	0.27971700
H	0.33404100	-2.80709300	0.14988100
N	1.02617000	-1.78859600	-1.54907000
H	1.87468300	-1.72438700	-2.10192700
H	2.05371300	1.05139700	0.07160100
C	6.52716900	-0.49416500	-0.68636900
C	5.72275000	0.58514200	-0.31640900
C	4.79578400	0.46770400	0.72647700
C	4.68916200	-0.75804700	1.40015500
C	5.48999900	-1.83819900	1.02776200
C	6.41227600	-1.71063500	-0.01429500
H	7.23948800	-0.38308200	-1.49865200
H	5.82015900	1.53170600	-0.84212600
H	3.97166200	-0.86978700	2.20861100
H	5.39774100	-2.78225800	1.55727800
H	7.03733400	-2.55264900	-0.29708000
C	3.97557100	1.66881400	1.14718800
H	4.17457300	2.50876300	0.47833800
H	4.26201200	1.98867100	2.15610900
N	2.50380900	1.44728800	1.13777800
H	2.22947600	0.76867300	1.85902500
H	2.05899800	2.35517500	1.36073500
S	1.57042300	5.42850800	1.23191400
O	1.90205000	4.10053200	1.91482200
C	0.33970900	5.09824800	-0.07131200
H	-0.57630100	4.77474000	0.42441000
H	0.16338100	6.02343500	-0.62640100
H	0.69318000	4.30896200	-0.73786100
C	2.96670400	5.82722200	0.11941600

H	2.75426700	6.77024300	-0.39141800
H	3.85309000	5.93897900	0.74654500
H	3.10260200	5.02240700	-0.60734400

Int5D

C	7.61988300	1.82406000	0.67359100
C	6.49378300	1.36991300	-0.01163000
C	6.57696800	0.25369100	-0.85622000
C	7.80848200	-0.39478400	-1.00026700
C	8.93788500	0.06108500	-0.31812200
C	8.84530900	1.17143100	0.52099200
H	7.54264800	2.69100000	1.32349700
H	5.54228900	1.88044600	0.11040900
H	7.88344100	-1.26071800	-1.65297200
H	9.88743100	-0.45131800	-0.44239400
H	9.72292200	1.52823600	1.05216500
C	5.35537900	-0.23666700	-1.59987700
H	5.63188100	-0.94863100	-2.38634100
H	4.83704600	0.58756200	-2.10304800
N	4.40518600	-0.87549500	-0.68859900
H	4.69483600	-1.06244700	0.27208300
C	3.21038700	-1.33453600	-1.05578600
S	2.63233600	-1.24570300	-2.63338600
C	2.34787800	-1.95239500	0.05055300
C	3.09786000	-2.65405100	1.19843600
O	4.16630200	-2.25716800	1.64701400
C	2.42178700	-3.88151700	1.76223000
H	1.33743200	-3.75133200	1.80556500
H	2.61497400	-4.71934400	1.07916000
H	2.84121500	-4.12346000	2.73998000
H	1.73726500	-2.71278300	-0.42964100
C	1.37373300	-0.93628500	0.69447500
C	1.88321100	0.43322600	1.01313800
C	2.87897100	0.68198200	1.97268100
C	1.34560100	1.52802800	0.31188400
C	3.32073300	1.98356200	2.21931100
H	3.30899500	-0.14004000	2.53332300
C	1.78874100	2.82870200	0.55725100
H	0.56145400	1.34449300	-0.41675500

C	2.78191600	3.06044100	1.51219500
H	4.08486300	2.15426200	2.97259400
H	1.35128500	3.65427900	0.00214300
H	3.12856100	4.07141500	1.70753300
C	0.07299600	-1.26986200	0.89229300
C	-0.90691200	-0.38883800	1.65494100
H	-1.66506600	-0.02394200	0.95115400
C	-1.59043500	-1.12362700	2.79887100
C	-0.84409100	-1.57239900	3.89945800
C	-2.97023000	-1.36233100	2.78364000
C	-1.46114800	-2.23803800	4.95676400
H	0.22793800	-1.39299500	3.92278900
C	-3.59109500	-2.02998500	3.84293700
H	-3.56592200	-1.01242400	1.94434300
C	-2.83922200	-2.46984300	4.93139300
H	-0.86839900	-2.57486400	5.80274700
H	-4.66329000	-2.20176500	3.81380600
H	-3.32074100	-2.98809900	5.75561300
S	-1.46551600	1.57289100	-3.14068600
O	-1.62893300	0.91960700	-1.76225600
C	-0.64192700	0.33153300	-4.19694400
H	-1.35754700	-0.47587700	-4.36279000
H	-0.37345800	0.78993200	-5.15235400
H	0.24101600	-0.05213100	-3.67840800
C	-0.07624600	2.75200300	-3.02896100
H	0.07495000	3.20304300	-4.01371600
H	-0.36554500	3.51749500	-2.30380200
H	0.82502400	2.22895200	-2.70072400
C	-2.10676500	-6.08802200	-1.30133800
C	-1.32734700	-4.98090200	-0.96798900
C	-1.70579500	-3.69163000	-1.36869800
C	-2.88632700	-3.54067700	-2.10684900
C	-3.66590200	-4.64813800	-2.44776000
C	-3.27815400	-5.92594300	-2.04466100
H	-1.79906900	-7.07997100	-0.98218000
H	-0.42022400	-5.10835000	-0.38492000
H	-3.19580300	-2.54594000	-2.41809400
H	-4.57750600	-4.51014200	-3.02233300
H	-3.88435600	-6.78897200	-2.30441700

C	-0.85685700	-2.48555100	-1.03231400
H	-1.39065600	-1.56397200	-1.30037000
H	0.06044300	-2.48858600	-1.63294800
N	-0.47654800	-2.49183900	0.40755700
H	-1.30628700	-2.72029200	0.94971900
H	-0.38923200	0.48843000	2.04716000
C	-7.35679900	0.52582300	0.55112400
C	-6.73764700	1.64274700	-0.01465800
C	-5.54076400	1.51730700	-0.72743400
C	-4.96999600	0.24224100	-0.85952300
C	-5.58389600	-0.87628100	-0.29415000
C	-6.78183000	-0.73742100	0.41252200
H	-8.28781600	0.64363100	1.09880400
H	-7.19062400	2.62481600	0.09790500
H	-4.03088900	0.13501000	-1.39759500
H	-5.13137800	-1.85739400	-0.41347400
H	-7.26408900	-1.60853500	0.84711600
C	-4.85810300	2.72073500	-1.34737400
H	-5.53749200	3.58027700	-1.30972500
H	-4.68050700	2.50752500	-2.41576800
N	-3.62445700	3.06959200	-0.62147500
H	-2.97305900	2.28556100	-0.69475100
H	-3.13795800	3.83685500	-1.08674600
S	-1.26758800	5.52068800	0.70077900
O	-1.14525100	4.96235100	-0.71571500
C	-1.60804000	4.12018800	1.82774200
H	-0.71126900	3.49835000	1.84221400
H	-1.80302200	4.51423500	2.82915300
H	-2.46347200	3.56103600	1.43608300
C	-2.92972400	6.28134000	0.82330000
H	-3.07515400	6.66681800	1.83590100
H	-2.95997300	7.10301900	0.10555400
H	-3.67952900	5.52560400	0.57873700

TS4'D

C	6.94885600	-0.61614600	-1.12297200
C	5.77563100	-0.28312200	-0.44868000
C	5.44381700	1.05834600	-0.21286200
C	6.31247800	2.05636300	-0.66530400

C	7.49157700	1.72553300	-1.33608500
C	7.81215500	0.38829800	-1.56748500
H	7.19223600	-1.65998100	-1.30009900
H	5.10517300	-1.06512200	-0.10261800
H	6.06284500	3.10024100	-0.49331200
H	8.15461700	2.51321800	-1.68223700
H	8.72709300	0.12872100	-2.09211000
C	4.18650400	1.41601200	0.54911200
H	4.06549600	2.50676600	0.60772400
H	4.23729100	1.06787100	1.58839000
N	3.00421800	0.82154700	-0.05437800
H	2.86174500	0.80278100	-1.11862000
C	1.84434700	0.70169400	0.59418100
S	1.53283200	1.23472500	2.16504300
C	0.73645000	0.14680400	-0.26355800
C	0.76565100	0.52510400	-1.70783000
O	1.87380600	0.90835500	-2.28872500
C	-0.22609400	-0.15474200	-2.66433000
H	-1.24421000	-0.23222200	-2.28494000
H	-0.22249800	0.41322600	-3.59638300
H	0.14850600	-1.15986200	-2.88319800
H	0.15647400	1.45217000	-1.21812300
C	-0.24367800	-0.73152200	0.36213300
C	0.40905800	-1.81484300	1.17150800
C	1.40097800	-2.61918500	0.58452800
C	0.06168300	-2.05719200	2.51121900
C	2.02216300	-3.63657800	1.31046400
H	1.67805100	-2.45117600	-0.45231000
C	0.67227000	-3.07966300	3.23247200
H	-0.67143900	-1.41667900	2.99006000
C	1.65691100	-3.87194500	2.63539800
H	2.78466400	-4.24829800	0.83702100
H	0.39238800	-3.24905800	4.26820600
H	2.13660300	-4.66460700	3.20203900
C	-1.62201700	-0.71200500	0.23997100
C	-2.48480400	-1.93129700	0.56920100
H	-2.95060600	-1.78518900	1.55141600
C	-3.57518900	-2.18781600	-0.45836500
C	-3.25476500	-2.71733700	-1.71774500

C	-4.91639900	-1.89982900	-0.17461600
C	-4.24876800	-2.95018000	-2.66582500
H	-2.21892700	-2.94898200	-1.95084900
C	-5.91511600	-2.13063400	-1.12496800
H	-5.18352800	-1.50482700	0.80276800
C	-5.58331700	-2.65584900	-2.37260800
H	-3.98352300	-3.36476000	-3.63401500
H	-6.94988900	-1.90453400	-0.88486400
H	-6.35743600	-2.83952400	-3.11158900
C	-5.03580000	3.99698700	-0.46040300
C	-3.91802300	3.21150300	-0.74743700
C	-3.14919400	2.66231700	0.28555500
C	-3.51541800	2.91558300	1.61409400
C	-4.62888100	3.70352100	1.90273900
C	-5.39252500	4.24412100	0.86552800
H	-5.62143600	4.42048900	-1.27101100
H	-3.63442600	3.03033800	-1.78136100
H	-2.91817500	2.49976200	2.42123900
H	-4.89799200	3.90004900	2.93639200
H	-6.25794500	4.86032300	1.09082300
C	-1.95777600	1.78291500	-0.02701400
H	-1.18354100	1.88001100	0.74159400
H	-1.50143900	2.10790400	-0.98150400
N	-2.35927900	0.38739200	-0.09020700
H	-3.33352200	0.22098600	-0.30760100
H	-1.83959100	-2.80635400	0.65016600

Int5WD

C	7.00664000	0.67568000	-0.39732200
C	5.83767800	0.25683100	-1.03496500
C	5.01212000	-0.70918400	-0.44936400
C	5.37305000	-1.24931300	0.79424800
C	6.53783800	-0.82568600	1.43375600
C	7.35907800	0.13501300	0.83923200
H	7.63920900	1.42397300	-0.86607300
H	5.56284700	0.68286700	-1.99631500
H	4.73711900	-1.99635200	1.26356600
H	6.80876600	-1.25148400	2.39578000
H	8.26855500	0.45895700	1.33693500

C	3.75609800	-1.17435200	-1.15135900
H	3.73218400	-2.26655000	-1.24572500
H	3.70541700	-0.77693900	-2.17093400
N	2.55656000	-0.75609100	-0.42322600
H	2.67353600	-0.20029100	0.42109700
C	1.32050200	-1.14765400	-0.72252200
S	0.95863600	-2.17949800	-2.00320200
C	0.19305100	-0.57976400	0.14369800
C	0.49117300	-0.43369100	1.64073900
O	1.61410700	-0.18151800	2.08030800
C	-0.68034100	-0.63270600	2.56325500
H	-1.60395800	-0.24420300	2.12815300
H	-0.80580000	-1.71787000	2.66300200
H	-0.47376900	-0.19199300	3.54014400
H	-0.62356900	-1.29090700	0.08472600
C	-0.33466800	0.77089800	-0.38587700
C	0.67259600	1.82516800	-0.72177300
C	1.29173600	2.59885300	0.27394400
C	1.03476900	2.04811800	-2.06081300
C	2.23744100	3.56941500	-0.06050200
H	1.03298200	2.44064900	1.31614900
C	1.97758100	3.02050100	-2.39505100
H	0.57263200	1.44635900	-2.83749800
C	2.58243800	3.78417200	-1.39541500
H	2.70188800	4.15980400	0.72403700
H	2.23962300	3.18008700	-3.43715300
H	3.31672200	4.54132700	-1.65442700
C	-1.66578100	0.95955500	-0.55513800
C	-2.26711100	2.29429400	-0.97749500
H	-2.79268400	2.15054600	-1.93091100
C	-3.24754800	2.84611800	0.04597700
C	-2.78031200	3.39929500	1.24764300
C	-4.62951700	2.80238200	-0.17560100
C	-3.67020700	3.89738200	2.19713400
H	-1.70995600	3.44292500	1.43158600
C	-5.52503800	3.29753300	0.77620600
H	-5.00852500	2.38984500	-1.10773100
C	-5.04743700	3.84607000	1.96523500
H	-3.29015800	4.32800900	3.11922100

H	-6.59330700	3.25663200	0.58408300
H	-5.74068700	4.23400800	2.70564900
C	-4.28856000	-4.09454700	0.41802900
C	-3.39190200	-3.11669600	-0.00873100
C	-3.78923100	-2.14406200	-0.93848800
C	-5.10028000	-2.17505100	-1.42584600
C	-6.00106800	-3.15387400	-0.99941200
C	-5.59619200	-4.11561000	-0.07493100
H	-3.96431700	-4.84545900	1.13277500
H	-2.37619900	-3.11599600	0.37778700
H	-5.41724200	-1.42963800	-2.15187600
H	-7.01434800	-3.16465500	-1.39102400
H	-6.29235800	-4.88033700	0.25758400
C	-2.82398600	-1.07033300	-1.39117400
H	-3.21115000	-0.59116300	-2.30507000
H	-1.85716300	-1.51093200	-1.65257200
N	-2.60524700	-0.08116700	-0.30520300
H	-3.50259200	0.31883300	-0.04302000
H	-1.47296200	3.02165400	-1.15594000
O	2.78285500	-2.78316300	2.54573200
H	2.85706700	-3.06695000	3.46562400
H	2.53269600	-1.84378200	2.58741100
O	0.30785700	-3.50370100	1.30046900
H	1.19831700	-3.44749900	1.69565700
H	0.46761200	-3.59217300	0.34953300

TS4WD

C	7.53987900	-0.05413500	0.94386100
C	6.48984500	0.21813300	0.06506100
C	5.41087700	-0.66442800	-0.05391700
C	5.39777500	-1.82902700	0.72830500
C	6.44326000	-2.09870900	1.61041300
C	7.51798900	-1.21306300	1.71945500
H	8.37163700	0.63987300	1.02313600
H	6.50816600	1.12342100	-0.53625500
H	4.56345500	-2.52118800	0.64511600
H	6.42254900	-3.00401900	2.21046500
H	8.33337000	-1.42661400	2.40444600
C	4.28164000	-0.37645100	-1.01785700

H	4.11992100	-1.21235100	-1.70835100
H	4.51527900	0.49344700	-1.64171000
N	3.02737600	-0.13582400	-0.30232400
H	3.06242300	-0.09293400	0.71355200
C	1.81119600	-0.14283100	-0.85260400
S	1.60643200	-0.43069300	-2.52845500
C	0.62261500	0.03229800	0.03898500
C	0.75474000	-0.17571800	1.46392900
O	1.71604700	-0.82247300	1.98174900
C	-0.33716400	0.27709400	2.41308300
H	-0.65331500	1.30648700	2.23270300
H	-1.22255600	-0.35271500	2.27457100
H	0.02718600	0.16370500	3.43511400
H	0.09527400	-1.42391700	-0.27246400
C	-0.39450200	1.03017500	-0.46588800
C	0.17376900	2.35264400	-0.89068800
C	0.95888300	3.10591500	-0.00242300
C	-0.02860900	2.85760900	-2.18502100
C	1.49297400	4.33739400	-0.38192900
H	1.15078800	2.72529500	0.99690800
C	0.50974700	4.08560400	-2.56863000
H	-0.59412700	2.26457300	-2.89632100
C	1.26884900	4.83342200	-1.66718600
H	2.08677900	4.90794600	0.32683500
H	0.34511700	4.45254000	-3.57777200
H	1.68976900	5.78897800	-1.96620500
C	-1.73080100	0.80907300	-0.46758000
C	-2.77860900	1.89171600	-0.71876500
H	-3.44820700	1.57111800	-1.52702500
C	-3.61006800	2.17963800	0.52258400
C	-3.11686100	3.03480600	1.51986700
C	-4.86577300	1.58837900	0.71413800
C	-3.85675300	3.28978400	2.67339700
H	-2.14824700	3.50826400	1.38060700
C	-5.60819100	1.83818600	1.87150300
H	-5.27440200	0.93729600	-0.05528300
C	-5.10534700	2.68915100	2.85466400
H	-3.46120200	3.96081500	3.43071700
H	-6.58072200	1.37130700	1.99916000

H	-5.68232000	2.88817400	3.75298400
C	-3.86725200	-4.42279200	0.48207700
C	-3.13643500	-3.28744900	0.13269400
C	-3.56409200	-2.45629400	-0.91206800
C	-4.74106500	-2.79044100	-1.59335100
C	-5.46973500	-3.93062100	-1.25119100
C	-5.03515300	-4.75042500	-0.20960900
H	-3.52367700	-5.05521100	1.29619400
H	-2.22800700	-3.03391000	0.66751300
H	-5.08968900	-2.15128900	-2.40114000
H	-6.37965800	-4.17262000	-1.79303700
H	-5.60285500	-5.63524700	0.06353400
C	-2.77277700	-1.23019500	-1.31925100
H	-3.40677800	-0.60479100	-1.96859000
H	-1.90923500	-1.52046900	-1.92782100
N	-2.26164300	-0.49126100	-0.14281700
H	-3.04308700	-0.37067200	0.50183300
H	-2.29966600	2.81208900	-1.05239500
O	2.03113900	-3.18534900	0.86186800
H	1.84634600	-3.84624800	1.54160400
H	2.05364500	-2.30322600	1.33749000
O	0.12427400	-2.48193100	-0.69476900
H	0.86880100	-2.91512600	-0.13255000
H	0.52342700	-2.24473700	-1.57344000

Int6WD

C	7.59636800	-0.09880000	0.85111400
C	6.53397600	0.12064000	-0.02775400
C	5.46183400	-0.77646300	-0.08810800
C	5.46673000	-1.90138000	0.75034700
C	6.52601300	-2.11828600	1.63072400
C	7.59349500	-1.21863900	1.68280500
H	8.42382100	0.60401400	0.88496700
H	6.53836900	0.99361200	-0.67562200
H	4.63485900	-2.59995600	0.70709700
H	6.52204300	-2.99362100	2.27407900
H	8.41950500	-1.39166300	2.36658300
C	4.31046300	-0.54473100	-1.04056400
H	4.07142900	-1.45085900	-1.60705300

H	4.56071600	0.22594200	-1.77885900
N	3.10546100	-0.14322800	-0.31167100
H	3.21889500	0.08380300	0.66905900
C	1.86310700	-0.14295800	-0.81640900
S	1.56968600	-0.53092600	-2.43996400
C	0.75991900	0.23534400	0.10890800
C	0.76749100	-0.06594000	1.44475800
O	1.70843800	-0.82711100	2.05595200
C	-0.24088300	0.41384100	2.44981700
H	-0.87927100	1.21254000	2.07855000
H	-0.87317900	-0.42457500	2.76655700
H	0.29594400	0.75366500	3.34181800
H	-0.59105400	-2.06030900	-0.26432600
C	-0.32584000	1.09038800	-0.46466800
C	0.13327400	2.44948300	-0.90255700
C	0.83582600	3.28626000	-0.02066200
C	-0.08098400	2.89826400	-2.21597200
C	1.27402700	4.54749300	-0.42512600
H	1.03722400	2.94449300	0.99033000
C	0.36338200	4.15546400	-2.62374100
H	-0.57913800	2.23989700	-2.92023900
C	1.03755000	4.98768100	-1.72832000
H	1.80465000	5.18412100	0.27733300
H	0.19291800	4.48010700	-3.64624300
H	1.38494000	5.96628100	-2.04654100
C	-1.62721700	0.71986000	-0.52722900
C	-2.76547900	1.71849500	-0.74364900
H	-3.48220800	1.33648100	-1.47828000
C	-3.49901100	2.01362300	0.55887200
C	-3.04318300	3.03307300	1.40911500
C	-4.62259900	1.27388800	0.95149400
C	-3.69027200	3.30245700	2.61467800
H	-2.17692500	3.62096000	1.11691100
C	-5.27006000	1.53861100	2.16097100
H	-5.00499300	0.48948300	0.30382500
C	-4.80587800	2.55358300	2.99660000
H	-3.32582700	4.10093500	3.25488200
H	-6.14067400	0.95398100	2.44441600
H	-5.31080600	2.76400400	3.93478500

C	-4.07855200	-4.62666800	-0.16205700
C	-3.18566600	-3.63532600	-0.56963700
C	-3.65932000	-2.39173800	-1.01397000
C	-5.04383100	-2.17571900	-1.05180000
C	-5.93798700	-3.16771800	-0.64579800
C	-5.45549800	-4.39649200	-0.19537900
H	-3.69747400	-5.58653800	0.17533300
H	-2.11624500	-3.82196800	-0.56037000
H	-5.42700000	-1.22693400	-1.42090200
H	-7.00746300	-2.98222700	-0.68787100
H	-6.14731000	-5.17246100	0.11945600
C	-2.70962700	-1.29288700	-1.44300400
H	-3.27281800	-0.55836300	-2.03103500
H	-1.92798000	-1.68713600	-2.09762100
N	-2.02907600	-0.65254700	-0.26799200
H	-2.69419400	-0.65851600	0.50650400
H	-2.37252500	2.65097400	-1.14738700
O	2.16584100	-3.10866600	0.82646300
H	2.00108100	-3.76801700	1.51263300
H	1.98616300	-1.62178900	1.51184700
O	-0.03727500	-2.78639200	-0.63675200
H	1.34497300	-3.10511800	0.25944600
H	0.35443400	-2.36088000	-1.42510600

Int6'D

C	-7.16891800	-0.20494500	1.26858900
C	-6.12367900	-0.40288700	0.36471900
C	-5.32763500	0.67073000	-0.05284500
C	-5.59962700	1.94962500	0.45203900
C	-6.64250600	2.15056100	1.35537000
C	-7.42941000	1.07220300	1.76606900
H	-7.78097100	-1.04646700	1.57963400
H	-5.92736200	-1.39775200	-0.02734600
H	-4.99458400	2.79268000	0.12728300
H	-6.84473700	3.14791600	1.73464400
H	-8.24438500	1.22847400	2.46660200
C	-4.18069800	0.44862800	-1.01216300
H	-4.06859400	1.28709000	-1.70465900
H	-4.34735400	-0.44290800	-1.62944400

N	-2.91998100	0.30563600	-0.27008900
H	-3.02017900	-0.11442300	0.64829300
C	-1.70501600	0.09961400	-0.88199900
S	-1.54528800	0.14311100	-2.54301900
C	-0.56486800	-0.11788600	0.04676900
C	-0.44916300	0.60412200	1.20685600
O	-1.28842200	1.61585800	1.56757200
C	0.64060700	0.45759800	2.22141500
H	1.08280000	-0.53699100	2.18741900
H	1.44052200	1.17906100	2.02265100
H	0.23262000	0.65713700	3.21619000
C	0.45986300	-1.12917100	-0.34736000
C	-0.07295000	-2.50961700	-0.54804700
C	-0.86938500	-3.10832700	0.44483700
C	0.15145300	-3.23418800	-1.73167200
C	-1.39402500	-4.38891400	0.27678100
H	-1.06715700	-2.56083900	1.36262000
C	-0.36944600	-4.51692000	-1.90098600
H	0.71959200	-2.76992000	-2.53147100
C	-1.14279100	-5.10193000	-0.89714600
H	-1.99561600	-4.83293600	1.06543100
H	-0.18399700	-5.05374700	-2.82723300
H	-1.55245400	-6.09884800	-1.03151500
C	1.78199700	-0.82249800	-0.50431700
C	2.86662500	-1.88623400	-0.65592900
H	3.31211000	-1.79924500	-1.65580600
C	3.97141300	-1.76928600	0.38337100
C	3.73627800	-2.15321200	1.71224700
C	5.23974400	-1.28122800	0.04599800
C	4.73775400	-2.04603300	2.67480700
H	2.76048700	-2.54647700	1.98576800
C	6.24624900	-1.16945700	1.00934900
H	5.44703000	-0.99925900	-0.98391500
C	5.99727700	-1.55013500	2.32671400
H	4.53818200	-2.35271500	3.69768500
H	7.22388400	-0.78984700	0.72632700
H	6.77809600	-1.46721100	3.07692800
C	2.23999400	4.85902500	0.46338600
C	1.72497300	3.62495900	0.06926000

C	2.33470000	2.89099400	-0.95851600
C	3.46788000	3.42521800	-1.58233900
C	3.98800100	4.66033600	-1.18907100
C	3.37504200	5.37946900	-0.16344200
H	1.75294200	5.41843700	1.25715600
H	0.83659900	3.22992900	0.55474300
H	3.94242100	2.87217200	-2.38991300
H	4.86672800	5.06084400	-1.68665600
H	3.77456500	6.34202600	0.14272200
C	1.79462500	1.53843700	-1.37105200
H	2.08454000	1.32823400	-2.41217400
H	0.70558800	1.53892600	-1.35036600
N	2.28400400	0.48595500	-0.46332700
H	3.29469000	0.50594500	-0.39365200
H	2.41765600	-2.87783200	-0.59064400
H	-1.98599200	1.70885600	0.89418200

Int5aD

C	-7.45375600	-1.36717300	-0.38501600
C	-6.29364500	-1.07584800	0.33123700
C	-5.46742500	-2.10890400	0.79780200
C	-5.83118500	-3.43431500	0.53587600
C	-6.99635100	-3.72781200	-0.17525300
C	-7.80933100	-2.69391600	-0.63932300
H	-8.08436400	-0.55758200	-0.74113300
H	-6.02513300	-0.04173200	0.53104700
H	-5.19941700	-4.24217700	0.89675900
H	-7.26684100	-4.76241000	-0.36634900
H	-8.71581900	-2.91914100	-1.19367400
C	-4.21398900	-1.79361700	1.58292300
H	-3.74136200	-2.71115000	1.95315500
H	-4.44065300	-1.19268300	2.47217500
N	-3.25697000	-1.04808300	0.76901100
H	-3.44180700	-0.91607800	-0.22732400
C	-2.11579700	-0.54029900	1.23572600
S	-1.61433500	-0.71401500	2.82942000
C	-1.26681800	0.27153100	0.24559800
C	-1.47020200	0.02200700	-1.25670200
O	-2.51496200	-0.41474000	-1.73889900

C	-0.30084100	0.35385600	-2.14948300
H	0.30221900	1.17756700	-1.76090400
H	0.32864900	-0.54386300	-2.20732000
H	-0.66433000	0.57622100	-3.15538900
H	-0.23515700	0.00023500	0.46482600
C	-1.45836400	1.78975300	0.44235000
C	-2.88452300	2.23424600	0.60607400
C	-3.73432200	2.41119900	-0.49918100
C	-3.41309600	2.46066200	1.88888300
C	-5.06150100	2.81083700	-0.32963800
H	-3.35492000	2.23541700	-1.50082300
C	-4.73888800	2.86104100	2.06026600
H	-2.77224600	2.31200900	2.75171200
C	-5.56860700	3.03769900	0.95122600
H	-5.69631600	2.95068100	-1.20026200
H	-5.12305900	3.03495000	3.06148700
H	-6.59941500	3.35418100	1.08349300
C	-0.44094900	2.69816300	0.44246200
C	-0.73394100	4.19667900	0.53883100
H	-0.34418800	4.56052500	1.49868900
C	-0.11972200	5.01831300	-0.58349600
C	-0.53570700	4.83235500	-1.91064000
C	0.85824000	5.98467700	-0.32087400
C	0.01079000	5.59175600	-2.94234100
H	-1.29402300	4.08508300	-2.12833200
C	1.41055300	6.74742200	-1.35396300
H	1.18458700	6.14984500	0.70335100
C	0.98829600	6.55286400	-2.66756100
H	-0.32621500	5.43631000	-3.96344500
H	2.16738000	7.49315900	-1.12794300
H	1.41345100	7.14510800	-3.47259600
S	5.00848100	-2.53079700	-2.29540300
O	4.47664100	-3.08474700	-0.98178100
C	6.36431300	-1.36908100	-1.88484900
H	7.17505400	-1.96307800	-1.45874600
H	6.70783300	-0.87623100	-2.79852700
H	6.01525800	-0.63555000	-1.15369500
C	3.81866200	-1.27534300	-2.89137800
H	4.19331900	-0.84910000	-3.82643900

H	2.87027400	-1.79240800	-3.05902400
H	3.69060400	-0.49694900	-2.13453600
C	5.08879300	2.48548800	-0.51408100
C	3.71236300	2.29605900	-0.36723900
C	3.19575600	1.64254300	0.76155600
C	4.09055700	1.16839000	1.73026000
C	5.46504200	1.34771700	1.57843600
C	5.97100600	2.01214600	0.45830300
H	5.46906000	3.00486400	-1.38969500
H	3.03468200	2.65892100	-1.13438700
H	3.70911900	0.64831800	2.60375400
H	6.13926400	0.96982600	2.34141300
H	7.04114000	2.16384900	0.34774300
C	1.71078500	1.38049000	0.92180800
H	1.46258100	1.26007100	1.98538800
H	1.51141100	0.40823500	0.45364700
N	0.92759100	2.46287200	0.30959300
H	1.44605900	3.33175100	0.33517800
H	-1.81197000	4.35708200	0.55664600
C	3.06805900	-1.37512200	4.68345000
C	2.18247200	-1.74743900	3.66849900
C	2.64118900	-2.42152900	2.52981000
C	4.01025700	-2.70882000	2.42279400
C	4.89605700	-2.33417000	3.43357600
C	4.42814800	-1.66863200	4.56972200
H	2.69329000	-0.85897500	5.56337600
H	1.12544300	-1.51075600	3.75401900
H	4.38255100	-3.21313900	1.53463000
H	5.95326500	-2.56772200	3.33751600
H	5.11728400	-1.38524100	5.36080600
C	1.68641800	-2.83316300	1.42617200
H	0.65769100	-2.73648900	1.78924300
H	1.85742600	-3.90275600	1.20813800
N	1.84088800	-1.98350600	0.22913800
H	2.80484300	-2.08612100	-0.09527500
H	1.28604600	-2.37659300	-0.53300500
S	-0.11651200	-3.86553700	-3.23067900
O	0.79270000	-2.79394000	-2.63527400
C	-1.76744100	-3.64759500	-2.47796300

H	-2.12846800	-2.65749900	-2.76271400
H	-2.43948600	-4.42152200	-2.85823900
H	-1.68669800	-3.70263700	-1.38946800
C	0.30901200	-5.43497500	-2.39353600
H	-0.38055100	-6.21935500	-2.71631600
H	1.32850700	-5.68889000	-2.68836200
H	0.26420900	-5.29320500	-1.31099200

TS4aD

C	6.94318200	-2.47648800	0.97453200
C	5.85136100	-1.96676200	0.27411400
C	4.95492000	-2.82839700	-0.37475200
C	5.17802400	-4.20766000	-0.30505100
C	6.27448600	-4.72019900	0.39121600
C	7.15960900	-3.85548100	1.03439500
H	7.62887100	-1.79667900	1.47252100
H	5.68489800	-0.89400600	0.22909400
H	4.48712100	-4.88590700	-0.79982400
H	6.43186100	-5.79422300	0.43528000
H	8.01123000	-4.25144000	1.58014400
C	3.78959400	-2.27382800	-1.16691700
H	3.14620100	-3.09411100	-1.51451900
H	4.13275800	-1.74981300	-2.06518300
N	3.01577700	-1.32084200	-0.38355300
H	2.89917300	-1.47779500	0.62182200
C	2.38015000	-0.24158200	-0.87000200
S	2.37178300	0.13232500	-2.52681300
C	1.60047100	0.59315700	0.10148700
C	1.64844000	0.29383600	1.54503400
O	2.00298200	-0.81112500	2.00874900
C	1.05687700	1.30191200	2.52002700
H	1.48373600	2.29881000	2.39659700
H	-0.02376500	1.38044200	2.35949000
H	1.23884000	0.94474400	3.53557800
H	0.35558600	-0.04549300	-0.03610600
C	1.59339200	2.07628700	-0.23798600
C	2.94656400	2.72460100	-0.27274700
C	3.89951500	2.50939700	0.73852500
C	3.32876600	3.52539100	-1.36364900

C	5.16002900	3.10444100	0.68392200
H	3.66262700	1.86951300	1.58182500
C	4.58888100	4.11797800	-1.42346400
H	2.63624400	3.64944200	-2.18890000
C	5.51028600	3.91624400	-0.39526400
H	5.87027600	2.92890400	1.48726700
H	4.85643400	4.72408700	-2.28450300
H	6.49433800	4.37373400	-0.44137700
C	0.46525500	2.79278300	-0.45853500
C	0.41832400	4.31789600	-0.56111000
H	0.29494900	4.62013900	-1.60974200
C	-0.71161100	4.94015000	0.24561700
C	-0.72857900	4.84742500	1.64567400
C	-1.75702200	5.62903600	-0.38427200
C	-1.75689600	5.42372400	2.39044400
H	0.07469400	4.32051100	2.15285700
C	-2.78906800	6.20916100	0.35789700
H	-1.75546100	5.72230500	-1.46772800
C	-2.79250200	6.10701700	1.74882600
H	-1.74822900	5.34254800	3.47375100
H	-3.58564600	6.74365800	-0.15220000
H	-3.59218600	6.55809800	2.32900000
S	-5.00047000	-2.75774600	1.53747100
O	-3.72695800	-3.58957000	1.67543000
C	-5.92331200	-3.43467300	0.10747900
H	-6.22192500	-4.45104300	0.36990900
H	-6.80962100	-2.82108700	-0.07402400
H	-5.27357900	-3.44881900	-0.77042900
C	-4.54634300	-1.15792300	0.78357800
H	-5.44827600	-0.55292800	0.65926500
H	-3.85210800	-0.68073700	1.47949700
H	-4.06100200	-1.32002100	-0.18141100
C	-4.95851400	1.73269900	-2.09052400
C	-3.66889600	2.22187300	-1.88653400
C	-2.54642500	1.48719600	-2.30062100
C	-2.75283800	0.25303100	-2.93050500
C	-4.04463900	-0.23890700	-3.14062400
C	-5.15084500	0.49967700	-2.72043000
H	-5.81500700	2.31971900	-1.77039700

H	-3.53270500	3.19187200	-1.41323400
H	-1.89827100	-0.32425500	-3.27091900
H	-4.17673300	-1.19658700	-3.63572200
H	-6.15644900	0.12509900	-2.89065000
C	-1.14894000	2.03263200	-2.09518700
H	-1.08326500	3.01495900	-2.59379200
H	-0.40619700	1.38719800	-2.57195000
N	-0.79593500	2.12438600	-0.65245600
H	-1.52692000	2.65896500	-0.18559800
H	1.37101900	4.73987100	-0.23340300
C	-0.77030200	-3.21198100	-3.76673800
C	-0.34643700	-2.64494000	-2.56348000
C	-1.03922800	-2.91148200	-1.37257300
C	-2.14792900	-3.76903100	-1.40721600
C	-2.56388700	-4.34146600	-2.61205200
C	-1.88001400	-4.06025600	-3.79576400
H	-0.22413600	-2.99660700	-4.68073600
H	0.52070800	-1.98819000	-2.55797900
H	-2.67505800	-3.98874700	-0.48137200
H	-3.41682500	-5.01526100	-2.62360600
H	-2.20084000	-4.50732300	-4.73257400
C	-0.60471200	-2.30700200	-0.05502500
H	0.44896100	-2.52507600	0.14029600
H	-1.19762000	-2.75077700	0.74903500
N	-0.76766700	-0.81873300	0.01036600
H	-1.40078000	-0.47300800	-0.70736000
H	-1.18016100	-0.57454800	0.92005200
S	-1.49118900	-1.08703300	4.09079400
O	-1.90897400	-0.52614300	2.72570300
C	-0.27822000	-2.41857400	3.80219200
H	0.59746100	-1.96060800	3.33333000
H	-0.00645200	-2.85069100	4.76940400
H	-0.71722700	-3.17687600	3.14975200
C	-2.86391300	-2.15328900	4.65458600
H	-2.56068700	-2.66537900	5.57169000
H	-3.71307700	-1.49978100	4.86459800
H	-3.11370700	-2.86225600	3.85929800

C	-1.62006500	5.64563200	-2.15933100
C	-0.76975900	5.00297300	-1.26132800
C	-1.27530100	4.41068000	-0.09403700
C	-2.65196100	4.48080100	0.15069800
C	-3.50666000	5.12682600	-0.74636600
C	-2.99264800	5.71015700	-1.90391300
H	-1.21188000	6.10256500	-3.05653500
H	0.29777900	4.95818900	-1.45990400
H	-3.05530700	4.02980700	1.05394900
H	-4.57197500	5.17342100	-0.53849800
H	-3.65449700	6.21504700	-2.60184700
C	-0.34523100	3.72483500	0.88422400
H	-0.89610700	3.42038300	1.78226900
H	0.43451400	4.41299200	1.23440100
N	0.29996000	2.57742800	0.25937800
H	-0.01647300	2.24664000	-0.65297900
C	1.36880600	1.91858700	0.77071400
S	1.91138300	2.27307700	2.34520700
C	2.01271600	0.90654800	-0.08394400
C	1.36471100	0.35988800	-1.18921400
O	0.11669500	0.62651000	-1.50962300
C	2.03810300	-0.60328000	-2.14390900
H	3.07505200	-0.81608500	-1.89468000
H	1.47604900	-1.54382900	-2.16394900
H	1.98248900	-0.18216300	-3.15511900
H	-0.90260400	-0.02211000	-0.61291900
C	3.44727200	0.58126200	0.21827300
C	4.41220400	1.70047800	-0.01595700
C	4.42197300	2.37346300	-1.25037600
C	5.30560900	2.14200400	0.97521800
C	5.31325400	3.41632000	-1.49875800
H	3.71925900	2.06997600	-2.02091400
C	6.19951700	3.18420200	0.72913600
H	5.26940500	1.67732500	1.95486400
C	6.21156100	3.82455100	-0.51080500
H	5.30670200	3.91131700	-2.46656500
H	6.87563100	3.50847500	1.51580800
H	6.90359100	4.64020900	-0.70106200
C	3.86646600	-0.64274900	0.64013900

C	5.33443700	-1.04674600	0.74467500
H	5.58338800	-1.22002700	1.80057000
C	5.67820400	-2.29927200	-0.04689700
C	5.76486500	-2.25117000	-1.44686700
C	5.91743600	-3.52293400	0.59116400
C	6.07575500	-3.39209500	-2.18367500
H	5.59375100	-1.30576800	-1.95494800
C	6.22616100	-4.67080000	-0.14442700
H	5.87679800	-3.57437500	1.67711400
C	6.30524400	-4.60861400	-1.53458600
H	6.14334700	-3.33294400	-3.26646700
H	6.41063700	-5.60900000	0.37155500
H	6.54908400	-5.49748300	-2.10924200
S	-6.34573200	-2.11188600	-0.75995200
O	-5.80852200	-0.68385800	-0.77945100
C	-7.54338300	-2.20524300	0.62186400
H	-8.36959300	-1.53666400	0.37432100
H	-7.91033600	-3.23053500	0.71726800
H	-7.06273500	-1.87652100	1.54623400
C	-5.05816000	-3.17832800	-0.02378800
H	-5.45377700	-4.19152800	0.08931400
H	-4.21800100	-3.16698500	-0.72169100
H	-4.74917600	-2.76895400	0.94129800
C	-0.57088100	-3.95703400	0.33615000
C	0.56116200	-3.16029300	0.53150500
C	0.72436000	-2.42297900	1.71086300
C	-0.27825900	-2.50117400	2.69155600
C	-1.41031300	-3.29413800	2.49877000
C	-1.55868900	-4.03017800	1.31917500
H	-0.68141700	-4.51594600	-0.58841800
H	1.33358700	-3.10031000	-0.22754300
H	-0.16886800	-1.93481500	3.61305100
H	-2.17241100	-3.33877200	3.27180600
H	-2.43278600	-4.65792000	1.17149800
C	1.93476100	-1.53628600	1.95245000
H	2.31104100	-1.73628200	2.97040100
H	1.62882000	-0.48762700	1.96103800
N	2.98159900	-1.69941300	0.95251000
H	3.47286800	-2.57860400	1.05945900

H	5.96218700	-0.22473000	0.40019900
C	-2.22710400	0.87707600	4.07031100
C	-1.98477500	0.83676000	2.69695100
C	-3.02310700	0.52643500	1.80539800
C	-4.30513300	0.27262400	2.30947900
C	-4.54525700	0.31973400	3.68452200
C	-3.50619800	0.61645800	4.56744000
H	-1.41458100	1.12697100	4.74581900
H	-0.98552700	1.06196300	2.33124200
H	-5.10861300	0.05453200	1.61055100
H	-5.54471700	0.12857900	4.06587000
H	-3.69302400	0.65423800	5.63678500
C	-2.78847500	0.49177300	0.31239300
H	-2.44442700	1.46625400	-0.04544200
H	-3.71375000	0.23396500	-0.20697700
N	-1.73863500	-0.51213100	-0.09891700
H	-1.37854800	-1.03742200	0.70137500
H	-2.12914600	-1.18876600	-0.78797100
S	-2.76534000	-1.60052000	-3.60889900
O	-2.74637100	-2.11643600	-2.15879000
C	-2.23571300	0.14420000	-3.59144200
H	-1.24727400	0.19873200	-3.11858400
H	-2.18341900	0.48844400	-4.62805300
H	-2.95254200	0.74695800	-3.02778000
C	-4.52269600	-1.30512400	-4.01043400
H	-4.58865900	-0.75473700	-4.95246900
H	-5.00128200	-2.28018500	-4.12022800
H	-4.98122300	-0.75250800	-3.18492600

TS4bD

C	0.79084100	6.19148800	2.16762900
C	0.18790200	5.36272100	1.22317100
C	0.94767400	4.76693400	0.20532100
C	2.32242200	5.02445400	0.15473100
C	2.92833300	5.85859100	1.09735800
C	2.16417700	6.44253700	2.10702300
H	0.18871000	6.64689300	2.94875800
H	-0.88127500	5.17317000	1.26892400
H	2.92106400	4.57142300	-0.63176000

H	3.99639000	6.04904500	1.04205200
H	2.63314300	7.09101400	2.84143600
C	0.28711200	3.87857000	-0.82688500
H	1.02344800	3.54264800	-1.56763700
H	-0.47522400	4.42716600	-1.39335200
N	-0.36133300	2.73969300	-0.18728900
H	-0.11869600	2.51316900	0.77337300
C	-1.25812200	1.92266600	-0.78505500
S	-1.61193200	2.09638300	-2.43401100
C	-1.92429000	0.91236800	0.07162300
C	-1.35056800	0.44023700	1.23585500
O	-0.10435300	0.74012500	1.61427300
C	-2.05675900	-0.46565100	2.21294000
H	-3.12169700	-0.56686000	2.01460400
H	-1.60749400	-1.46546000	2.18810400
H	-1.90295200	-0.06802600	3.22248300
H	0.76426400	0.32618500	0.83541900
C	-3.31495300	0.51065800	-0.31979900
C	-4.33019600	1.60774000	-0.27906700
C	-4.46024700	2.40226800	0.87330600
C	-5.15411300	1.90690400	-1.37750600
C	-5.40212200	3.42822100	0.94055100
H	-3.81326900	2.20707900	1.72365300
C	-6.09709800	2.93250200	-1.31278700
H	-5.02671600	1.34351500	-2.29592500
C	-6.22937300	3.69582700	-0.15184200
H	-5.49051100	4.01976000	1.84811200
H	-6.71818600	3.14628700	-2.17845900
H	-6.96044700	4.49790600	-0.10295900
C	-3.64431200	-0.76815300	-0.64474900
C	-5.07773500	-1.25925700	-0.82166700
H	-5.21717800	-1.58605200	-1.86124800
C	-5.43472100	-2.41223600	0.10385200
C	-5.69140600	-2.17393300	1.46273800
C	-5.51274400	-3.72918200	-0.36626800
C	-6.01165500	-3.22120900	2.32421400
H	-5.64599100	-1.15507900	1.83853700
C	-5.82952500	-4.78311200	0.49531800
H	-5.33864600	-3.93014300	-1.42107300

C	-6.07885100	-4.53190400	1.84352600
H	-6.21289000	-3.01566000	3.37191600
H	-5.88640700	-5.79705200	0.10932500
H	-6.32924200	-5.34812700	2.51493400
S	6.09250600	-2.18476800	0.80851700
O	5.64880500	-0.78183100	1.21676500
C	7.40442300	-1.98343700	-0.45413500
H	8.23844100	-1.47312800	0.03061700
H	7.72363000	-2.96921000	-0.80259400
H	7.02854000	-1.38230500	-1.28489100
C	4.81359400	-2.87984300	-0.29421600
H	5.15509300	-3.84828500	-0.66980800
H	3.91809300	-2.99880400	0.31865700
H	4.61806400	-2.18763000	-1.11646500
C	0.99363000	-4.01571800	-0.59385000
C	-0.02888300	-3.06645800	-0.64097000
C	-0.64612700	-2.73351800	-1.85528500
C	-0.21659200	-3.38074900	-3.02119300
C	0.80487000	-4.33096500	-2.97905600
C	1.41282400	-4.65240000	-1.76427800
H	1.45981700	-4.24212500	0.36006700
H	-0.36734800	-2.58697800	0.27168600
H	-0.69098900	-3.13935400	-3.96932900
H	1.11938700	-4.82515100	-3.89425200
H	2.20165100	-5.39901900	-1.72968800
C	-1.72969900	-1.67578000	-1.91929200
H	-2.24030600	-1.74280900	-2.89447400
H	-1.28912400	-0.67476600	-1.89147200
N	-2.66489100	-1.78278100	-0.79331100
H	-3.08896000	-2.70447900	-0.77284000
H	-5.77203000	-0.43614800	-0.64983400
C	2.96515200	1.07294900	-3.93228200
C	2.44953900	1.05500800	-2.63588400
C	3.30163900	0.86868900	-1.53651600
C	4.67671300	0.71794100	-1.75948700
C	5.19101500	0.74795200	-3.05814000
C	4.33633000	0.92029000	-4.14766100
H	2.29222700	1.21916000	-4.77186400
H	1.38030000	1.20201700	-2.49272300

H	5.33334100	0.57407400	-0.90540200
H	6.26080800	0.64107000	-3.21849100
H	4.73549900	0.94269200	-5.15755000
C	2.76233400	0.87534300	-0.12143300
H	2.33163500	1.85596300	0.10699800
H	3.57543100	0.68933900	0.58338700
N	1.69728200	-0.14353500	0.13556000
H	1.30341400	-0.49810200	-0.73555900
H	2.06979300	-0.95305700	0.65693100
S	2.40273500	-2.01461100	3.46766700
O	2.42118300	-2.27811400	1.95420500
C	2.19165400	-0.21953600	3.71584600
H	1.24638700	0.07188300	3.24653400
H	2.16097900	-0.02501700	4.79148300
H	3.02597700	0.31454700	3.25387900
C	4.13824400	-2.11112600	4.03082300
H	4.19106000	-1.79263000	5.07527100
H	4.44856700	-3.15460600	3.94914200
H	4.75300800	-1.47922800	3.38280900

Int6D

C	-3.49433400	6.35554100	1.14313700
C	-2.93133000	5.29978500	0.42795100
C	-1.54404900	5.23687700	0.22774600
C	-0.73809600	6.25069700	0.75638000
C	-1.30186700	7.31159400	1.46798100
C	-2.68153000	7.36544100	1.66419800
H	-4.56997400	6.39337500	1.28996900
H	-3.56710000	4.51674600	0.02293700
H	0.33831800	6.21006800	0.60936500
H	-0.66233000	8.09129900	1.87153900
H	-3.12209200	8.18845600	2.21936500
C	-0.93666500	4.10000400	-0.56475400
H	0.15386100	4.21541500	-0.62300700
H	-1.29935200	4.08934900	-1.59835600
N	-1.28621500	2.80953400	0.01901800
H	-1.48390200	2.79230800	1.01155000
C	-1.33754000	1.63206900	-0.63097700
S	-0.95323600	1.49451400	-2.26978000

C	-1.80728000	0.47827900	0.19942700
C	-1.21653500	0.19763700	1.40008800
O	-0.08795700	0.80788700	1.84752200
C	-1.71538000	-0.82865600	2.37496800
H	-2.76168900	-1.08038800	2.20629300
H	-1.12630800	-1.75092700	2.29807300
H	-1.58170400	-0.44183800	3.39055300
H	0.58383300	0.98977100	1.09516300
C	-2.98449900	-0.27328400	-0.32013600
C	-4.18249400	0.56825300	-0.61076200
C	-4.66230400	1.47890700	0.34954200
C	-4.84329500	0.52630100	-1.85189300
C	-5.76903500	2.28767100	0.09335200
H	-4.16188000	1.53794200	1.31220900
C	-5.95381900	1.33007900	-2.10972600
H	-4.45986600	-0.13070900	-2.62631200
C	-6.42418700	2.21500600	-1.13859200
H	-6.12763300	2.96853000	0.86123000
H	-6.44180400	1.27675600	-3.07919400
H	-7.28542400	2.84536800	-1.34045100
C	-2.99381800	-1.63128200	-0.52166000
C	-4.28606100	-2.41994200	-0.74603800
H	-4.28818500	-2.81773500	-1.76881900
C	-4.46259500	-3.57431200	0.22717200
C	-4.87978600	-3.33425700	1.54514300
C	-4.21342800	-4.89712700	-0.16102200
C	-5.03576500	-4.38407000	2.44804400
H	-5.09017900	-2.31453800	1.85734500
C	-4.36532700	-5.95228100	0.74273300
H	-3.90745600	-5.10403700	-1.18403100
C	-4.77609800	-5.69844600	2.05039900
H	-5.36477300	-4.17827100	3.46282500
H	-4.16790200	-6.97070600	0.42029700
H	-4.89954600	-6.51672900	2.75378600
S	6.49505600	-1.43289700	0.95329000
O	5.96711300	-0.32108300	1.85603300
C	7.97369500	-0.76802100	0.10126500
H	8.72337000	-0.56731300	0.86858200
H	8.35134200	-1.51429700	-0.60271500

H	7.70953300	0.15544600	-0.41795200
C	5.40830500	-1.53773500	-0.51041600
H	5.79253900	-2.31028200	-1.18219900
H	4.42162900	-1.80973900	-0.12817200
H	5.36211500	-0.56818200	-1.01095700
C	1.99385700	-4.78851600	-1.87871500
C	1.37005000	-3.75366000	-1.17668000
C	0.15925100	-3.21733300	-1.63093700
C	-0.41430400	-3.73830500	-2.80030800
C	0.20721000	-4.77126500	-3.49994300
C	1.41531800	-5.30158100	-3.03935600
H	2.93195100	-5.19824800	-1.51320700
H	1.82296400	-3.34937600	-0.27464400
H	-1.35242600	-3.32462600	-3.16074300
H	-0.24769000	-5.16084200	-4.40663100
H	1.89967200	-6.10799700	-3.58301700
C	-0.51418600	-2.08447300	-0.87743500
H	-0.55907100	-1.18715900	-1.50660200
H	0.09076800	-1.83107700	0.00274300
N	-1.88237200	-2.44494700	-0.52394500
H	-2.05264200	-3.43089000	-0.39159500
H	-5.13797200	-1.74549900	-0.66025200
C	4.36445600	2.91050600	-3.21536000
C	3.39999200	2.72420100	-2.22586500
C	3.77295000	2.39079800	-0.91541000
C	5.13376200	2.24611400	-0.61639200
C	6.10122400	2.44648100	-1.60566400
C	5.72030400	2.77847000	-2.90623300
H	4.05858700	3.16839700	-4.22518600
H	2.34618400	2.83740800	-2.47269300
H	5.43571900	1.95644400	0.38746300
H	7.15547500	2.35624800	-1.35602100
H	6.47302200	2.93716800	-3.67312400
C	2.71477000	2.22021200	0.15960500
H	2.06784900	3.10528800	0.16735600
H	3.19397600	2.17316400	1.14187700
N	1.83799200	1.04033700	0.03141700
H	1.42835100	0.99488800	-0.90219400
H	2.34963900	0.17098500	0.20034900

S	2.42194500	-1.71330000	2.79682100
O	2.62742500	-1.69781000	1.27656800
C	2.80311600	-0.03592500	3.40828900
H	1.97503800	0.60096700	3.09580600
H	2.86047400	-0.06391500	4.49987700
H	3.75636500	0.27349600	2.97140200
C	3.89263100	-2.52917000	3.51753000
H	3.77270900	-2.57426900	4.60348000
H	3.92881900	-3.54112900	3.10990000
H	4.78437500	-1.96174300	3.24097600

TS5'D

C	-6.37417000	0.05610500	2.33128700
C	-5.38749100	-0.34319500	1.43141400
C	-5.27884600	0.26311600	0.17067800
C	-6.18197700	1.27930100	-0.16150600
C	-7.17481500	1.67858600	0.73598400
C	-7.27303400	1.06909400	1.98651100
H	-6.44633000	-0.42668600	3.30214900
H	-4.68882800	-1.13111500	1.69794600
H	-6.10678900	1.76082500	-1.13347800
H	-7.86722800	2.46863500	0.45860200
H	-8.04274100	1.37903900	2.68758000
C	-4.22846100	-0.19408200	-0.81937600
H	-4.24018300	0.45723600	-1.70714300
H	-4.44218400	-1.20359200	-1.18378400
N	-2.91158100	-0.23098500	-0.20218000
H	-2.70114100	0.56293100	0.38487900
C	-1.83397100	-0.91744500	-0.71428100
S	-2.07201200	-2.04851400	-1.96508000
C	-0.55154200	-0.66721200	-0.11302500
C	-0.16281100	0.55646500	0.56617200
O	-0.93724900	1.66106600	0.32379600
C	0.35710500	0.51395400	1.99521100
H	1.05753100	-0.30884000	2.13567400
H	0.85356600	1.45159800	2.28309500
H	-0.49747800	0.35460800	2.66094400
C	0.65979200	-1.41746100	-0.43699300
C	0.71209600	-2.89757700	-0.56065300

C	0.18670400	-3.68798000	0.47296100
C	1.33319200	-3.53620000	-1.64429500
C	0.29403500	-5.07626300	0.43195400
H	-0.31757800	-3.20065600	1.30179100
C	1.43460200	-4.92554300	-1.68836400
H	1.69455000	-2.93917600	-2.47562100
C	0.92065200	-5.70118900	-0.64787700
H	-0.11913100	-5.67232300	1.24085000
H	1.90444400	-5.40362200	-2.54325700
H	0.99731300	-6.78404300	-0.68394200
C	1.78288300	-0.64529500	-0.52961900
C	3.22922300	-1.02303000	-0.70652300
H	3.64547500	-0.56658000	-1.61627600
C	4.10384800	-0.62910700	0.47888600
C	3.91149000	-1.23579800	1.73002000
C	5.10395600	0.34337800	0.35689700
C	4.69633500	-0.87802500	2.82506900
H	3.14694300	-2.00185100	1.83415500
C	5.89076700	0.70719800	1.45376500
H	5.28267300	0.80626600	-0.61146800
C	5.68769200	0.09839100	2.69139900
H	4.53959900	-1.36544200	3.78319400
H	6.66478900	1.46050100	1.33698700
H	6.29923100	0.37640900	3.54461200
C	0.57492500	5.30166000	-1.16645900
C	0.45206600	3.93678800	-1.43309800
C	1.54901300	3.07920500	-1.27975800
C	2.77158200	3.61757000	-0.85144100
C	2.89350800	4.97939700	-0.57574900
C	1.79424900	5.82551600	-0.73455600
H	-0.28268600	5.95510300	-1.29708200
H	-0.49930100	3.52957500	-1.76131400
H	3.63671500	2.96780700	-0.73724400
H	3.84732700	5.38075000	-0.24630600
H	1.88907300	6.88705000	-0.52642500
C	1.42872100	1.59894600	-1.56304900
H	2.22336100	1.26511900	-2.24014700
H	0.47087800	1.35332100	-2.03104400
N	1.49712600	0.77984100	-0.31746900

H	2.15027000	1.19720600	0.34643900
H	3.28242800	-2.10443200	-0.85488800
H	-0.71109100	2.36448900	0.94943600

TS5D

C	-6.22524400	-3.56409600	-0.43566800
C	-4.85145500	-3.35367700	-0.33390300
C	-3.99792300	-3.71520200	-1.38805400
C	-4.55158800	-4.28888300	-2.53744500
C	-5.92875900	-4.50120000	-2.64020500
C	-6.76917800	-4.13774100	-1.58889500
H	-6.87511100	-3.28561800	0.38949900
H	-4.42410300	-2.91551200	0.56397100
H	-3.89877000	-4.57535200	-3.35929900
H	-6.34173900	-4.94867700	-3.54009100
H	-7.84051300	-4.30136900	-1.66439400
C	-2.50094400	-3.48323500	-1.27874400
H	-1.99985500	-3.95677600	-2.13341500
H	-2.11227500	-3.92964600	-0.35970400
N	-2.13849300	-2.07280700	-1.23808900
H	-2.42484200	-1.54227300	-2.04831600
C	-1.79473200	-1.34124900	-0.11702100
S	-1.55540900	-2.16269600	1.37924000
C	-1.62160900	0.05772900	-0.29918900
C	-1.24481400	0.63624400	-1.60712000
O	-0.44516200	-0.02489500	-2.42305600
C	-2.22191700	1.51414600	-2.36543600
H	-2.74910600	2.19538000	-1.69610200
H	-1.71717200	2.07728200	-3.15650300
H	-2.96571200	0.86278800	-2.83933700
H	0.17580900	-0.73117600	-1.92710100
C	-1.64443900	1.06314600	0.75078600
C	-2.46015600	0.92962000	1.98919300
C	-3.82729300	0.62655200	1.89836200
C	-1.91106500	1.15776800	3.25955400
C	-4.62121000	0.56304400	3.04167000
H	-4.25880100	0.43256300	0.92124300
C	-2.70322500	1.08941300	4.40529300
H	-0.84933700	1.37117300	3.34258000

C	-4.06307700	0.79374100	4.30064800
H	-5.67822700	0.32907400	2.95036900
H	-2.25772200	1.26292700	5.38119700
H	-4.68126200	0.73866500	5.19202100
C	-0.94916300	2.20832100	0.48212700
C	-0.94750600	3.53167700	1.20735200
H	0.08172300	3.84223200	1.43665700
C	-1.62146600	4.63567800	0.39947300
C	-3.02033500	4.67656200	0.29157700
C	-0.87158400	5.60610400	-0.27624500
C	-3.64877700	5.66512000	-0.46392400
H	-3.61402500	3.92717700	0.80907100
C	-1.49872200	6.59563200	-1.03890600
H	0.21345300	5.59165300	-0.20240100
C	-2.88910700	6.62868400	-1.13353200
H	-4.73306400	5.68667200	-0.52865000
H	-0.89865000	7.34000600	-1.55467500
H	-3.37925600	7.39846800	-1.72235800
S	2.51064200	0.20117000	3.19522400
O	4.03371400	0.22210100	3.34329300
C	1.83215800	0.08544700	4.89168800
H	2.05508500	1.02522600	5.40015800
H	0.75137000	-0.06831300	4.83618800
H	2.31682200	-0.74245200	5.41492500
C	2.02533400	-1.46837500	2.65480800
H	0.93439000	-1.52238300	2.56507900
H	2.48225800	-1.59946900	1.67332900
H	2.41012500	-2.20907500	3.36095300
C	2.56397500	3.03366300	-4.08699500
C	1.87629400	2.34540400	-3.08722100
C	2.00662600	2.72742400	-1.74310600
C	2.84145100	3.80794200	-1.42738400
C	3.53698200	4.49098700	-2.42732400
C	3.39721800	4.10601800	-3.76098000
H	2.45413900	2.72745400	-5.12348500
H	1.23665700	1.50441700	-3.33989700
H	2.94893000	4.11464700	-0.38949400
H	4.18252500	5.32409900	-2.16420400
H	3.93427100	4.63717200	-4.54142000

C	1.25204200	1.99950100	-0.65593700
H	1.56904800	2.35072200	0.33137900
H	1.46811700	0.92898000	-0.68426800
N	-0.22615700	2.16416200	-0.77900600
H	-0.43457000	2.97815400	-1.35716000
H	-1.46052700	3.41620500	2.16422400
C	2.68954500	-5.47392000	0.60595000
C	1.84919600	-4.60410900	-0.08747600
C	2.28599400	-3.97484700	-1.26315300
C	3.57902000	-4.24105600	-1.72785200
C	4.42291000	-5.11379400	-1.03579800
C	3.97966400	-5.73150800	0.13424000
H	2.33618400	-5.95494100	1.51351400
H	0.84929100	-4.40201500	0.29117900
H	3.92748300	-3.76331500	-2.64058400
H	5.42138700	-5.31458600	-1.41437500
H	4.63169600	-6.41326900	0.67270200
C	1.38127300	-2.99654400	-1.98921600
H	0.40568100	-3.45301800	-2.18459500
H	1.81688800	-2.73841900	-2.95999500
N	1.14138200	-1.73962500	-1.24653800
H	0.67802100	-1.95762000	-0.36067700
H	2.04293800	-1.31314300	-1.00084900
S	5.03174400	-0.33442100	-0.23235800
O	3.50317800	-0.41723700	-0.13041300
C	5.70695700	-1.46625400	1.03276100
H	5.41354500	-2.47684000	0.74085500
H	6.79739900	-1.38190600	1.03078300
H	5.28567800	-1.19522300	2.00509600
C	5.50159300	1.22898700	0.58287600
H	6.59217100	1.30885600	0.59732500
H	5.07887600	2.03379800	-0.02189200
H	5.08242900	1.22670200	1.59429700

Int7'D

C	-5.94825800	0.79951500	2.43356500
C	-5.06833300	-0.06753900	1.78867200
C	-5.15273100	-0.27919900	0.40382200
C	-6.14060000	0.40270000	-0.31528600

C	-7.02674600	1.27083300	0.32756900
C	-6.93226100	1.47300700	1.70393800
H	-5.87249000	0.94679400	3.50761900
H	-4.30587900	-0.59431300	2.35612400
H	-6.21698100	0.24909600	-1.38886700
H	-7.78841800	1.78898600	-0.24857900
H	-7.62009200	2.14700900	2.20664900
C	-4.20414200	-1.23493800	-0.28860400
H	-4.45774800	-1.31652700	-1.35584600
H	-4.29662500	-2.24677300	0.11661700
N	-2.82444900	-0.80517200	-0.09712100
H	-2.68886000	0.19101200	-0.20912600
C	-1.73443200	-1.58952500	-0.45129200
S	-1.99269100	-3.20556500	-0.92416700
C	-0.45934600	-0.95420200	-0.37335400
C	-0.26430400	0.47998000	0.07587600
O	-1.14302500	1.38451900	-0.54304100
C	-0.25728000	0.66805800	1.59507500
H	0.51446800	0.04258500	2.04933200
H	-0.07266100	1.71483400	1.88043300
H	-1.23020200	0.35764900	1.98117500
C	0.84647200	-1.50819800	-0.53799400
C	1.22979000	-2.94384700	-0.63482900
C	1.05172000	-3.79852100	0.46302100
C	1.87725400	-3.43365000	-1.77548100
C	1.50806400	-5.11208800	0.41686000
H	0.53393300	-3.42997700	1.34253600
C	2.31943300	-4.75722500	-1.82816100
H	2.01234200	-2.77997100	-2.63208600
C	2.13951900	-5.59841500	-0.73150800
H	1.35994300	-5.76350200	1.27336100
H	2.80511600	-5.12754500	-2.72659100
H	2.48573400	-6.62729400	-0.76953600
C	1.84095800	-0.55771900	-0.51506100
C	3.33410000	-0.62928100	-0.49367000
H	3.79301600	-0.17272900	-1.38631300
C	3.96334700	0.01259400	0.74062500
C	3.65131500	-0.46152700	2.02447500
C	4.85046400	1.09018100	0.62579800

C	4.21316600	0.12458200	3.15748200
H	2.97126200	-1.30376900	2.12433400
C	5.41212000	1.68409700	1.76060300
H	5.11936300	1.45588200	-0.36324800
C	5.09344500	1.20340400	3.02958500
H	3.96921300	-0.26327100	4.14245000
H	6.10088700	2.51688900	1.64958100
H	5.52916100	1.66047700	3.91302200
C	-0.01261800	5.15813200	-1.87225500
C	0.07894200	3.77624800	-2.04138800
C	1.17304500	3.06703200	-1.52751600
C	2.17431700	3.77100200	-0.84139900
C	2.07595800	5.15093800	-0.66020300
C	0.98273400	5.84770600	-1.17720400
H	-0.86254600	5.69532100	-2.28232600
H	-0.70167900	3.23933500	-2.57150700
H	3.04236700	3.24178100	-0.45323500
H	2.85778100	5.68171100	-0.12536600
H	0.90882600	6.92260200	-1.04291500
C	1.29856000	1.57457100	-1.72369300
H	2.27371300	1.32389800	-2.14556400
H	0.52152100	1.16840900	-2.36945200
N	1.21656200	0.78550800	-0.42008600
H	1.68637400	1.34097700	0.30246300
H	3.59903100	-1.69036500	-0.53731500
H	-1.16941500	2.20907700	-0.03478100

Int7D

C	-1.06286800	7.15611700	-0.21107200
C	-0.63431200	5.90506800	-0.65027100
C	0.63009300	5.41406900	-0.29184400
C	1.45008900	6.20721600	0.51791600
C	1.02511100	7.46322200	0.95741100
C	-0.23357200	7.94102500	0.59501100
H	-2.04406500	7.52280300	-0.50008800
H	-1.27823200	5.29519400	-1.27761500
H	2.43122500	5.83752200	0.80650600
H	1.67622000	8.06378800	1.58652800
H	-0.56827700	8.91596400	0.93763500

C	1.10709200	4.06788200	-0.79871300
H	2.09903400	3.84709300	-0.37318900
H	1.24357000	4.08081200	-1.88406100
N	0.13997200	3.02371600	-0.50470800
H	-0.22047800	3.02434100	0.44067600
C	-0.03679900	1.86262700	-1.23856500
S	0.93822200	1.62023100	-2.64340800
C	-0.98607100	0.93871400	-0.74255800
C	-1.56672000	1.04552200	0.66198600
O	-0.69536300	1.33789000	1.67772600
C	-2.79376800	1.95270300	0.79367500
H	-3.58941100	1.63404800	0.11527100
H	-3.16176100	1.95006100	1.82603400
H	-2.50994200	2.97365600	0.53041300
H	0.24701600	1.01346100	1.46446300
C	-1.61731000	-0.16886900	-1.39833800
C	-1.65126600	-0.43823200	-2.86065100
C	-2.09227700	0.55087900	-3.75298400
C	-1.32945900	-1.70529100	-3.36781000
C	-2.21253300	0.27740300	-5.11239700
H	-2.32829500	1.53818700	-3.37078600
C	-1.43750700	-1.97550400	-4.73414500
H	-0.97491200	-2.47648600	-2.69051500
C	-1.88234500	-0.98611300	-5.61017700
H	-2.55578100	1.05514500	-5.78847700
H	-1.18086400	-2.96246700	-5.10975900
H	-1.97117300	-1.19517800	-6.67243000
C	-2.35237400	-0.94761000	-0.53926100
C	-3.36506900	-2.03028800	-0.76167100
H	-3.07380000	-2.97470100	-0.27638100
C	-4.76748000	-1.66246900	-0.28328500
C	-5.46032000	-0.59523700	-0.87559500
C	-5.38888900	-2.36635400	0.75552900
C	-6.73836000	-0.24662700	-0.44238400
H	-4.99011300	-0.04502600	-1.68667500
C	-6.66893500	-2.01571700	1.19652900
H	-4.87309400	-3.20805800	1.21308700
C	-7.34660700	-0.95445700	0.59857400
H	-7.26345700	0.57621000	-0.91911500

H	-7.13447600	-2.57595600	2.00250500
H	-8.34148600	-0.68070300	0.93697600
S	1.90856300	-3.50388400	-2.40899600
O	2.80362400	-4.47235200	-1.63006500
C	2.61435100	-3.35891400	-4.09021800
H	2.05981500	-2.59390400	-4.63958300
H	3.67240600	-3.09675900	-4.01477500
H	2.50397200	-4.32927200	-4.57751100
C	2.31284600	-1.82427900	-1.84220100
H	1.71315200	-1.07641700	-2.37303700
H	2.07542900	-1.81522300	-0.77619200
H	3.38105200	-1.63860100	-1.98339000
C	-0.63761100	-0.80724700	5.39678700
C	-0.46042400	-0.94184300	4.02027400
C	-1.55136900	-1.21546500	3.18778000
C	-2.82216200	-1.36124600	3.76166900
C	-3.00267900	-1.21142600	5.13709300
C	-1.90920800	-0.93422200	5.95845000
H	0.21832900	-0.59678500	6.03142700
H	0.52697700	-0.84574900	3.58112200
H	-3.68084800	-1.60460900	3.13805300
H	-3.99421500	-1.32147500	5.56641900
H	-2.04688200	-0.82215900	7.02987000
C	-1.34992500	-1.40705800	1.70305400
H	-1.66700900	-2.41047300	1.40597300
H	-0.30746600	-1.29880300	1.40936100
N	-2.17200900	-0.46204700	0.84662900
H	-3.08247900	-0.35502800	1.30286900
H	-3.38762000	-2.24078000	-1.83462000
C	5.85789400	0.87377300	-0.79721200
C	4.60345200	1.21672000	-0.29403300
C	4.31115400	1.04872200	1.06868200
C	5.30461700	0.53387500	1.90992300
C	6.56314100	0.19052900	1.40770800
C	6.84196100	0.35911200	0.05134700
H	6.06953500	1.01389100	-1.85347700
H	3.84274100	1.60914900	-0.96668900
H	5.09379200	0.40663500	2.96951000
H	7.32403500	-0.20195300	2.07679900

H	7.81957400	0.09606100	-0.34224300
C	2.93474200	1.39845300	1.60710500
H	2.69611000	2.44236000	1.37577400
H	2.93198900	1.30996600	2.69862900
N	1.83915000	0.56248700	1.07730200
H	1.81556900	0.64117200	0.05893400
H	2.02327300	-0.42296100	1.28937000
S	2.79640600	-3.46338000	2.11263900
O	1.89595800	-2.36627900	1.52408800
C	4.33707400	-3.49783100	1.13074000
H	4.81396600	-2.52267400	1.24966200
H	4.98388700	-4.27747800	1.54363400
H	4.09742000	-3.70119200	0.08270200
C	2.11909400	-5.05342300	1.52561700
H	2.74909800	-5.86167500	1.90752300
H	1.11495700	-5.14195000	1.94462300
H	2.10045900	-5.05112200	0.43109800

Int8'D

C	-5.11829700	4.09662800	1.86891800
C	-4.82546100	2.77189200	1.55115400
C	-5.47016600	2.12858800	0.48351800
C	-6.41532100	2.84905200	-0.25474000
C	-6.71435800	4.17666500	0.06179800
C	-6.06535000	4.80517400	1.12372700
H	-4.61245500	4.57730000	2.70201100
H	-4.09460200	2.21986200	2.13619000
H	-6.92247400	2.36386600	-1.08512300
H	-7.45197200	4.71838200	-0.52389500
H	-6.29506000	5.83751800	1.37187800
C	-5.15897300	0.68399200	0.15153200
H	-5.81902400	0.33620000	-0.65726800
H	-5.36010600	0.02702500	1.00326100
N	-3.75637100	0.51923300	-0.19758100
H	-3.39509500	1.19446300	-0.86021300
C	-3.08989200	-0.69560200	-0.18525100
S	-3.89564800	-2.08726000	0.41255200
C	-1.74722000	-0.66327400	-0.64592900
C	-0.95566700	0.62204000	-0.72320300

O	-1.50031700	1.47668500	-1.71329200
C	-0.77178400	1.36269900	0.60273500
H	-0.36111700	0.69417800	1.36188800
H	-0.11235000	2.23178100	0.48993300
H	-1.75271200	1.70000500	0.94148500
C	-0.92596800	-1.73268500	-1.10229200
C	-1.37086600	-3.13499200	-1.34913500
C	-0.92776200	-4.19887100	-0.55320100
C	-2.18217600	-3.41485800	-2.45766200
C	-1.29708100	-5.51108000	-0.85013600
H	-0.31979400	-3.99127100	0.32221700
C	-2.54822600	-4.72534500	-2.75638500
H	-2.53431100	-2.59431900	-3.07497500
C	-2.10777300	-5.77921900	-1.95320700
H	-0.95347300	-6.32410500	-0.21629200
H	-3.18178700	-4.92426100	-3.61620800
H	-2.39601500	-6.80063900	-2.18478800
C	0.34493700	-1.34554700	-1.44756100
C	1.39288500	-2.10775400	-2.20373800
H	1.55165500	-1.70281100	-3.21539100
C	2.76091800	-2.26601900	-1.54550200
C	2.89264300	-2.93533900	-0.31930200
C	3.92065300	-1.78731000	-2.16602800
C	4.14496200	-3.11859300	0.26619000
H	2.00126800	-3.31577800	0.17085800
C	5.17801900	-1.95951400	-1.58022600
H	3.84258700	-1.28536200	-3.12802300
C	5.29499500	-2.62676200	-0.36091600
H	4.22719500	-3.65101100	1.20983400
H	6.06359500	-1.57847600	-2.08092400
H	6.27089400	-2.77302000	0.09295200
C	0.88306400	4.62144600	-3.01006600
C	0.61291600	3.25464800	-3.09113400
C	1.27517100	2.34147500	-2.25620000
C	2.22319400	2.82694200	-1.34494800
C	2.48589800	4.19466700	-1.25706400
C	1.81797500	5.09513100	-2.08847500
H	0.36327500	5.31277400	-3.66679500
H	-0.11610300	2.88957800	-3.80958700

H	2.75998300	2.13689000	-0.70173400
H	3.22155900	4.54780900	-0.54146400
H	2.02788600	6.15858200	-2.02235200
C	1.02881900	0.85618600	-2.41655800
H	1.97637800	0.36387600	-2.64326900
H	0.33179400	0.66177600	-3.23091200
N	0.48962100	0.12671900	-1.20555500
H	1.16607300	0.27706000	-0.41061700
H	0.96914500	-3.10528400	-2.35806300
H	-1.17283100	2.37824100	-1.56632100
C	5.19394200	3.96144100	1.76843600
C	4.06252400	3.19173200	2.04670500
C	4.03211400	1.81945100	1.76346300
C	5.17129300	1.23648200	1.18905800
C	6.29981700	2.00423600	0.89975200
C	6.31707400	3.36960200	1.18948100
H	5.19589000	5.02223800	2.00336200
H	3.19050900	3.66056200	2.49589700
H	5.18828800	0.17280500	0.96575100
H	7.16987000	1.53278400	0.45155000
H	7.19762000	3.96532500	0.96780800
C	2.82066700	0.99119600	2.14237600
H	1.99272100	1.66061300	2.39542000
H	3.05171000	0.43676300	3.06610400
N	2.35036800	0.07084500	1.08492200
H	3.11921900	-0.52187100	0.77837600
H	1.68786900	-0.56421900	1.54780900
S	-0.10529500	-2.54789200	3.13095000
O	0.45678200	-1.13920000	2.92293200
C	-1.87875000	-2.37606200	3.49269100
H	-2.39578500	-2.13207500	2.55647500
H	-2.25372700	-3.33277200	3.86661600
H	-2.01008100	-1.58576900	4.23637900
C	0.43074800	-3.05109000	4.80734200
H	-0.01170700	-4.01848600	5.05815100
H	1.51894000	-3.13407400	4.78871600
H	0.12986900	-2.28636600	5.52752100
Int8D			
C	8.61037000	-1.23740000	1.86358800

C	7.64632500	-1.33943700	0.86183800
C	6.96777200	-2.55061000	0.64970500
C	7.27930100	-3.64740400	1.46252200
C	8.24654900	-3.54616900	2.46499700
C	8.91386000	-2.33873600	2.66899400
H	9.13245500	-0.29612300	2.01296600
H	7.41353200	-0.49135700	0.22339500
H	6.76153700	-4.59127400	1.30603100
H	8.47604200	-4.40873900	3.08475200
H	9.66682200	-2.25564700	3.44786100
C	5.91226800	-2.66915000	-0.43108700
H	5.60990900	-3.71903400	-0.52679900
H	6.30656700	-2.33045100	-1.39351000
N	4.70714700	-1.86142500	-0.16982700
H	4.55151400	-1.77469200	0.83055000
C	4.46630700	-0.60490300	-0.83826600
S	5.58082300	0.00748800	-1.97003000
C	3.22657700	-0.04040400	-0.51183900
C	2.06215100	-0.81526700	0.10094400
O	2.04884000	-2.18413000	-0.14655800
C	1.83349300	-0.56828100	1.59765900
H	1.67859100	0.48916200	1.82158200
H	0.97421800	-1.14732100	1.94756800
H	2.71658200	-0.91147900	2.14309100
H	2.98707600	-2.41021900	-0.36865300
C	2.69254300	1.24042200	-0.90402000
C	3.49052200	2.46465300	-1.17531500
C	4.38464500	2.94430700	-0.20699100
C	3.33331700	3.18991500	-2.36430000
C	5.09348500	4.12447900	-0.41788400
H	4.52793300	2.37383100	0.70557700
C	4.04885900	4.36746100	-2.57901800
H	2.67391800	2.80646800	-3.13717200
C	4.92769500	4.84157700	-1.60460300
H	5.78307600	4.48147500	0.34184100
H	3.92562600	4.90990700	-3.51216600
H	5.48612500	5.75811300	-1.77172300
C	1.32666700	1.24357800	-0.88530900
C	0.32680000	2.34481900	-1.06206800

H	-0.51963600	1.99916300	-1.67162900
C	-0.23146400	2.99512200	0.20531100
C	0.58269400	3.23776400	1.31942300
C	-1.55647700	3.44694900	0.23809100
C	0.08198000	3.90162000	2.44072500
H	1.62059600	2.92047200	1.29587400
C	-2.05921700	4.11766100	1.35556200
H	-2.19927600	3.28638600	-0.62346100
C	-1.24261800	4.34298500	2.46544200
H	0.73116800	4.08250900	3.29280900
H	-3.08735200	4.47058900	1.35484400
H	-1.63050800	4.86442600	3.33562900
S	-6.69705000	-2.14339800	-1.20602800
O	-7.43563500	-0.82278400	-1.40888700
C	-7.94627200	-3.35018200	-0.62899600
H	-7.45238400	-4.28914500	-0.36582800
H	-8.47932100	-2.93466800	0.22951600
H	-8.64186900	-3.51408900	-1.45371400
C	-5.75922400	-2.01458300	0.35337600
H	-5.27148800	-2.97153500	0.55699400
H	-5.01367900	-1.23303700	0.19009800
H	-6.42695300	-1.73559600	1.17191900
C	-0.98901200	-4.32515500	-2.05197000
C	-0.05631700	-3.29117200	-1.97945100
C	-0.47154800	-1.95234700	-1.97895700
C	-1.84392600	-1.67463700	-2.06151900
C	-2.77908200	-2.70888200	-2.12665200
C	-2.35331800	-4.03782300	-2.12389800
H	-0.64801300	-5.35647000	-2.05719400
H	1.00101100	-3.51534900	-1.91396100
H	-2.19946600	-0.64813000	-2.06979000
H	-3.83598000	-2.46991000	-2.19491900
H	-3.07791000	-4.84513900	-2.18720200
C	0.52580800	-0.81451800	-1.99528600
H	0.13889700	-0.00670400	-2.61906400
H	1.49022900	-1.12192900	-2.39966600
N	0.84400300	-0.15020100	-0.65191600
H	-0.01791200	-0.17474600	-0.04321700
H	0.81099900	3.13474400	-1.64670900

C	-4.76468200	-1.48244900	4.02997900
C	-3.51147200	-1.31081700	3.44051200
C	-3.09380200	-0.05106800	2.98896400
C	-3.96108300	1.03719300	3.15305100
C	-5.21524000	0.87121400	3.74401900
C	-5.62240200	-0.39050600	4.18168900
H	-5.06576100	-2.46426800	4.38488200
H	-2.84244000	-2.16332000	3.34163500
H	-3.63802500	2.02267200	2.82711800
H	-5.86939300	1.72886100	3.87600800
H	-6.59344000	-0.51937700	4.65102100
C	-1.73724700	0.12804800	2.33075100
H	-0.98783800	-0.45399000	2.87792800
H	-1.43187300	1.17585800	2.39181400
N	-1.66876700	-0.27458500	0.90898200
H	-1.92047300	-1.25828300	0.81860900
H	-2.38365800	0.22625800	0.37205600
S	-4.74984400	1.84074000	-1.30127500
O	-4.01884900	0.54360100	-0.92738900
C	-6.21517700	1.96924600	-0.21753300
H	-5.84416900	2.02666300	0.80753400
H	-6.75527200	2.88556800	-0.47167600
H	-6.84217500	1.08414300	-0.35654800
C	-5.64581600	1.51153300	-2.85698600
H	-6.20834600	2.40806500	-3.13220500
H	-4.89232200	1.30267800	-3.61874500
H	-6.30941700	0.65482400	-2.70778100

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C	-5.64350800	3.46690400	1.72873600
C	-5.15763800	2.20221000	1.40338200
C	-5.66661300	1.49658200	0.30209200
C	-6.67403400	2.09423700	-0.46278000
C	-7.16579000	3.36172600	-0.13971600
C	-6.65106100	4.05264900	0.95640200
H	-5.24115200	3.99656500	2.58824000
H	-4.37682200	1.74498800	2.00519200
H	-7.07669100	1.56021300	-1.32007700
H	-7.94844200	3.80829300	-0.74698200

H	-7.03082800	5.03846600	1.20969000
C	-5.14383300	0.11545400	-0.03614000
H	-5.72295300	-0.30555800	-0.87239500
H	-5.28118200	-0.57688700	0.80020400
N	-3.72138700	0.15051100	-0.33208300
H	-3.44641100	0.82530800	-1.03641000
C	-2.87834800	-0.95184500	-0.25198500
S	-3.48496200	-2.43109500	0.38886800
C	-1.55107600	-0.73509000	-0.68460800
C	-0.94566200	0.64630800	-0.82618100
O	-1.58477900	1.34330400	-1.91022100
C	-1.00675300	1.51481500	0.43921400
H	-0.62601700	0.96291600	1.30066000
H	-0.43369900	2.44139000	0.31781600
H	-2.04693700	1.76535600	0.65047000
C	-0.59228300	-1.68487400	-1.16061200
C	-0.84879900	-3.12750000	-1.43128900
C	-0.24224600	-4.14039100	-0.67712800
C	-1.65681200	-3.49504600	-2.51734700
C	-0.43970600	-5.48498800	-0.99372300
H	0.35491500	-3.86988300	0.18847000
C	-1.85347100	-4.83664900	-2.83631400
H	-2.13832100	-2.71691300	-3.10110900
C	-1.24490600	-5.83803600	-2.07626900
H	0.03143600	-6.25651000	-0.39043800
H	-2.48586200	-5.10219300	-3.67896300
H	-1.40078700	-6.88417800	-2.32432700
C	0.59193700	-1.09237900	-1.51255500
C	1.71508200	-1.68582200	-2.31563200
H	1.82594600	-1.18686000	-3.29006000
C	3.10153500	-1.76089200	-1.67747800
C	3.31936600	-2.52872700	-0.52143600
C	4.20372600	-1.12059300	-2.25776500
C	4.59611400	-2.65715500	0.02824100
H	2.47825700	-3.04950900	-0.07264500
C	5.48352500	-1.23975100	-1.70888100
H	4.06240900	-0.53694000	-3.16462300
C	5.68615400	-2.01106600	-0.56460800
H	4.74455200	-3.27534300	0.90968500

H	6.32180600	-0.73631700	-2.18227800
H	6.68155500	-2.11811700	-0.14331200
C	0.46014400	4.95697900	-2.62738300
C	0.37213100	3.57432000	-2.80161100
C	1.15418500	2.69882500	-2.03324900
C	2.04721900	3.24822000	-1.10380600
C	2.13341500	4.62865400	-0.92238700
C	1.33643200	5.48824000	-1.68065200
H	-0.15286900	5.61641500	-3.23482700
H	-0.30136000	3.16689300	-3.55109200
H	2.69549700	2.59517800	-0.52865400
H	2.83482100	5.02831600	-0.19617900
H	1.40625000	6.56320000	-1.54300500
C	1.10018300	1.20273700	-2.27574400
H	2.12429400	0.85168600	-2.42699400
H	0.53706200	0.99957400	-3.19023100
N	0.54208600	0.35481500	-1.17451600
H	1.29031900	0.39156100	-0.00241000
H	1.40075600	-2.70842300	-2.54801300
H	-1.44105000	2.29423600	-1.78685500
C	4.93050700	3.81672600	2.07552100
C	3.70389700	3.16037800	2.17617400
C	3.58588200	1.79928000	1.85994700
C	4.73096700	1.10986600	1.44130600
C	5.95654300	1.76835200	1.32744400
C	6.06221300	3.12228000	1.64527400
H	5.00007900	4.87069900	2.32861300
H	2.82513000	3.70940100	2.50458400
H	4.68907200	0.05103800	1.20176600
H	6.82921800	1.21631100	0.99150400
H	7.01693300	3.63212200	1.55847000
C	2.25140800	1.11183700	2.06362800
H	1.45055200	1.85493300	2.07055000
H	2.22989800	0.62091700	3.04344400
N	1.89190000	0.07968200	1.04945400
H	2.70527500	-0.46853600	0.76695900
H	1.25138200	-0.58186600	1.53550200
S	-0.28759000	-2.54877900	3.16323500
O	0.37587800	-1.17618700	2.96130100

C	-2.00213200	-2.23143000	3.67084600
H	-2.55463100	-1.95155700	2.76652200
H	-2.42455700	-3.15848200	4.06758600
H	-2.00363200	-1.44021500	4.42513300
C	0.33864900	-3.13227900	4.77978700
H	-0.15609400	-4.06965700	5.04594000
H	1.41200600	-3.29812900	4.67130400
H	0.15545800	-2.36629100	5.53700900

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C	8.54600200	-1.86544200	1.62083800
C	7.56062300	-1.75982900	0.64035300
C	6.78672900	-2.87758300	0.28732500
C	7.02654000	-4.09353000	0.93931700
C	8.01467300	-4.20020600	1.92072800
C	8.77663200	-3.08414000	2.26545000
H	9.14182500	-0.99408400	1.87947200
H	7.38251700	-0.81963500	0.12464800
H	6.43485500	-4.96662500	0.67237500
H	8.18688400	-5.15297200	2.41438800
H	9.54641600	-3.16239600	3.02838900
C	5.70801600	-2.76982200	-0.77118200
H	5.32624600	-3.77287200	-0.99907400
H	6.11480100	-2.33365000	-1.68886800
N	4.57237300	-1.91694000	-0.37579700
H	4.47801600	-1.91087500	0.63606700
C	4.41154600	-0.57113200	-0.90299600
S	5.59513500	0.10600300	-1.93145400
C	3.20078400	0.01276500	-0.53536300
C	1.99398100	-0.73927200	0.02855200
O	1.91746500	-2.09496900	-0.32670200
C	1.87427600	-0.63088700	1.55754400
H	1.74246800	0.40343500	1.88540200
H	1.03945600	-1.24423900	1.91488300
H	2.78574900	-1.02059700	2.01975500
H	2.84855600	-2.34582000	-0.56278500
C	2.71948800	1.35157100	-0.80276100
C	3.56577400	2.56406300	-0.95630400
C	4.46721800	2.92049400	0.05843300

C	3.45164300	3.40307800	-2.07369500
C	5.22018500	4.08822800	-0.03478400
H	4.58282600	2.26061700	0.91295500
C	4.20995400	4.56988800	-2.17111400
H	2.78958300	3.11663700	-2.88551000
C	5.09319000	4.91994100	-1.14962700
H	5.91466100	4.34633700	0.76002200
H	4.11691100	5.20061900	-3.05100600
H	5.68556000	5.82738200	-1.22556100
C	1.35471500	1.38644500	-0.76115100
C	0.42092600	2.55504900	-0.86883300
H	-0.40743900	2.32443300	-1.55542200
C	-0.17496100	3.08642100	0.43439100
C	0.61302900	3.21871000	1.58709000
C	-1.50390400	3.52632100	0.48593400
C	0.08358200	3.76187700	2.75869300
H	1.65243400	2.90684100	1.55079700
C	-2.03790800	4.07335600	1.65630100
H	-2.12560000	3.45613500	-0.40291000
C	-1.24661200	4.18802300	2.80090200
H	0.71338300	3.86017100	3.63845900
H	-3.06862200	4.41896400	1.66899400
H	-1.65693800	4.61468500	3.71156300
S	-6.69182900	-2.24114100	-1.33585700
O	-7.23063700	-0.83890600	-1.61068900
C	-8.09278100	-3.21118600	-0.66849800
H	-7.73361200	-4.18785600	-0.33379100
H	-8.55060000	-2.65912300	0.15576700
H	-8.81463700	-3.33753600	-1.47710200
C	-5.71509800	-2.15292600	0.20363600
H	-5.28514000	-3.13574100	0.41272200
H	-4.92828900	-1.41703200	0.02032300
H	-6.34521700	-1.81976000	1.03182800
C	-1.95579100	-3.48242200	-1.53012100
C	-0.84016800	-2.65663200	-1.37647800
C	-0.75641900	-1.43061300	-2.06192000
C	-1.81840300	-1.07290600	-2.90497600
C	-2.92668300	-1.90505200	-3.07128100
C	-3.00162200	-3.11420700	-2.38048700

H	-1.99497600	-4.43110700	-1.00074200
H	-0.00944700	-2.95590100	-0.74680600
H	-1.76622000	-0.13499400	-3.45335600
H	-3.72941800	-1.61016600	-3.74116500
H	-3.86080900	-3.76536600	-2.51302600
C	0.45193700	-0.51653500	-1.97295000
H	0.27216300	0.35031500	-2.61221400
H	1.33971800	-1.02390200	-2.35883400
N	0.79808500	0.02569800	-0.59620000
H	-0.47558700	-0.02647100	0.22992700
H	0.97178500	3.37992800	-1.33371700
C	-4.20757000	-1.98910600	3.89345300
C	-3.02660900	-1.58815700	3.26857900
C	-2.83850800	-0.25399100	2.88248200
C	-3.85213100	0.67489200	3.14582900
C	-5.03135900	0.27852000	3.77810800
C	-5.21354900	-1.05485300	4.14970900
H	-4.33496800	-3.02452800	4.19551100
H	-2.23739400	-2.31649400	3.09359600
H	-3.70360000	1.71420900	2.86679300
H	-5.80397700	1.01197400	3.99070600
H	-6.12753400	-1.36175500	4.64974900
C	-1.55646300	0.17308000	2.20491600
H	-0.69499400	-0.29651200	2.68363100
H	-1.42034200	1.25307200	2.26086600
N	-1.51018600	-0.19689500	0.75457900
H	-1.69726500	-1.19460700	0.62943200
H	-2.27294000	0.28651200	0.23891500
S	-4.61989900	1.87517600	-0.98129100
O	-3.91776800	0.61730600	-0.44697300
C	-6.26204200	1.92798900	-0.18768300
H	-6.08809700	2.02221600	0.88569200
H	-6.79787900	2.80716700	-0.55597500
H	-6.80228800	1.00613800	-0.42233100
C	-5.19001400	1.48847600	-2.67006200
H	-5.72013300	2.36076700	-3.06256600
H	-4.29742700	1.30007000	-3.26890200
H	-5.84138400	0.61034800	-2.63526100

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C	5.93758400	-3.04331200	2.02730300
C	5.26977600	-1.84707600	1.77342200
C	5.74785800	-0.94387600	0.81168900
C	6.91236700	-1.27577700	0.11072000
C	7.58700300	-2.47334100	0.36224100
C	7.10117400	-3.36156300	1.32075300
H	5.55473600	-3.72793800	2.77958000
H	4.36669800	-1.59964400	2.32495500
H	7.29420700	-0.58731900	-0.63912500
H	8.48976700	-2.71148400	-0.19362400
H	7.62311300	-4.29362900	1.51824000
C	5.02777200	0.36330700	0.55198800
H	5.60316100	0.96852800	-0.16553800
H	4.96586400	0.96610400	1.46271200
N	3.66766700	0.12321000	0.09027300
H	3.61318800	-0.52019900	-0.69230500
C	2.69820500	1.13154100	0.01734500
S	3.02265100	2.65117500	0.78485300
C	1.50503300	0.78897400	-0.64080500
C	1.11034000	-0.64329900	-0.96438000
O	2.03837200	-1.18638500	-1.93917500
C	1.07371900	-1.60213400	0.23838800
H	0.43364700	-1.20345000	1.02813400
H	0.69107300	-2.58762200	-0.04943500
H	2.07665100	-1.71409800	0.65268700
C	0.50633600	1.65267500	-1.23206900
C	0.58819000	3.13151600	-1.37116100
C	1.57711300	3.70360700	-2.18725100
C	-0.34575700	3.98564500	-0.76830200
C	1.62657500	5.07940600	-2.39187400
H	2.31233900	3.05533400	-2.65249900
C	-0.29695500	5.36701100	-0.96839700
H	-1.10420400	3.56193200	-0.11597700
C	0.68988200	5.91924400	-1.78312700
H	2.40180000	5.50045000	-3.02605800
H	-1.02969000	6.00919900	-0.48655900
H	0.73200700	6.99308400	-1.94192100
C	-0.48759300	0.91912300	-1.81530600

C	-1.59120000	1.41788500	-2.71163400
H	-1.47644800	1.03441900	-3.73640200
C	-3.02496400	1.13685700	-2.26565400
C	-3.56172100	1.77317900	-1.13374300
C	-3.85545100	0.25901700	-2.97467800
C	-4.86966500	1.52186800	-0.71292500
H	-2.94558400	2.48160800	-0.58787100
C	-5.16360700	-0.00271500	-2.55560400
H	-3.48067400	-0.21740000	-3.87734200
C	-5.67437600	0.62146500	-1.41839200
H	-5.26359900	2.03498700	0.16003800
H	-5.78319800	-0.69053500	-3.12428500
H	-6.69023900	0.42244500	-1.09080000
C	0.09202700	-5.14293900	-2.58740800
C	0.26462600	-3.77803400	-2.83179900
C	-0.71030400	-2.84715600	-2.45115000
C	-1.88492800	-3.32718900	-1.85299400
C	-2.06339100	-4.68830200	-1.60630800
C	-1.06829700	-5.60119300	-1.96420400
H	0.86145100	-5.84657500	-2.89159300
H	1.15661000	-3.43302200	-3.34887000
H	-2.67960800	-2.62478000	-1.61374800
H	-2.98452700	-5.04080200	-1.15019100
H	-1.20544700	-6.66152300	-1.77452400
C	-0.54812800	-1.36690000	-2.74055900
H	-1.48547000	-1.02105900	-3.17570300
H	0.23759400	-1.21923400	-3.48923900
N	-0.29314900	-0.50716200	-1.55484900
H	-1.48218600	-0.62813200	-0.08766100
H	-1.45858900	2.50104000	-2.78547300
H	2.02599300	-2.15170800	-1.85740500
C	-6.03737200	-2.07375800	2.83751700
C	-4.90345600	-2.22421800	2.03768400
C	-3.72330000	-1.53381400	2.33746000
C	-3.69163700	-0.68180600	3.45215800
C	-4.82782000	-0.52848800	4.24560300
C	-6.00070800	-1.22462800	3.94328100
H	-6.94513700	-2.61891000	2.59653500
H	-4.93520300	-2.88741900	1.17672200

H	-2.78298600	-0.13103500	3.68175900
H	-4.79584600	0.13352000	5.10596900
H	-6.88123000	-1.10567100	4.56779800
C	-2.50122200	-1.71197300	1.46594100
H	-2.65229000	-2.51248000	0.73997800
H	-1.62075800	-1.96228400	2.06273000
N	-2.15296400	-0.45971900	0.71642900
H	-2.98776300	-0.02192000	0.31538100
H	-1.69770900	0.23694800	1.40671700
S	0.25732100	1.76609400	2.33130200
O	-1.07113200	0.98860600	2.62754900
C	1.46225700	1.00101700	3.46387200
H	1.68533600	0.01176000	3.06274200
H	2.37100300	1.60231500	3.45757600
H	1.00809700	0.92083800	4.45465600
C	0.06063800	3.34329700	3.22335300
H	1.00397600	3.88655100	3.15123600
H	-0.72502500	3.90238100	2.71326800
H	-0.22298500	3.14921100	4.26033700

Int9D

C	0.81312000	7.02693900	-0.86946500
C	1.80484700	6.05181500	-0.75738000
C	1.70294100	5.02620800	0.19336400
C	0.58077600	5.00570300	1.03428100
C	-0.40816700	5.98718600	0.93395100
C	-0.29651400	6.99931500	-0.02242100
H	0.91252800	7.81606300	-1.60937400
H	2.67712900	6.08861800	-1.40553800
H	0.49334300	4.21891100	1.77981500
H	-1.25538900	5.97322400	1.61526600
H	-1.06122600	7.76700400	-0.09832200
C	2.77417800	3.96622200	0.29543200
H	2.77730200	3.51841300	1.29360200
H	3.77281300	4.37869500	0.11140100
N	2.52333300	2.85718700	-0.66696900
H	2.55448000	3.25942700	-1.60465500
C	3.60820700	1.81625000	-0.60569800
S	5.17542300	2.33951400	-1.04865300

C	3.13130400	0.59942300	-0.17620300
C	1.64842200	0.22302000	-0.05204600
O	0.80336600	1.31797100	0.27355500
C	1.14376500	-0.41723700	-1.35829800
H	1.73088200	-1.30186900	-1.61417400
H	0.09901600	-0.72315200	-1.23737100
H	1.21822700	0.30211400	-2.18000500
H	1.35327900	2.12048800	-0.17698500
C	3.82522100	-0.61410200	0.26160500
C	5.23257100	-0.99045900	-0.02088400
C	5.70382100	-1.05830700	-1.34235800
C	6.11249300	-1.33090700	1.01744700
C	7.00087500	-1.48460600	-1.61494200
H	5.04628700	-0.75959300	-2.15166100
C	7.41683200	-1.74837100	0.74609100
H	5.77414100	-1.24389300	2.04587300
C	7.86311600	-1.83324300	-0.57198900
H	7.34622400	-1.53117900	-2.64404900
H	8.08397000	-2.00019500	1.56611000
H	8.87789200	-2.15688100	-0.78648300
C	2.94280300	-1.40957400	0.93720300
C	3.13440700	-2.80079800	1.47559300
H	2.83070000	-2.85655100	2.53046200
C	2.36552700	-3.86073700	0.69733300
C	2.73282400	-4.17175700	-0.62038200
C	1.29678400	-4.55805600	1.27205900
C	2.05475600	-5.15660900	-1.33786500
H	3.56287900	-3.63872200	-1.07679200
C	0.61133300	-5.54350500	0.55582700
H	1.00591800	-4.33542200	2.29605400
C	0.98980800	-5.84786400	-0.75218500
H	2.36427100	-5.39289200	-2.35249500
H	-0.21099000	-6.07825200	1.02377100
H	0.46834100	-6.62331500	-1.30665000
S	-5.21237700	-3.35089300	0.62402400
O	-4.75304600	-4.09136100	-0.62730400
C	-6.78677300	-4.12670700	1.14152500
H	-7.21926600	-3.55790500	1.96874700
H	-7.47027300	-4.16225600	0.28977400

H	-6.55232500	-5.14043200	1.47056600
C	-5.90537400	-1.75196400	0.07729700
H	-6.30743800	-1.21373800	0.93975600
H	-5.07021600	-1.20389900	-0.36546900
H	-6.68419000	-1.92896000	-0.66907100
C	-2.03750500	1.11012900	3.53895100
C	-0.67249900	0.97300300	3.27157200
C	-0.17551800	-0.16501400	2.62443900
C	-1.07870000	-1.17151700	2.25505400
C	-2.44302700	-1.04259800	2.52081800
C	-2.92978500	0.10193800	3.16055800
H	-2.40346700	1.99996300	4.04416200
H	0.01721000	1.76168600	3.56089100
H	-0.69503400	-2.05009300	1.74571700
H	-3.12649800	-1.83522600	2.22940300
H	-3.99068400	0.20477300	3.37152600
C	1.30865700	-0.32638800	2.36047500
H	1.70021200	-1.06255300	3.07184000
H	1.82986400	0.61874800	2.56770800
N	1.61665800	-0.83628600	1.00924700
H	-0.71020200	1.20348400	0.04324100
H	4.20085900	-3.04033200	1.44953300
C	-5.27178800	4.51461000	-0.22530600
C	-3.93103800	4.12749600	-0.26742100
C	-3.56216000	2.90107000	-0.83177000
C	-4.55717200	2.06359900	-1.35799300
C	-5.89601800	2.44954000	-1.31016800
C	-6.25676100	3.67527800	-0.74486000
H	-5.54407900	5.47091600	0.21119100
H	-3.16254300	4.78611100	0.12845500
H	-4.27795800	1.10763000	-1.79326900
H	-6.65993400	1.79653300	-1.72257000
H	-7.30007300	3.97530400	-0.71436500
C	-2.10522300	2.50389900	-0.88213800
H	-1.47068700	3.30968500	-0.50607600
H	-1.78555600	2.27991200	-1.90385700
N	-1.79290400	1.27927300	-0.07543100
H	-2.19629000	1.33435700	0.86418300
H	-2.16919400	0.41999100	-0.53697100

S	-2.28111300	-1.82414000	-2.43250800
O	-2.96183500	-0.90579800	-1.38507200
C	-3.64765600	-2.62162200	-3.33570300
H	-4.18084000	-1.83258800	-3.86927000
H	-3.21952600	-3.32588300	-4.05392200
H	-4.29693500	-3.13290900	-2.61982300
C	-1.68153600	-3.29028400	-1.53690600
H	-1.22573600	-3.97059600	-2.26066600
H	-0.91363200	-2.95338600	-0.83926600
H	-2.52307000	-3.76129300	-1.02204500

Int10D

C	-0.49306400	5.19225600	2.73280400
C	0.32415900	4.36167400	1.96685800
C	1.16887900	3.42569500	2.58576800
C	1.17349300	3.35063500	3.98468400
C	0.35635900	4.18271600	4.75338600
C	-0.48111800	5.10614800	4.12759100
H	-1.13908200	5.91399100	2.24010800
H	0.32164800	4.42893700	0.88236200
H	1.82899400	2.63516700	4.47790000
H	0.37667600	4.11115700	5.83764900
H	-1.11777900	5.75629900	4.72126000
C	2.03540000	2.49941200	1.75248400
H	2.82753700	2.07649100	2.38234100
H	2.50349300	3.04449800	0.92983500
N	1.31102400	1.37341800	1.14115700
H	0.82658900	0.82028600	1.83974400
C	0.51904100	1.57285200	-0.03680000
S	1.26423000	2.53493000	-1.28860900
C	-0.67940800	0.88915100	-0.14977800
C	-1.28433000	-0.00604000	0.93392600
O	-0.27662300	-0.95187600	1.40114300
C	-1.84474100	0.75714000	2.14503100
H	-2.65404600	1.40617300	1.80366400
H	-2.25932200	0.06990900	2.89079200
H	-1.08321800	1.38540900	2.61404800
C	-1.59023900	0.79254000	-1.30064500
C	-1.67272700	1.70812100	-2.46864300

C	-1.90918200	3.08070400	-2.27737000
C	-1.61207600	1.22805200	-3.78518300
C	-2.08936600	3.93455400	-3.36066400
H	-1.94129800	3.46958600	-1.26493600
C	-1.78551600	2.08465200	-4.87529300
H	-1.40967400	0.17441400	-3.95703400
C	-2.02734500	3.44109500	-4.66750800
H	-2.27332700	4.99148200	-3.18742100
H	-1.72867800	1.68839100	-5.88581800
H	-2.16398500	4.10986700	-5.51286000
C	-2.52652100	-0.17178200	-1.05646900
C	-3.72043600	-0.54512700	-1.89452000
H	-3.64933100	-1.58493200	-2.24495100
C	-5.06318900	-0.36406500	-1.19878000
C	-5.39350100	0.85762400	-0.59457200
C	-6.00763300	-1.39614900	-1.17234300
C	-6.63178900	1.03809000	0.01891800
H	-4.66870500	1.66697300	-0.61074800
C	-7.25033400	-1.22008200	-0.55809500
H	-5.77016500	-2.34863300	-1.64142100
C	-7.56625700	-0.00144500	0.04093300
H	-6.87028400	1.99273700	0.47990800
H	-7.96816800	-2.03576000	-0.54848300
H	-8.53100900	0.13991200	0.51979600
C	-2.49766900	-3.96511800	3.79646900
C	-2.13654400	-3.54102700	2.51350300
C	-2.90285700	-2.58945300	1.82911600
C	-4.04462500	-2.06676000	2.45539100
C	-4.40603800	-2.48878600	3.73329000
C	-3.63331400	-3.43865200	4.40912800
H	-1.89192700	-4.70539000	4.31166200
H	-1.25750100	-3.96342800	2.03096100
H	-4.63953500	-1.32478500	1.93157200
H	-5.29453000	-2.07813000	4.20463900
H	-3.91769300	-3.76472300	5.40543700
C	-2.53129400	-2.16547500	0.41803700
H	-3.33711300	-2.48496600	-0.24915600
H	-1.62800400	-2.70902800	0.10213400
N	-2.39666500	-0.71951200	0.24399500

H	1.24731200	-1.30592100	0.30584200
H	-3.69394300	0.07326100	-2.79688500
H	-0.64865700	-1.44376200	2.14989700
C	-0.29415500	-3.85593100	-2.95713700
C	0.22717800	-2.63139000	-2.53449200
C	1.54522700	-2.54451500	-2.06808100
C	2.32963500	-3.70584400	-2.01940500
C	1.80606900	-4.92880200	-2.43768900
C	0.49494600	-5.00575700	-2.91252800
H	-1.31513500	-3.90941200	-3.32389600
H	-0.39167300	-1.73811900	-2.55656600
H	3.34328500	-3.65065100	-1.63217600
H	2.42281300	-5.82213500	-2.39658700
H	0.09069600	-5.95768200	-3.24480300
C	2.10483500	-1.21394300	-1.62407800
H	1.50085700	-0.37506000	-1.97429500
H	3.13117700	-1.06681400	-1.96358600
N	2.16285100	-1.10213600	-0.12699000
H	2.90507800	-1.72641000	0.24892700
H	2.37892300	-0.12638800	0.15898200
S	4.89809600	1.86524800	-0.92559900
O	4.62792600	0.46398400	-0.36015100
C	4.47566100	1.81807100	-2.69758600
H	3.38659600	1.73945100	-2.73665000
H	4.79641200	2.75509600	-3.16072100
H	4.96668100	0.96043900	-3.16502200
C	6.71899800	1.94011200	-1.14442600
H	6.98847100	2.86447500	-1.66183400
H	7.16581500	1.93539100	-0.14835900
H	7.05642200	1.06636800	-1.70737000
S	5.70750900	-2.35493200	0.87478400
O	4.25462600	-2.79974100	0.66479700
C	6.45429700	-3.69017300	1.87492500
H	6.47795200	-4.58429900	1.24972900
H	7.47138500	-3.40930500	2.16032500
H	5.83470200	-3.87112500	2.75618600
C	5.68407600	-1.07366300	2.17188900
H	6.71087300	-0.84796700	2.47257800
H	5.22143700	-0.20080500	1.70666900

H	5.09881200	-1.43367500	3.02172300
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TS7D

C	2.02698900	5.25280200	-3.25404800
C	1.80298200	3.88428000	-3.11771400
C	2.76942700	3.05230700	-2.53183100
C	3.96466100	3.63154500	-2.09133400
C	4.19546100	5.00261200	-2.22887600
C	3.22527000	5.81881300	-2.80898800
H	1.26752900	5.88035700	-3.71232700
H	0.87384400	3.44422100	-3.46789700
H	4.72646100	2.99805900	-1.64163100
H	5.13096100	5.43212400	-1.88008800
H	3.39902600	6.88584000	-2.91498000
C	2.53771300	1.55910600	-2.41564600
H	3.39212400	1.09407600	-1.89688200
H	2.50086000	1.08798000	-3.40355300
N	1.28129000	1.25374700	-1.76027000
H	1.13431400	1.67842900	-0.85090800
C	0.52274100	0.10924000	-1.98314600
S	1.09711500	-1.02654200	-3.15293200
C	-0.65481300	-0.01755500	-1.21429300
C	-1.18943500	1.07480400	-0.35506600
O	0.00098100	1.33981000	0.81093300
C	-1.40683700	2.48132900	-0.91335000
H	-2.24142300	2.44986400	-1.61824000
H	-1.67197700	3.19607700	-0.12894400
H	-0.52680100	2.84521200	-1.43887200
C	-1.45074200	-1.20948100	-0.90857700
C	-1.37690500	-2.57116800	-1.49924200
C	-1.64768700	-2.79211900	-2.86216300
C	-1.12708600	-3.69393900	-0.69300500
C	-1.67929600	-4.08020500	-3.38803700
H	-1.82332300	-1.93754700	-3.50480400
C	-1.14857800	-4.98976000	-1.22050500
H	-0.92183700	-3.55015400	0.36468500
C	-1.42634800	-5.18724800	-2.57116000
H	-1.89723600	-4.22284500	-4.44290200
H	-0.95411800	-5.83962100	-0.57115100

H	-1.44987100	-6.19134700	-2.98582000
C	-2.40161100	-0.87480000	0.01863000
C	-3.53984000	-1.70902300	0.53606500
H	-3.57004200	-1.72712100	1.63521200
C	-4.92336200	-1.31186600	0.02749700
C	-5.15253100	-1.13711100	-1.34472900
C	-5.99759100	-1.14982300	0.90898700
C	-6.42205700	-0.80847400	-1.81839900
H	-4.32479100	-1.25939600	-2.03742500
C	-7.27037200	-0.81769300	0.43886100
H	-5.83729000	-1.28469500	1.97664000
C	-7.48667900	-0.64511600	-0.92766700
H	-6.58175800	-0.68009100	-2.88556000
H	-8.08932100	-0.69060500	1.14153200
H	-8.47463200	-0.38544200	-1.29714700
C	-4.53639700	4.53322200	2.04464300
C	-3.69685200	3.42420400	2.16956600
C	-3.78183500	2.35341000	1.27237900
C	-4.72775300	2.41234300	0.24105700
C	-5.56501700	3.51980700	0.11270700
C	-5.47374800	4.58408700	1.01324000
H	-4.45315100	5.35667000	2.74866200
H	-2.96565600	3.39036000	2.97480000
H	-4.79869400	1.58806500	-0.46063800
H	-6.29355900	3.55040800	-0.69264900
H	-6.12649200	5.44619900	0.90953300
C	-2.90140500	1.12805100	1.47668500
H	-3.50671600	0.36242600	1.96895800
H	-2.09433800	1.37153600	2.18069900
N	-2.33879100	0.52340500	0.27577000
H	1.20447200	0.26158300	1.14640100
H	-3.34110600	-2.74135800	0.23288400
H	-0.13464300	2.19753000	1.23884800
C	-1.16034000	-1.21499700	4.63719800
C	-0.56430400	-1.42834000	3.39348800
C	0.82983700	-1.46189400	3.27242700
C	1.62153800	-1.27022000	4.41325900
C	1.02442200	-1.05221300	5.65453700
C	-0.36707300	-1.02840100	5.76997500

H	-2.24305000	-1.19649600	4.72125700
H	-1.17684800	-1.56281200	2.50612200
H	2.70414800	-1.26962000	4.32097600
H	1.64577000	-0.90460800	6.53315800
H	-0.83054900	-0.86486500	6.73864300
C	1.46713500	-1.70074000	1.92475400
H	0.74962300	-2.12041400	1.21795800
H	2.32244200	-2.37639600	1.99669400
N	1.98517900	-0.43791600	1.30430100
H	2.73147600	-0.03870600	1.90419300
H	2.44900700	-0.68835600	0.41064900
S	3.99770600	-2.43005600	-1.65024800
O	3.87431600	-1.58863500	-0.36054800
C	2.72316300	-3.72549200	-1.55258900
H	1.76389100	-3.22518700	-1.70006500
H	2.88865700	-4.43633200	-2.36649200
H	2.78656600	-4.22141900	-0.58064100
C	5.43669100	-3.51641000	-1.31539000
H	5.54204100	-4.23922700	-2.12846600
H	6.32174700	-2.87884100	-1.27537900
H	5.29991500	-4.02429000	-0.35775100
S	5.69034300	0.12257700	2.43514100
O	4.22891900	0.19223000	2.88965400
C	6.53122200	1.49875000	3.29376300
H	6.52181200	1.26643800	4.35992600
H	7.56195500	1.57428500	2.93810500
H	5.98359700	2.42610500	3.11067800
C	5.76570400	0.80943800	0.74804000
H	6.81266900	0.87763200	0.43965400
H	5.22131800	0.10767600	0.10875500
H	5.29217300	1.79470400	0.73327200

Pr

C	-5.98875300	1.34168100	0.25058000
C	-5.08656100	0.28409500	0.36065800
C	-4.97166000	-0.66366800	-0.66717900
C	-5.77970400	-0.53045400	-1.80195400
C	-6.68838700	0.52365400	-1.91015800
C	-6.79336700	1.46339900	-0.88450300

H	-6.06611800	2.06832300	1.05414500
H	-4.46832900	0.19138900	1.24985500
H	-5.69774200	-1.25900400	-2.60434100
H	-7.31092500	0.61105100	-2.79592800
H	-7.49882600	2.28505600	-0.96756200
C	-3.99249100	-1.81028800	-0.54897000
H	-4.11864000	-2.52263700	-1.37144500
H	-4.15469600	-2.38138700	0.37430400
N	-2.61569300	-1.31888800	-0.55107000
H	-2.48461800	-0.31868300	-0.62467000
C	-1.52188500	-2.09365600	-0.41510400
S	-1.62750700	-3.76945500	-0.30320000
C	-0.25202200	-1.34290400	-0.34666200
C	0.89598100	-1.60625900	-1.08392000
C	1.17344500	-2.65617000	-2.11204300
H	0.31795700	-3.32703800	-2.18315400
H	1.35941500	-2.21845000	-3.10131100
H	2.04581800	-3.26538400	-1.84871400
H	3.06294700	0.95175700	1.12520100
C	-0.00404400	-0.15319900	0.43762200
C	-0.89585300	0.44565000	1.45522700
C	-1.13691900	1.83030600	1.49898600
C	-1.51655200	-0.36582100	2.42398600
C	-1.95610900	2.38631300	2.48335500
H	-0.68674600	2.47419400	0.74929200
C	-2.33993600	0.18955100	3.40149200
H	-1.33678000	-1.43657200	2.41144100
C	-2.56205900	1.56945600	3.43780700
H	-2.12511700	3.45933700	2.49712100
H	-2.80103600	-0.45559600	4.14412100
H	-3.19942900	2.00127100	4.20392400
C	1.29060900	0.25337200	0.15620800
C	2.10981300	1.35467400	0.75999200
H	1.57451900	1.70440800	1.65012900
C	2.40305400	2.55620300	-0.13642400
C	1.56732000	2.91307600	-1.20230700
C	3.52254700	3.35739100	0.13005700
C	1.83772800	4.04503600	-1.97452200
H	0.70511900	2.29360000	-1.43182500

C	3.79394900	4.48908700	-0.63794000
H	4.18552800	3.09089000	0.94991600
C	2.95039900	4.83813100	-1.69464900
H	1.17758300	4.30415100	-2.79754500
H	4.66663100	5.09615100	-0.41404100
H	3.16169400	5.71729500	-2.29617700
C	4.84693400	-2.80300900	1.38016900
C	3.86538000	-2.19629700	0.59327800
C	4.21815900	-1.23505300	-0.35979500
C	5.56765800	-0.88776300	-0.50649200
C	6.54764700	-1.49647700	0.27611900
C	6.18908900	-2.45800800	1.22325600
H	4.55800600	-3.54640900	2.11732600
H	2.82272000	-2.46773500	0.72661900
H	5.85196800	-0.13454200	-1.23791500
H	7.58938200	-1.21526900	0.15140300
H	6.95047300	-2.93058000	1.83665800
C	3.18784700	-0.58181900	-1.27235400
H	3.20063900	-1.07053500	-2.25112300
H	3.45675300	0.46359100	-1.44647800
N	1.81775400	-0.62579000	-0.77763600

H₂O

O	0.00000000	0.11793200	0.00000000
H	0.76889600	-0.46143300	0.00000000
H	-0.76889600	-0.48202200	0.00000000

Re'

C	4.95343300	3.23304600	-1.00142800
C	4.41804300	2.09633900	-1.60971100
C	3.85302300	1.07418400	-0.83934000
C	3.82835100	1.21258900	0.55654200
C	4.35496100	2.35128200	1.16469500
C	4.92109200	3.36383000	0.38688900
H	5.39035900	4.01687000	-1.61309400
H	4.43977300	2.00081800	-2.69212100
H	3.39374600	0.42597200	1.16826900
H	4.32796500	2.44572100	2.24627400
H	5.33435900	4.24897800	0.86125500

C	3.29263400	-0.16576200	-1.49955300
H	3.83933600	-1.06621600	-1.19471800
H	3.38784500	-0.10786400	-2.59031000
N	1.88747900	-0.35695700	-1.14125800
H	1.41690200	0.41923400	-0.68920700
C	1.16961500	-1.45742400	-1.40905500
S	1.78421400	-2.78234600	-2.22004900
C	-0.31071100	-1.33806200	-1.02802500
C	-1.12676200	-2.65988700	-0.90078100
O	-2.19931700	-2.70163800	-1.47272200
C	-0.67805200	-3.79123000	-0.00253000
H	0.39053300	-3.98821500	-0.08640000
H	-0.89977200	-3.52689600	1.03768800
H	-1.24850300	-4.68321900	-0.26568300
H	-0.77370400	-0.87202100	-1.90386300
C	-0.63174300	-0.40385900	0.15905500
C	-0.19873200	-0.69961200	1.56050300
C	0.90438200	-1.52108800	1.84954300
C	-0.89522800	-0.12574100	2.64021400
C	1.29848100	-1.75278800	3.16888300
H	1.46455200	-1.98881300	1.04867800
C	-0.49975500	-0.35642800	3.95409300
H	-1.75828600	0.50055300	2.43789800
C	0.60207800	-1.17092100	4.22685600
H	2.15334200	-2.39359000	3.36440000
H	-1.05902400	0.09497300	4.76837500
H	0.90855900	-1.35432200	5.25222900
C	-1.36558100	0.65907800	-0.11533400
C	-2.12370700	1.69062000	-0.40968100
H	-1.63890900	2.64207900	-0.63592800
C	-3.60102900	1.68747500	-0.45325100
C	-4.33609000	0.49151800	-0.52831900
C	-4.29242700	2.90862500	-0.43173100
C	-5.72721900	0.52394600	-0.55871700
H	-3.81059300	-0.45705300	-0.59211400
C	-5.68589400	2.93684800	-0.46263600
H	-3.73163700	3.83875400	-0.38521200
C	-6.40804900	1.74440100	-0.52203500
H	-6.28287700	-0.40694000	-0.62319900

H	-6.20643300	3.88992700	-0.44237500
H	-7.49344700	1.76472500	-0.55036100

Com1W'

C	-7.36395000	0.81588000	-0.43782200
C	-6.50016200	0.47566400	0.60470200
C	-5.42279200	-0.38914500	0.38415700
C	-5.22088600	-0.90584700	-0.90434800
C	-6.07781000	-0.56001600	-1.94828700
C	-7.15333800	0.30039700	-1.71665500
H	-8.19705600	1.48689600	-0.25070900
H	-6.66405600	0.88410700	1.59843600
H	-4.38839000	-1.57982000	-1.09050100
H	-5.90887100	-0.96610500	-2.94120100
H	-7.82272400	0.56688300	-2.52914000
C	-4.49883500	-0.77111100	1.51899900
H	-4.52671400	-1.84954900	1.71600600
H	-4.80067000	-0.28285800	2.45302600
N	-3.11508300	-0.41224400	1.20716100
H	-2.95990700	0.18936700	0.40508600
C	-2.04539400	-0.79412400	1.91522100
S	-2.12335100	-1.74842900	3.28486400
C	-0.72281500	-0.18740500	1.42420200
C	0.51862100	-0.88955300	2.02618600
O	1.25016300	-0.24150300	2.76664300
C	0.90510000	-2.29304200	1.64361600
H	0.04546100	-2.93819100	1.47406500
H	1.49520000	-2.24692400	0.71987500
H	1.53793400	-2.70489000	2.43112300
H	-0.69303500	0.81347500	1.86981400
C	-0.62824700	0.03688000	-0.10097300
C	-0.54154200	-1.08417200	-1.09046300
C	-1.20961900	-2.30723500	-0.90924600
C	0.19301600	-0.89932500	-2.27524400
C	-1.14776200	-3.30627400	-1.88182600
H	-1.78590600	-2.48785100	-0.00904200
C	0.25035100	-1.89628800	-3.24680700
H	0.72226700	0.03611700	-2.42610100
C	-0.42078900	-3.10618500	-3.05523800

H	-1.67243800	-4.24313200	-1.71831900
H	0.82565400	-1.72821500	-4.15250400
H	-0.37420800	-3.88497400	-3.81044000
C	-0.64039300	1.28707900	-0.52634700
C	-0.68807700	2.52677600	-0.95864900
H	-1.67359900	2.93863500	-1.18602800
C	0.44661000	3.44424200	-1.17156800
C	1.75136600	3.13345800	-0.75140200
C	0.20741300	4.67965200	-1.79458100
C	2.78408800	4.04564300	-0.94861300
H	1.96203800	2.18716400	-0.26035900
C	1.24700900	5.58444100	-2.00121100
H	-0.80074500	4.92859600	-2.11690600
C	2.53831400	5.27054200	-1.57569300
H	3.77769900	3.80626300	-0.58526100
H	1.04650200	6.53537400	-2.48652900
H	3.34794800	5.97943000	-1.72271400
C	5.93517100	-3.52289400	-0.51313600
C	5.97045300	-2.27655800	0.11560900
C	4.95829800	-1.33381900	-0.09754700
C	3.90021400	-1.67126800	-0.95292400
C	3.85792700	-2.91773300	-1.57833200
C	4.87698800	-3.84852200	-1.36203600
H	6.72983200	-4.24157000	-0.33201400
H	6.79307000	-2.03354900	0.78462100
H	3.10943600	-0.94538100	-1.11195800
H	3.02571500	-3.16090500	-2.23346500
H	4.84397800	-4.82005600	-1.84713400
C	5.01894700	0.03260100	0.56227900
H	5.42956500	0.75523100	-0.15711300
H	5.75203500	-0.01613900	1.38750400
N	3.69747700	0.51837000	0.95948400
H	3.32243000	-0.06022200	1.70803300
H	3.76278300	1.46853900	1.33309900
O	0.94157800	2.49445100	3.00518900
H	0.63607300	2.70170500	3.89695400
H	1.07400000	1.52173800	2.99964600
O	3.54294400	3.28602600	2.28668500
H	3.98945400	3.12318300	3.12688700

H	2.59373400	3.15138200	2.49465600
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TS1W'

C	5.96871800	-1.77670500	-1.26045600
C	5.06760400	-1.02396300	-0.50698300
C	5.25537300	0.35765800	-0.35249200
C	6.35665100	0.96309100	-0.96821200
C	7.26171300	0.20810500	-1.71601400
C	7.06961800	-1.16555600	-1.86511400
H	5.81168900	-2.84605600	-1.37213900
H	4.20796800	-1.50407200	-0.04820400
H	6.50695600	2.03477000	-0.86154400
H	8.11107100	0.69506700	-2.18683100
H	7.76991400	-1.75511600	-2.44987300
C	4.31623500	1.18237600	0.50632000
H	4.45061800	2.24958500	0.28758000
H	4.53463700	1.04520600	1.57087700
N	2.91982500	0.81828500	0.30456100
H	2.64152000	0.58536300	-0.66749000
C	2.04576300	0.55378100	1.28096000
S	2.39190300	0.70795500	2.91924000
C	0.66638900	0.11097900	0.72452100
C	0.63307600	-1.46257600	0.58324400
O	1.65121000	-1.91209900	-0.18346900
C	0.55398800	-2.29077400	1.85974900
H	1.41304000	-2.03401200	2.48194200
H	-0.34836000	-2.11753700	2.44497200
H	0.63122900	-3.34911600	1.59139800
H	0.67038300	0.44409000	-0.31449900
C	-0.52197500	0.90371400	1.33255100
C	-1.40819300	0.53109000	2.48987900
C	-0.92872700	-0.00098000	3.69763200
C	-2.78951100	0.78588000	2.38418600
C	-1.80350000	-0.28333200	4.74843200
H	0.13783800	-0.14873200	3.81883600
C	-3.65974300	0.50724900	3.43576700
H	-3.17983700	1.21286200	1.46469000
C	-3.17062800	-0.03645200	4.62483200
H	-1.40507800	-0.68692300	5.67515500

H	-4.72043800	0.71321300	3.32321100
H	-3.84622700	-0.25810900	5.44593300
C	-0.78288000	2.04848000	0.72922500
C	-1.01338500	3.22707800	0.19670400
H	-0.50520400	4.08495500	0.64214500
C	-1.92391000	3.52457900	-0.92967400
C	-2.21618200	2.57513400	-1.92417200
C	-2.50469800	4.79982200	-1.02241900
C	-3.09047300	2.89262600	-2.96205900
H	-1.72244900	1.60734500	-1.91108900
C	-3.38052400	5.11166500	-2.06090500
H	-2.27220800	5.54601600	-0.26700600
C	-3.68159000	4.15649000	-3.03302100
H	-3.29786000	2.15370800	-3.73146800
H	-3.82521500	6.10145500	-2.11206800
H	-4.35890500	4.39944600	-3.84658600
C	-4.29559500	-2.77995700	-2.79450400
C	-3.48927800	-2.02485500	-1.94348800
C	-2.99303600	-2.58232300	-0.75658900
C	-3.32139300	-3.90622000	-0.43777300
C	-4.12763500	-4.66235400	-1.28945700
C	-4.61518200	-4.10013200	-2.46987600
H	-4.68017100	-2.33622200	-3.70806000
H	-3.24124300	-0.99747100	-2.19593100
H	-2.95353800	-4.34396700	0.48728100
H	-4.37956000	-5.68562200	-1.02772200
H	-5.24640400	-4.68578600	-3.13143800
C	-2.09400800	-1.77700000	0.15299400
H	-2.14286100	-2.14030100	1.17970800
H	-2.36772900	-0.72389500	0.15255900
N	-0.66778400	-1.85784600	-0.31259700
H	-0.44080600	-2.82941800	-0.53641400
H	-0.58769800	-1.33281300	-1.23034200
O	2.00946700	-0.37575000	-2.02810100
H	2.72658100	-0.63132900	-2.62119200
H	1.86112400	-1.24303000	-1.09013100
O	-0.44133400	-0.39844600	-2.61823300
H	-0.62549900	-0.86853800	-3.44060600
H	0.58473800	-0.31470300	-2.55153800

Int1W' (Int1W'')

C	5.96178000	-1.72373500	-1.16476100
C	5.08069300	-0.96029900	-0.39914000
C	5.16650600	0.44039200	-0.40549300
C	6.14808100	1.05402100	-1.19114800
C	7.03432700	0.28934700	-1.95250800
C	6.94269800	-1.10237700	-1.94234700
H	5.88668200	-2.80753900	-1.14863600
H	4.31480100	-1.44655400	0.19866600
H	6.21973700	2.13881400	-1.20747400
H	7.79081800	0.78221900	-2.55649700
H	7.62946200	-1.69948300	-2.53534100
C	4.23753100	1.27505300	0.45336500
H	4.32870400	2.33578200	0.18710200
H	4.49156000	1.18852500	1.51493000
N	2.84821700	0.85240300	0.31688100
H	2.55960400	0.58626600	-0.62470700
C	1.99650700	0.62194000	1.32919600
S	2.38187700	0.91345600	2.93539200
C	0.63250600	0.08902800	0.83085200
C	0.55749600	-1.49041300	0.91458200
O	1.73035200	-2.01156800	0.31821600
C	0.51814200	-2.10635900	2.30998500
H	1.37283400	-1.75554000	2.88956800
H	-0.39131300	-1.85391600	2.85316200
H	0.58810500	-3.19414400	2.20762200
H	0.64144000	0.25504400	-0.24868800
C	-0.55582400	0.97706200	1.28970600
C	-1.46142400	0.78436500	2.47409200
C	-1.00062000	0.45669200	3.75908800
C	-2.84081200	1.00887300	2.30236400
C	-1.89311500	0.34644400	4.82665000
H	0.06299100	0.32614100	3.92015000
C	-3.72875400	0.90038000	3.37049900
H	-3.21346900	1.27262900	1.31689700
C	-3.25850000	0.56353100	4.64064900
H	-1.51109900	0.09929200	5.81326600
H	-4.78832300	1.07602100	3.20746000

H	-3.94782200	0.47498100	5.47538800
C	-0.79196400	2.02913500	0.52954200
C	-1.00486100	3.12709900	-0.16083700
H	-0.48760100	4.03166600	0.16620300
C	-1.90990000	3.28490200	-1.31844000
C	-2.27249100	2.20252900	-2.13911700
C	-2.41859600	4.55863000	-1.61986200
C	-3.14315000	2.39383500	-3.21008600
H	-1.83296900	1.22410700	-1.96754900
C	-3.29113900	4.74491000	-2.69087300
H	-2.13304400	5.40503400	-1.00047100
C	-3.66198200	3.66109500	-3.48801800
H	-3.40617300	1.55044700	-3.84303300
H	-3.67936600	5.73693700	-2.90351900
H	-4.33772300	3.80455200	-4.32613100
C	-4.29828400	-2.56464300	-2.41413100
C	-3.50306800	-1.95726500	-1.44121300
C	-2.83704300	-2.72892200	-0.47828100
C	-2.98992900	-4.12089800	-0.51050000
C	-3.78193700	-4.73175100	-1.48419800
C	-4.43710900	-3.95411600	-2.43984300
H	-4.81729900	-1.95246000	-3.14625900
H	-3.40617800	-0.87515000	-1.41954000
H	-2.49156500	-4.73076300	0.23978300
H	-3.89300200	-5.81218000	-1.49133800
H	-5.05922600	-4.42642200	-3.19438600
C	-1.94083400	-2.07937700	0.55557600
H	-1.98177300	-2.65699000	1.48802800
H	-2.29750600	-1.07543000	0.78308400
N	-0.55668500	-1.98462100	0.02686000
H	-0.25438200	-2.93180900	-0.20392500
H	-0.60483900	-1.24414900	-1.57291600
O	2.07762300	-0.62204200	-2.10684700
H	2.72324500	-0.93071500	-2.75282600
H	1.85824000	-1.60862300	-0.56815700
O	-0.52637500	-0.82181300	-2.48096200
H	-1.03751800	-1.38708400	-3.07322500
H	1.17081000	-0.68054300	-2.50450700

TS1W''

C	6.14633200	2.41123900	-0.20024200
C	5.21241200	1.42996700	-0.53268200
C	5.53155900	0.06982400	-0.40121700
C	6.80256900	-0.28267300	0.06610300
C	7.74051900	0.69868500	0.38968000
C	7.41410000	2.04872600	0.25876500
H	5.88443500	3.46011200	-0.30476600
H	4.22761300	1.72272400	-0.88868600
H	7.05912900	-1.33305500	0.17663900
H	8.72280200	0.40751900	0.75011200
H	8.14147300	2.81358200	0.51414100
C	4.53664800	-1.00272600	-0.78816200
H	4.88910100	-1.99227500	-0.47419100
H	4.41124700	-1.06084800	-1.87728600
N	3.22475000	-0.74069400	-0.20318600
H	3.16820400	0.03289600	0.44688800
C	2.07095000	-1.30556900	-0.61044800
S	1.99564100	-2.47324200	-1.79507500
C	0.85706800	-0.68743300	0.08850300
C	0.43862600	0.67466800	-0.60436500
O	1.26291400	1.72628100	-0.15031200
C	0.53531000	0.65445900	-2.12274400
H	1.56827100	0.46857700	-2.41419800
H	-0.08385300	-0.13609300	-2.55039400
H	0.24668500	1.62460200	-2.53233500
H	1.18688000	-0.38360600	1.09499300
C	-0.39248700	-1.52756500	0.24288300
C	-0.35224400	-2.97088600	0.58428400
C	0.67270600	-3.48518500	1.39595600
C	-1.35961800	-3.84987000	0.15043900
C	0.69018200	-4.83013700	1.76353500
H	1.46608500	-2.83102600	1.74609800
C	-1.33738200	-5.19297600	0.51334100
H	-2.15618600	-3.47176700	-0.48086300
C	-0.31386300	-5.69165100	1.32355800
H	1.49296100	-5.20354000	2.39320000
H	-2.12113600	-5.85554500	0.15724400
H	-0.29839000	-6.74064400	1.60439100

C	-1.55540300	-0.85220100	0.27070200
C	-2.84226100	-0.93774100	0.77539500
H	-2.90265100	-1.40238100	1.76186900
C	-4.08441100	-0.94105100	-0.00070000
C	-4.10751600	-0.97637900	-1.41443800
C	-5.33541200	-0.93745700	0.65684800
C	-5.30728500	-0.97768400	-2.12255600
H	-3.16568000	-1.02516700	-1.95586800
C	-6.53200200	-0.95287800	-0.05345500
H	-5.35564500	-0.92319500	1.74441500
C	-6.53206900	-0.96359000	-1.45135400
H	-5.28420100	-1.00723600	-3.20916000
H	-7.47432900	-0.95291200	0.48884500
H	-7.46627700	-0.97088100	-2.00446900
C	-3.50069100	4.88398200	0.52205400
C	-3.33351100	3.57148900	0.07381200
C	-2.08316000	3.11816500	-0.37531300
C	-0.99989200	4.00922400	-0.36604000
C	-1.16847800	5.31898800	0.08358300
C	-2.41619700	5.76118100	0.52813700
H	-4.47652400	5.21754800	0.86265600
H	-4.18443100	2.89415000	0.05802500
H	-0.01994200	3.66775200	-0.68342900
H	-0.31968400	5.99664400	0.08858400
H	-2.54115000	6.78171600	0.87756200
C	-1.96601700	1.68848700	-0.87282400
H	-1.73804700	1.65165600	-1.93815600
H	-2.92887700	1.19516300	-0.73423900
N	-0.97626500	0.84305800	-0.14602800
H	-0.96010400	1.18007500	0.81835700
H	-2.52871000	0.66841400	2.09088700
O	0.60579600	1.77661500	2.57408100
H	1.01358100	1.20726700	3.23754500
H	1.14762600	1.81307800	0.82325000
O	-2.12796400	1.44443200	2.56025000
H	-2.62641100	2.21491300	2.25186600
H	-0.36399400	1.70788900	2.72778600
Int2W''			
C	-6.14452600	-2.68558500	-0.09559600

S100

C	-5.26598000	-1.67374200	-0.48252900
C	-5.62651300	-0.32494400	-0.34222000
C	-6.88309700	-0.01450800	0.18943600
C	-7.76645400	-1.02650900	0.56778100
C	-7.39851200	-2.36493400	0.42803800
H	-5.85068600	-3.72513500	-0.20766100
H	-4.29193600	-1.93295600	-0.89053000
H	-7.17105600	1.02680900	0.30783100
H	-8.73824100	-0.76807000	0.97808100
H	-8.08302000	-3.15334200	0.72652200
C	-4.68930100	0.77880500	-0.78195000
H	-5.06152400	1.75849100	-0.45934000
H	-4.61324700	0.83155000	-1.87555900
N	-3.34515600	0.56372100	-0.25440700
H	-3.24737600	-0.16345400	0.44238000
C	-2.22892100	1.17849800	-0.69396400
S	-2.23762800	2.35111200	-1.87414400
C	-0.97102600	0.61862400	-0.02187600
C	-0.46333600	-0.68529500	-0.73434800
O	-1.07701900	-1.84345600	-0.26919800
C	-0.60174200	-0.66581500	-2.24887600
H	-1.65285800	-0.53241000	-2.50228800
H	-0.04061800	0.15768500	-2.69304200
H	-0.28606000	-1.62029500	-2.67356600
H	-1.27322400	0.28818100	0.98751100
C	0.24972400	1.49639100	0.10277400
C	0.18339500	2.89899900	0.54551700
C	-0.86593500	3.35059300	1.36689500
C	1.17038000	3.83189300	0.17117600
C	-0.92428900	4.67362000	1.80246800
H	-1.64794800	2.66095900	1.67163300
C	1.10969500	5.15215400	0.60467900
H	1.98077900	3.51276200	-0.47511600
C	0.06340400	5.58261100	1.42564100
H	-1.74629700	4.99332200	2.43707600
H	1.87980500	5.85237500	0.29325700
H	0.01705800	6.61464900	1.76056700
C	1.40836900	0.77464500	0.04903000
C	2.67946800	0.97817800	0.68393000

H	2.62025700	1.79110800	1.41102100
C	3.99140200	0.94581400	0.00794200
C	4.15586300	1.07702300	-1.39056600
C	5.17574500	0.82917700	0.77223700
C	5.41688300	1.04662100	-1.98879200
H	3.27678500	1.24127000	-2.01008200
C	6.43429000	0.82228400	0.17802700
H	5.08917700	0.74165900	1.85288600
C	6.56791300	0.91683700	-1.21161500
H	5.49840700	1.15017600	-3.06809400
H	7.31997300	0.73308300	0.80236100
H	7.54981100	0.90129400	-1.67482200
C	4.09763900	-4.14110000	0.67367600
C	3.71064400	-2.94659500	0.06197900
C	2.41543200	-2.80181500	-0.45738900
C	1.51580900	-3.87277600	-0.35556900
C	1.90463700	-5.06362400	0.25788800
C	3.19509600	-5.20129700	0.77301900
H	5.10444300	-4.24220200	1.06805800
H	4.41477000	-2.12222600	-0.01374300
H	0.50419100	-3.76155000	-0.73376500
H	1.19822100	-5.88493300	0.33360300
H	3.49579300	-6.13032600	1.24826800
C	2.02614500	-1.50218000	-1.12748100
H	1.57782700	-1.68094600	-2.10174800
H	2.90400700	-0.88101900	-1.27352500
N	1.03625500	-0.68073800	-0.30399400
H	1.06801800	-1.12424100	0.62948600
H	2.35188100	-0.34819600	1.91256500
O	-0.68592100	-1.79388500	2.43807200
H	-1.17866200	-1.26844400	3.07946100
H	-1.04979300	-1.85964800	0.72013400
O	1.93280300	-1.14953900	2.40742600
H	2.56505600	-1.87514500	2.31207400
H	0.26794100	-1.57675300	2.58665100

TS2W''

C	-7.27941900	-2.26406300	-0.10005000
C	-6.29774800	-1.64545300	-0.87676800

C	-5.66068100	-0.48315500	-0.42876600
C	-6.02261200	0.04943900	0.81725000
C	-6.99872200	-0.56889500	1.59669500
C	-7.63032300	-1.72792500	1.13873800
H	-7.76749700	-3.16382600	-0.46294700
H	-6.02527000	-2.06647600	-1.84109000
H	-5.53753000	0.95519700	1.17193100
H	-7.27153300	-0.14388700	2.55820800
H	-8.39373200	-2.20759700	1.74414200
C	-4.59723100	0.18975400	-1.26684900
H	-4.80367300	1.25690700	-1.40207400
H	-4.55864900	-0.24436100	-2.27396400
N	-3.28675200	0.07714700	-0.62714500
H	-3.17768100	-0.66073200	0.05838100
C	-2.18753200	0.76567100	-0.99565900
S	-2.17489200	1.88083900	-2.23159500
C	-0.96124000	0.36418300	-0.17105000
C	-0.27635600	-0.93884200	-0.72076900
O	-0.78834800	-2.10032700	-0.15737900
C	-0.35491600	-1.08814400	-2.23294500
H	-1.40572600	-1.14546900	-2.51654400
H	0.08802700	-0.23361600	-2.74721000
H	0.12007900	-2.01678000	-2.55413900
H	-1.33150900	0.09360700	0.83138800
C	0.15831000	1.36162900	0.00288700
C	-0.07624500	2.76692400	0.38079600
C	-1.21092600	3.13637200	1.12454800
C	0.83414500	3.77802300	0.02063600
C	-1.42322100	4.46116100	1.50229500
H	-1.93401900	2.38129900	1.41837500
C	0.61965100	5.10060700	0.39649400
H	1.70677900	3.51868600	-0.56933000
C	-0.50945900	5.45085900	1.14131500
H	-2.30641000	4.71905900	2.08015100
H	1.33374000	5.86344100	0.09930900
H	-0.67674200	6.48410900	1.43099900
C	1.37358000	0.75742200	0.06942200
C	2.56096800	1.09642500	0.83925300
H	2.33548700	1.94317400	1.49396400

C	3.91311200	1.25577200	0.23831500
C	4.13922600	1.44328400	-1.14211400
C	5.05061100	1.26704300	1.07452900
C	5.42696800	1.59811000	-1.66004000
H	3.28497600	1.49089700	-1.81400900
C	6.33336900	1.44175500	0.56224100
H	4.90984700	1.13647800	2.14501100
C	6.53469100	1.59837200	-0.81305000
H	5.55991100	1.73899500	-2.72986100
H	7.18443700	1.44792500	1.23872400
H	7.53613200	1.72583000	-1.21318000
C	4.40141400	-4.12113000	0.62663300
C	3.97698800	-2.88811900	0.12845500
C	2.71563400	-2.75352700	-0.47068700
C	1.88334300	-3.87890700	-0.55687200
C	2.30812300	-5.10974900	-0.05633500
C	3.56725300	-5.23561200	0.53391900
H	5.38308500	-4.20914900	1.08271500
H	4.62929800	-2.02155000	0.19975100
H	0.89108000	-3.78730200	-0.98523300
H	1.65329500	-5.97322200	-0.12925300
H	3.89549200	-6.19665400	0.91884700
C	2.31796300	-1.40039300	-1.02304200
H	2.01753000	-1.45642400	-2.06737300
H	3.16870600	-0.72815700	-0.96558100
N	1.19604000	-0.72978600	-0.24344000
H	1.28051700	-1.14365000	0.71432800
H	2.36202100	-0.09715200	1.87062400
O	-0.63376000	-1.65224300	2.50504500
H	0.31952300	-1.39770100	2.64353400
H	-0.79379700	-2.01422400	0.83330200
O	1.93993700	-0.99719600	2.38948800
H	2.64347400	-1.65591500	2.46246100
H	-0.80135300	-2.39192500	3.10147500

Int3W''

C	7.24604200	1.73497500	-0.72015500
C	6.22255300	0.99802600	-1.31944100
C	5.50945700	0.04062200	-0.58939700

C	5.83925400	-0.16343100	0.75827900
C	6.85704100	0.57408100	1.36080900
C	7.56434000	1.52557100	0.62166600
H	7.79321600	2.47105900	-1.30204900
H	5.97601100	1.16434500	-2.36487900
H	5.29531200	-0.90809400	1.33370300
H	7.10350700	0.40232600	2.40463800
H	8.36118000	2.09676600	1.08907100
C	4.40269800	-0.76147300	-1.23591600
H	4.53401400	-1.83645900	-1.06671100
H	4.40394400	-0.62366800	-2.32434100
N	3.09959100	-0.38140200	-0.69548500
H	3.05143300	0.48252700	-0.15964000
C	1.95571800	-1.05081800	-0.93726600
S	1.88101400	-2.44853300	-1.84720900
C	0.75522200	-0.36468500	-0.30050200
C	0.02654200	0.67114800	-1.22677700
O	0.70299100	1.88409300	-1.39212100
C	-0.25984200	0.14663300	-2.63577100
H	0.68089400	-0.02816400	-3.15792300
H	-0.81331900	-0.79280200	-2.60621200
H	-0.82436300	0.88884200	-3.20501800
H	1.14828200	0.22650400	0.53958200
C	-0.39980700	-1.18356900	0.25756100
C	-0.22489500	-2.42544800	1.02758000
C	0.93482700	-2.62114800	1.80290900
C	-1.19522500	-3.44469700	1.03590300
C	1.10339000	-3.77007000	2.57049200
H	1.70936700	-1.86045700	1.81056400
C	-1.02706800	-4.59293000	1.80899500
H	-2.07337700	-3.35320700	0.40586800
C	0.12086800	-4.76217400	2.58279600
H	2.00641400	-3.89119900	3.16239400
H	-1.79136900	-5.36490000	1.79157300
H	0.25456600	-5.66000100	3.17896600
C	-1.51246500	-0.40732900	0.18996500
C	-2.84304000	-0.64558100	0.84948800
H	-2.69274900	-1.40020500	1.62973900
C	-3.99432600	-1.09729000	-0.04414300

C	-3.78373300	-1.81082700	-1.23113900
C	-5.31477000	-0.83594300	0.35105200
C	-4.86332900	-2.24979400	-2.00134700
H	-2.76876700	-2.02211400	-1.55416000
C	-6.39404100	-1.27498800	-0.41531100
H	-5.49646600	-0.28968300	1.27394400
C	-6.17142500	-1.98407700	-1.59743700
H	-4.67753600	-2.80028400	-2.91912500
H	-7.40846900	-1.06222900	-0.08992100
H	-7.01005300	-2.32460300	-2.19742800
C	-4.37225800	4.02398300	1.19356100
C	-3.99814000	2.92459300	0.41531000
C	-2.72702600	2.85809400	-0.16420400
C	-1.83979500	3.92874200	0.03109200
C	-2.21067300	5.02670500	0.80784700
C	-3.47869800	5.07459500	1.39648100
H	-5.36285200	4.05845800	1.63783000
H	-4.70255800	2.11332500	0.25050200
H	-0.86133000	3.88913600	-0.44043100
H	-1.51853800	5.85381700	0.94168500
H	-3.76862600	5.93054000	1.99871500
C	-2.31128700	1.67589800	-1.02476500
H	-1.92100100	2.07101400	-1.96521400
H	-3.18507300	1.06642400	-1.27083100
N	-1.24123600	0.84805800	-0.42596600
H	-0.58537300	1.73574000	1.24975300
H	-3.14253100	0.27308100	1.36876100
O	2.27568400	2.27229500	0.88421900
H	1.48658300	2.31862500	1.48253300
H	1.22757000	2.09821500	-0.59182300
O	-0.14854600	2.14273300	2.03207200
H	-0.64577000	2.96128100	2.16453900
H	2.77545200	3.08863200	1.00419200

TS3W''

C	-6.01672900	-1.57279500	-2.65551300
C	-5.10537800	-0.57438600	-2.30979700
C	-5.18256800	0.05460700	-1.06020800
C	-6.18651000	-0.33545700	-0.16419200

C	-7.09783100	-1.33467400	-0.50934300
C	-7.01475000	-1.95537700	-1.75692800
H	-5.95059500	-2.04936600	-3.62956000
H	-4.32638900	-0.27606700	-3.00542500
H	-6.24988300	0.14657400	0.80841200
H	-7.87502500	-1.62357500	0.19259400
H	-7.72618900	-2.72977800	-2.02899200
C	-4.17673800	1.12232500	-0.67097700
H	-4.63120600	1.82656700	0.03352400
H	-3.82773600	1.67299900	-1.54574500
N	-3.00532000	0.54816500	-0.00413100
H	-3.20473800	0.16813600	0.95113000
C	-1.79953100	0.43052800	-0.54670100
S	-1.36602200	0.88880100	-2.11232600
C	-0.75520900	-0.16848800	0.41980900
C	0.00319700	-1.31394500	-0.19800700
O	0.01516400	-2.55118200	1.76518400
C	-0.63670300	-2.43734100	-0.94026900
H	-1.62171600	-2.63389500	-0.51721300
H	-0.76642200	-2.14318000	-1.98828400
H	-0.04578100	-3.35233400	-0.89004800
H	-1.24041200	-0.52207200	1.34015500
C	0.34590200	0.81512000	0.76135500
C	0.09272700	2.06349600	1.49901100
C	-0.75495600	2.04462500	2.62239700
C	0.66823000	3.28424300	1.10551700
C	-1.00437000	3.21474700	3.33629500
H	-1.19304400	1.10381900	2.94390500
C	0.41619600	4.45077300	1.82634700
H	1.28864100	3.32424600	0.21604300
C	-0.41966900	4.42046300	2.94334400
H	-1.65734100	3.18308400	4.20360700
H	0.86379800	5.38678200	1.50508000
H	-0.61906700	5.33131800	3.50031100
C	1.51637300	0.31755400	0.31469900
C	2.90250100	0.87319900	0.41362100
H	2.85953000	1.68925200	1.14372200
C	3.50635600	1.39861600	-0.88670000
C	2.71107100	1.85047100	-1.94876200

C	4.90131700	1.46462900	-1.01275800
C	3.30260400	2.36506000	-3.10556700
H	1.62768700	1.78588100	-1.88299800
C	5.49008400	1.98311700	-2.16544200
H	5.52867300	1.10751100	-0.19971000
C	4.69087600	2.43678300	-3.21721200
H	2.67108600	2.70761600	-3.92016500
H	6.57265300	2.02875500	-2.24399100
H	5.14792800	2.83744200	-4.11725900
C	5.70343300	-3.01532500	0.17088100
C	4.69868900	-2.41031700	-0.58423500
C	3.38658600	-2.34225800	-0.09742400
C	3.08710300	-2.87575500	1.16326500
C	4.10174500	-3.46915000	1.91785900
C	5.40614400	-3.54615500	1.42689600
H	6.71644500	-3.06280800	-0.21809400
H	4.93679600	-1.98425900	-1.55575800
H	2.07004500	-2.81479400	1.55375800
H	3.86668700	-3.87533400	2.89769800
H	6.18748700	-4.01178500	2.02066000
C	2.31919700	-1.73577600	-0.99521400
H	1.81347600	-2.51801700	-1.56512700
H	2.78330500	-1.06580200	-1.72375100
N	1.27170700	-0.96369100	-0.31086000
H	-0.72486600	-2.03602200	2.51874100
H	3.57294300	0.11846700	0.83792900
O	-3.78985500	-0.46324600	2.42617100
H	-2.94219900	-0.86232100	2.83700400
H	-0.32762000	-3.44575500	1.63815300
O	-1.55894800	-1.41255100	3.19280100
H	-1.16128900	-1.10323500	4.01458900
H	-4.35125600	-1.22330300	2.22775600

Int4W''

C	-6.12664300	1.73641600	0.64560300
C	-5.21974600	0.73894100	0.99948900
C	-5.01866500	-0.36923000	0.16306400
C	-5.74453100	-0.45489300	-1.03180500
C	-6.65321100	0.54641200	-1.38844400

C	-6.84491000	1.64444100	-0.55008100
H	-6.27600500	2.58682500	1.30472400
H	-4.66160900	0.80855900	1.92901600
H	-5.60240700	-1.31454900	-1.68266900
H	-7.21144100	0.46366600	-2.31669300
H	-7.55188900	2.42239300	-0.82326600
C	-4.01516700	-1.44103300	0.54467400
H	-4.12768600	-2.31204500	-0.11114900
H	-4.15953200	-1.76300700	1.57857300
N	-2.64074800	-0.96086500	0.43493900
H	-2.36390000	-0.68337300	-0.51177500
C	-1.77614000	-0.80545000	1.45277200
S	-2.15780800	-1.09979100	3.07006200
C	-0.41535200	-0.39570300	1.02477200
C	0.37721400	0.61268500	1.57675500
O	-1.13340100	4.26106500	0.91719200
C	0.07995400	1.56530500	2.69352800
H	-0.87946900	1.29714900	3.13511300
H	0.82857100	1.48909400	3.49082900
H	0.02722100	2.60858000	2.36376500
H	-0.81173600	1.45310100	-0.28109700
C	0.35125200	-1.02799900	-0.02572400
C	-0.03710300	-2.22106900	-0.81557700
C	-0.04305000	-2.19467500	-2.21942200
C	-0.40103600	-3.41486100	-0.16849500
C	-0.38094100	-3.33131900	-2.95501900
H	0.19039600	-1.26811300	-2.73445700
C	-0.74685200	-4.54704900	-0.90392600
H	-0.40858400	-3.44881800	0.91694700
C	-0.73209700	-4.51168000	-2.30024200
H	-0.38203600	-3.28811100	-4.04036000
H	-1.02217300	-5.46085100	-0.38503300
H	-0.99835100	-5.39585900	-2.87218000
C	1.57816100	-0.38875100	-0.07457800
C	2.78895700	-0.74927300	-0.88638400
H	2.46491000	-1.50117000	-1.61412900
C	3.97039300	-1.31672600	-0.10272600
C	3.78512700	-2.07991500	1.05730800
C	5.27676900	-1.11987300	-0.57151900

C	4.87782800	-2.62741600	1.73112800
H	2.77940400	-2.24536000	1.43225300
C	6.37086600	-1.66825900	0.09923800
H	5.43652400	-0.53878300	-1.47708800
C	6.17434000	-2.42335100	1.25613800
H	4.71404000	-3.21573300	2.62950200
H	7.37509600	-1.50337100	-0.28097400
H	7.02348500	-2.84846900	1.78301200
C	4.32474100	3.53098000	-1.69210400
C	4.09694100	2.57745300	-0.69685100
C	2.91013800	2.58342800	0.04553600
C	1.95896300	3.58378100	-0.20931000
C	2.18618800	4.53243400	-1.20849000
C	3.36542100	4.50735300	-1.95673400
H	5.25179900	3.50895200	-2.25761400
H	4.85000500	1.82138300	-0.49131700
H	1.05039500	3.65881800	0.38306700
H	1.44368000	5.30503500	-1.38863800
H	3.53890200	5.24956400	-2.73027100
C	2.68985200	1.54338300	1.13453100
H	2.48475400	2.03880100	2.08494100
H	3.59922300	0.95203700	1.26768200
N	1.57540300	0.61814300	0.88649800
H	-1.28989800	3.61404400	0.20516300
H	3.13614500	0.10723900	-1.47589100
O	-2.58577700	0.21031400	-2.25211300
H	-2.08486400	1.01338900	-2.01440900
H	-1.33072900	5.11961700	0.52384400
O	-0.96798100	2.12946700	-0.97001300
H	-0.08334200	2.31066300	-1.32171000
H	-3.51526000	0.46069800	-2.15192200

TS2W'

C	6.39237600	2.23107700	-1.03529800
C	5.60064800	1.20094500	-1.54640100
C	4.91234900	0.33436500	-0.69012100
C	5.02845900	0.52377400	0.69524100
C	5.81208900	1.55684800	1.20780700
C	6.49832800	2.41289600	0.34350200

H	6.92107500	2.89327400	-1.71489600
H	5.51672700	1.06652600	-2.62182300
H	4.49857000	-0.13973400	1.37361400
H	5.89003000	1.69124400	2.28278500
H	7.11074300	3.21585600	0.74312800
C	4.07466600	-0.79700300	-1.24889700
H	4.49936500	-1.76865400	-0.97131500
H	4.08043700	-0.76717200	-2.34587700
N	2.70897900	-0.71947100	-0.73915700
H	2.45739500	0.13190800	-0.25554300
C	1.72951600	-1.64919400	-0.90863900
S	2.18965100	-3.09384700	-1.77016100
C	0.40638000	-1.33224800	-0.43373800
C	-0.65859600	-2.46506700	-0.25173300
O	-0.65071200	-3.36141000	-1.40392700
C	-0.42583200	-3.38404000	0.96012100
H	0.56650200	-3.83922800	0.89965500
H	-0.49369400	-2.83960800	1.90251600
H	-1.17394400	-4.18369000	0.95589900
H	-0.19473800	-0.61377200	-1.75904100
C	0.34661500	-0.15249400	0.53371400
C	0.62039800	-0.29000600	2.00823000
C	1.54398200	-1.23266600	2.48952800
C	-0.00131900	0.56478700	2.93389200
C	1.83866800	-1.31190500	3.85077600
H	2.03630400	-1.90293200	1.79367900
C	0.29035100	0.48152300	4.29417800
H	-0.71892100	1.29810400	2.57789100
C	1.21301700	-0.45717000	4.75963300
H	2.55901600	-2.04613800	4.20031800
H	-0.20868200	1.14813300	4.99175300
H	1.43869100	-0.52480400	5.81974900
C	0.18312200	1.07254600	0.06030400
C	0.12746700	2.30665200	-0.39590100
H	1.07335200	2.78494800	-0.66302800
C	-1.07207500	3.14741300	-0.57212300
C	-2.37320200	2.63206800	-0.44935900
C	-0.91566500	4.50923900	-0.87676300
C	-3.48106800	3.45794600	-0.61287900

H	-2.51321900	1.57678600	-0.24201400
C	-2.02618800	5.33624900	-1.04024800
H	0.08561700	4.92047500	-0.97949500
C	-3.31353500	4.81445800	-0.90702500
H	-4.47706600	3.03543600	-0.51768500
H	-1.88482200	6.38809100	-1.27211500
H	-4.17948400	5.45709100	-1.03609600
C	-5.74463300	0.00237300	-0.94737000
C	-4.44256000	-0.43928800	-0.70275800
C	-4.08073000	-0.92047600	0.56299800
C	-5.05138800	-0.95379200	1.57226000
C	-6.35065400	-0.50746100	1.33067700
C	-6.70245900	-0.02762700	0.06772800
H	-6.01087000	0.36662600	-1.93585200
H	-3.69471800	-0.42145900	-1.48877700
H	-4.78677200	-1.33573500	2.55557400
H	-7.09004200	-0.54263600	2.12587700
H	-7.71565100	0.31335200	-0.12480500
C	-2.66029200	-1.36860000	0.86121100
H	-2.68357900	-2.06305300	1.71680200
H	-2.07371800	-0.50490500	1.18758400
N	-2.03128200	-1.93294300	-0.33498000
H	-2.60212400	-2.71954400	-0.64062300
H	-0.82980100	-1.24738500	-3.28880300
O	-0.98366200	-2.39076600	-3.62332800
H	-0.93253000	-2.84470200	-2.64086400
H	0.32258200	-3.62097600	-1.52902400
O	-0.65281800	-0.21826800	-2.67206000
H	-0.00973800	0.38180400	-3.07450200
H	-0.17246300	-2.68825400	-4.06388200

Int2W'

C	5.06893542	1.91316330	-4.51040208
C	4.57191928	0.68555513	-4.06860510
C	4.21976689	0.49611712	-2.72769728
C	4.37058082	1.56725358	-1.83410508
C	4.85911459	2.79658497	-2.27469657
C	5.21176394	2.97266806	-3.61462136
H	5.33893320	2.04174993	-5.55464708

H	4.45717875	-0.13563077	-4.77155033
H	4.09973719	1.43669482	-0.78968501
H	4.96811544	3.61643122	-1.57064704
H	5.59475086	3.92955626	-3.95694258
C	3.70452641	-0.84496263	-2.24814612
H	4.40704306	-1.30071422	-1.54083606
H	3.62711014	-1.54457734	-3.09006909
N	2.41151221	-0.68777666	-1.58909079
H	1.96048008	0.21101990	-1.69281143
C	1.72951600	-1.64919400	-0.90863900
S	2.52384114	-3.19552086	-0.77120726
C	0.40638000	-1.33224800	-0.43373800
C	-0.55965719	-2.35982542	-0.26864170
O	-1.37249822	-4.22720526	-1.93269759
C	-0.32689319	-3.27879842	0.94321230
H	0.66544081	-3.73398642	0.88274630
H	-0.39475519	-2.73436642	1.88560730
H	-1.07500519	-4.07844842	0.93899030
H	-0.48044759	-0.29761366	-2.37280185
C	0.34661500	-0.15249400	0.53371400
C	0.62039800	-0.29000600	2.00823000
C	1.54398200	-1.23266600	2.48952800
C	-0.00131900	0.56478700	2.93389200
C	1.83866800	-1.31190500	3.85077600
H	2.03630400	-1.90293200	1.79367900
C	0.29035100	0.48152300	4.29417800
H	-0.71892100	1.29810400	2.57789100
C	1.21301700	-0.45717000	4.75963300
H	2.55901600	-2.04613800	4.20031800
H	-0.20868200	1.14813300	4.99175300
H	1.43869100	-0.52480400	5.81974900
C	0.18312200	1.07254600	0.06030400
C	0.12746700	2.30665200	-0.39590100
H	1.07335200	2.78494800	-0.66302800
C	-1.07207500	3.14741300	-0.57212300
C	-2.37320200	2.63206800	-0.44935900
C	-0.91566500	4.50923900	-0.87676300
C	-3.48106800	3.45794600	-0.61287900
H	-2.51321900	1.57678600	-0.24201400

C	-2.02618800	5.33624900	-1.04024800
H	0.08561700	4.92047500	-0.97949500
C	-3.31353500	4.81445800	-0.90702500
H	-4.47706600	3.03543600	-0.51768500
H	-1.88482200	6.38809100	-1.27211500
H	-4.17948400	5.45709100	-1.03609600
C	-5.64569419	0.10761458	-0.96427870
C	-4.34362119	-0.33404642	-0.71966670
C	-3.98179119	-0.81523442	0.54608930
C	-4.95244919	-0.84855042	1.55535130
C	-6.25171519	-0.40221942	1.31376830
C	-6.60352019	0.07761458	0.05081930
H	-5.91193119	0.47186758	-1.95276070
H	-3.59577919	-0.31621742	-1.50568570
H	-4.68783319	-1.23049342	2.53866530
H	-6.99110319	-0.43739442	2.10896830
H	-7.61671219	0.41859358	-0.14171370
C	-2.56135319	-1.26335842	0.84430230
H	-2.58464019	-1.95781142	1.69989330
H	-1.97477919	-0.39966342	1.17067530
N	-1.93234319	-1.82770142	-0.35188870
H	-2.50318519	-2.61430242	-0.65753170
H	-0.86325874	-1.49601815	-3.36154691
O	-0.98366200	-2.39076600	-3.62332800
H	-1.63906612	-3.93913756	-2.78683959
H	-0.39920422	-4.48677126	-2.05779459
O	-0.88191147	0.04900827	-3.17297683
H	-0.23883147	0.64908027	-3.57541883
H	-0.17246300	-2.68825400	-4.06388200

TS3W'

C	-6.61204700	0.81915600	-1.04270500
C	-5.62615600	0.13534200	-0.33191700
C	-5.30032800	-1.18785100	-0.66499700
C	-5.98169500	-1.81101300	-1.71642000
C	-6.97381100	-1.12928900	-2.42294100
C	-7.28904200	0.18793200	-2.08850500
H	-6.85509800	1.84331300	-0.77555400
H	-5.10905800	0.62901600	0.48726400

H	-5.73572500	-2.83620300	-1.98075500
H	-7.49738200	-1.62632600	-3.23430800
H	-8.05977700	0.71999000	-2.63836900
C	-4.22343100	-1.92349700	0.09924400
H	-4.20105200	-2.98503100	-0.16803800
H	-4.39616700	-1.87909800	1.18185600
N	-2.90642600	-1.33936700	-0.17172800
H	-2.88152000	-0.52530900	-0.77341200
C	-1.76813300	-1.70921800	0.42478400
S	-1.65191600	-2.99428700	1.50438600
C	-0.57480000	-0.87719600	0.11989300
C	0.50277900	-1.35253900	-0.56660500
O	1.71458700	-1.53441400	2.22674800
C	0.63645500	-2.60396100	-1.36989100
H	-0.30497700	-3.15548000	-1.34944900
H	0.87782900	-2.39110300	-2.41925000
H	1.42448200	-3.26157800	-0.98670400
H	2.97704100	1.27794300	2.28432300
C	-0.44178500	0.52055900	0.51615800
C	-1.54397000	1.34210400	1.07865100
C	-1.85617000	2.60112200	0.53223900
C	-2.29700300	0.89061200	2.17732600
C	-2.88982700	3.37210700	1.05781300
H	-1.27651000	2.97040200	-0.30750200
C	-3.33413500	1.66482900	2.70097300
H	-2.05775400	-0.06537500	2.63270500
C	-3.63813300	2.90779900	2.14356300
H	-3.11394000	4.33919700	0.61637500
H	-3.89540200	1.29841700	3.55615300
H	-4.44101500	3.51245600	2.55513400
C	0.77894400	1.06974500	0.21938200
C	1.53246600	2.17121800	0.53591800
H	1.37384900	2.57955200	1.53503300
C	2.30451000	3.00737700	-0.38006000
C	2.14531400	2.95728000	-1.78468700
C	3.22351900	3.95493100	0.12443000
C	2.88692900	3.77867200	-2.62988300
H	1.40490800	2.28210200	-2.20634300
C	3.95192000	4.78527800	-0.72177200

H	3.36022700	4.03165700	1.20078700
C	3.79935200	4.69922100	-2.10848300
H	2.73633900	3.71379600	-3.70472600
H	4.64897800	5.50243900	-0.29600700
H	4.37114100	5.34444000	-2.76841200
C	5.37581300	-2.60825100	0.03797300
C	4.41919700	-1.60295000	-0.08634700
C	3.71783500	-1.42747900	-1.28665600
C	4.01451100	-2.26126800	-2.37040300
C	4.98648200	-3.25670700	-2.25524500
C	5.66422800	-3.43650900	-1.04879200
H	5.88526800	-2.73447100	0.98763500
H	4.22325000	-0.95799500	0.76462800
H	3.48431800	-2.13084600	-3.31061300
H	5.20823200	-3.89424000	-3.10617300
H	6.41325000	-4.21749700	-0.95624100
C	2.68830500	-0.32263700	-1.40808600
H	2.24733600	-0.29169500	-2.40637300
H	3.15636500	0.64657600	-1.22647500
N	1.57966700	-0.41580600	-0.41397400
H	1.96271900	-0.63314500	0.52284300
H	4.06948900	-0.75481900	3.22317700
O	4.25493300	-1.72265000	3.23113900
H	2.50458500	-1.98573200	2.59106400
H	0.95375700	-2.13791500	2.23325000
O	3.02035200	0.71176500	3.07268600
H	2.23844400	0.13625300	2.96873600
H	4.43399000	-1.93600200	4.15519500

Int3W'

C	-6.61204700	0.81915600	-1.04270500
C	-5.62615600	0.13534200	-0.33191700
C	-5.30032800	-1.18785100	-0.66499700
C	-5.98169500	-1.81101300	-1.71642000
C	-6.97381100	-1.12928900	-2.42294100
C	-7.28904200	0.18793200	-2.08850500
H	-6.85509800	1.84331300	-0.77555400
H	-5.10905800	0.62901600	0.48726400
H	-5.73572500	-2.83620300	-1.98075500

H	-7.49738200	-1.62632600	-3.23430800
H	-8.05977700	0.71999000	-2.63836900
C	-4.22343100	-1.92349700	0.09924400
H	-4.20105200	-2.98503100	-0.16803800
H	-4.39616700	-1.87909800	1.18185600
N	-2.90642600	-1.33936700	-0.17172800
H	-2.88152000	-0.52530900	-0.77341200
C	-1.76813300	-1.70921800	0.42478400
S	-1.65191600	-2.99428700	1.50438600
C	-0.57480000	-0.87719600	0.11989300
C	0.50277900	-1.35253900	-0.56660500
O	1.71458700	-1.53441400	2.22674800
C	0.63645500	-2.60396100	-1.36989100
H	-0.30497700	-3.15548000	-1.34944900
H	0.87782900	-2.39110300	-2.41925000
H	1.42448200	-3.26157800	-0.98670400
H	2.97704100	1.27794300	2.28432300
C	-0.44178500	0.52055900	0.51615800
C	-1.54397000	1.34210400	1.07865100
C	-1.85617000	2.60112200	0.53223900
C	-2.29700300	0.89061200	2.17732600
C	-2.88982700	3.37210700	1.05781300
H	-1.27651000	2.97040200	-0.30750200
C	-3.33413500	1.66482900	2.70097300
H	-2.05775400	-0.06537500	2.63270500
C	-3.63813300	2.90779900	2.14356300
H	-3.11394000	4.33919700	0.61637500
H	-3.89540200	1.29841700	3.55615300
H	-4.44101500	3.51245600	2.55513400
C	0.83059383	0.97392103	0.17852801
C	1.58411583	2.07539403	0.49506401
H	1.42549883	2.48372803	1.49417901
C	2.35615983	2.91155303	-0.42091399
C	2.19696383	2.86145603	-1.82554099
C	3.27516883	3.85910703	0.08357601
C	2.93857883	3.68284803	-2.67073699
H	1.45655783	2.18627803	-2.24719699
C	4.00356983	4.68945403	-0.76262599
H	3.41187683	3.93583303	1.15993301

C	3.85100183	4.60339703	-2.14933699
H	2.78798883	3.61797203	-3.74557999
H	4.70062783	5.40661503	-0.33686099
H	4.42279083	5.24861603	-2.80926599
C	5.32416317	-2.51242703	0.07882699
C	4.36754717	-1.50712603	-0.04549301
C	3.66618517	-1.33165503	-1.24580201
C	3.96286117	-2.16544403	-2.32954901
C	4.93483217	-3.16088303	-2.21439101
C	5.61257817	-3.34068503	-1.00793801
H	5.83361817	-2.63864703	1.02848899
H	4.17160017	-0.86217103	0.80548199
H	3.43266817	-2.03502203	-3.26975901
H	5.15658217	-3.79841603	-3.06531901
H	6.36160017	-4.12167303	-0.91538701
C	2.63665517	-0.22681303	-1.36723201
H	2.19568617	-0.19587103	-2.36551901
H	3.10471517	0.74239997	-1.18562101
N	1.52801717	-0.31998203	-0.37312001
H	1.91106917	-0.53732103	0.56369699
H	4.06948900	-0.75481900	3.22317700
O	4.25493300	-1.72265000	3.23113900
H	2.50458500	-1.98573200	2.59106400
H	0.95375700	-2.13791500	2.23325000
O	3.02035200	0.71176500	3.07268600
H	2.23844400	0.13625300	2.96873600
H	4.43399000	-1.93600200	4.15519500

TS4W'

C	6.25382300	0.82819800	1.12200000
C	5.38351700	0.03598200	0.37421100
C	5.07769100	-1.26884500	0.78875900
C	5.66186900	-1.76278400	1.96040700
C	6.53907500	-0.97264700	2.70521100
C	6.83500200	0.32530500	2.28821600
H	6.48132800	1.83702900	0.79052900
H	4.94126500	0.43053700	-0.53705400
H	5.43021800	-2.77252800	2.28931400
H	6.98777600	-1.37040300	3.61073700

H	7.51594700	0.94192700	2.86749700
C	4.12945800	-2.12397200	-0.02057700
H	4.09607200	-3.14990200	0.36203300
H	4.44671400	-2.19719400	-1.06816700
N	2.77778900	-1.56076700	0.00369500
H	2.64533800	-0.71846000	0.54946900
C	1.74560900	-2.01852500	-0.72265300
S	1.84526600	-3.36201700	-1.71727200
C	0.51044900	-1.19595800	-0.58769300
C	-0.68340800	-1.64906200	-0.13861700
O	-2.72451000	-1.12916400	-2.49420300
C	-1.12083700	-3.01683800	0.25879800
H	-0.33035900	-3.72292200	0.00217500
H	-1.33477200	-3.09808200	1.32932100
H	-2.03173800	-3.32221000	-0.26687800
H	-2.62993300	2.00809600	-1.51924800
C	0.44648500	0.25234100	-0.83125900
C	1.56122300	1.08500200	-1.33667100
C	1.88294100	2.31498100	-0.73423300
C	2.32668000	0.66139000	-2.43846300
C	2.93181800	3.09434100	-1.22044200
H	1.30796900	2.65815100	0.11987300
C	3.37768400	1.44153200	-2.92016000
H	2.08662100	-0.27899200	-2.92538500
C	3.68503500	2.66182000	-2.31402800
H	3.16218600	4.04098500	-0.74012000
H	3.95018300	1.09859300	-3.77730500
H	4.50018700	3.27130600	-2.69312600
C	-0.81381000	0.70391500	-0.54703100
C	-1.45574000	1.99756300	-0.70819600
H	-0.80121700	2.60712000	-1.34356500
C	-1.79213500	2.79154600	0.53559500
C	-1.14366200	2.59504900	1.76967600
C	-2.76608100	3.80659500	0.46983400
C	-1.45191800	3.37211300	2.88856900
H	-0.37691000	1.82739000	1.84952800
C	-3.06340600	4.59245200	1.58189900
H	-3.30264600	3.94604600	-0.46378600
C	-2.41143500	4.38009100	2.79963900

H	-0.93260700	3.19469900	3.82721500
H	-3.81965300	5.36913300	1.50117600
H	-2.65095300	4.98957600	3.66632000
C	-5.71768600	-2.46646900	0.45851000
C	-4.71622800	-1.52258300	0.22662700
C	-3.66804000	-1.36839600	1.14661700
C	-3.67143400	-2.14527700	2.31273400
C	-4.67832900	-3.08159400	2.54708800
C	-5.70097200	-3.25057500	1.61336200
H	-6.52360700	-2.57454500	-0.26145500
H	-4.77555400	-0.90139600	-0.66267900
H	-2.88162500	-2.01069100	3.04787600
H	-4.66434900	-3.67369100	3.45731800
H	-6.48710300	-3.97857200	1.79091800
C	-2.60540000	-0.30890800	0.95835600
H	-2.00403800	-0.19265300	1.86088100
H	-3.07254200	0.65259400	0.74587300
N	-1.62826900	-0.51683100	-0.18995000
H	-2.18889100	-0.72112900	-1.11527800
H	-4.45676700	1.08491300	-2.48749000
O	-4.92932800	0.16938100	-2.67906300
H	-3.60624800	-0.66554500	-2.68578800
H	-2.89315200	-2.07692900	-2.56487000
O	-3.60467100	2.24088300	-2.19565700
H	-3.22051800	2.56154100	-3.02357400
H	-5.39648800	0.26615100	-3.51727000

Int4W'

C	-6.28622700	0.79962700	0.28075700
C	-5.24238600	-0.11594800	0.15382600
C	-5.05328100	-0.81662500	-1.04666300
C	-5.93143100	-0.58423100	-2.11109200
C	-6.98150700	0.32651200	-1.98215900
C	-7.15968400	1.02207700	-0.78617000
H	-6.41898700	1.33636500	1.21554700
H	-4.57087600	-0.28853800	0.99070000
H	-5.79224000	-1.12108300	-3.04589600
H	-7.65632000	0.49401000	-2.81655500
H	-7.97484000	1.73262600	-0.68482200

C	-3.91906500	-1.80749200	-1.18602400
H	-3.96965000	-2.32556000	-2.15013700
H	-3.96740300	-2.58801600	-0.41664500
N	-2.62552800	-1.13448700	-1.06569700
H	-2.63794600	-0.12499000	-0.99740700
C	-1.43388100	-1.75096000	-0.99901100
S	-1.29263600	-3.42958400	-1.14120900
C	-0.28781200	-0.85746000	-0.76480200
C	0.89460300	-0.83599500	-1.49753300
O	0.64703600	-3.24914600	1.62701400
C	1.32248300	-1.63434400	-2.68601800
H	0.55367900	-2.36424000	-2.93661000
H	1.49526800	-0.99291300	-3.55991400
H	2.25202600	-2.17912800	-2.49024500
H	2.63312400	1.50029900	1.26861300
C	-0.21516500	0.20468800	0.21365100
C	-1.18220100	0.48118700	1.30009500
C	-1.65942900	1.78120300	1.54225400
C	-1.63411100	-0.55907900	2.13640500
C	-2.54839300	2.03792100	2.58788900
H	-1.33403600	2.59543900	0.90142500
C	-2.52804900	-0.30080100	3.17527600
H	-1.26091500	-1.56769300	1.98339500
C	-2.98921700	0.99847300	3.40716800
H	-2.90009800	3.05188700	2.75619700
H	-2.85820400	-1.11699900	3.81204700
H	-3.68148900	1.19709900	4.22018700
C	1.01648300	0.81761000	0.05084500
C	1.67170000	1.87111700	0.89329800
H	1.04725300	1.99607400	1.78476300
C	1.87279000	3.23659900	0.24285900
C	1.01725800	3.71530900	-0.75806900
C	2.91622700	4.06548600	0.67857000
C	1.19274700	4.98976800	-1.30037300
H	0.21509100	3.07887600	-1.12115000
C	3.09413800	5.33933800	0.13898200
H	3.59437800	3.70750900	1.44967600
C	2.23076700	5.80763100	-0.85316000
H	0.51852600	5.34142200	-2.07640400

H	3.91012100	5.96428700	0.49085800
H	2.36945300	6.79797600	-1.27674800
C	5.01106200	-2.16053300	0.40448300
C	3.99433600	-1.26505900	0.06495700
C	4.08872500	-0.49275400	-1.09740200
C	5.22045300	-0.62369200	-1.91188900
C	6.24319600	-1.50699400	-1.56689800
C	6.13837900	-2.28088500	-0.40920400
H	4.90106700	-2.76515000	1.29998900
H	3.12504500	-1.17365400	0.70689800
H	5.30080400	-0.03439300	-2.82286700
H	7.11441700	-1.60012000	-2.20920300
H	6.92884200	-2.97854300	-0.14769500
C	3.01116300	0.51114100	-1.48225600
H	2.97242400	0.60740800	-2.57254900
H	3.26144300	1.50388800	-1.10029400
N	1.67064100	0.18614300	-0.99725700
H	0.91937600	-2.31319900	1.65059700
H	2.44891800	-1.80006200	3.04925200
O	3.00530200	-3.55065600	2.90865000
H	2.22039700	-3.72281400	2.33670800
H	0.30578300	-3.41091800	0.72693500
O	1.95438800	-1.00004200	2.76357600
H	1.25409200	-0.87887700	3.41689900
H	2.88604000	-4.12481300	3.67498800

Com1W

C	-4.29601000	0.88147500	3.09441100
C	-4.03951600	0.86103800	1.72066800
C	-2.93138100	1.53314300	1.19245100
C	-2.07747600	2.22316600	2.06592000
C	-2.33204400	2.24268900	3.43597500
C	-3.44318000	1.57199000	3.95486500
H	-5.16236600	0.35812500	3.48923200
H	-4.70497700	0.31942500	1.05332900
H	-1.21099800	2.74403300	1.66681100
H	-1.66577600	2.78545800	4.10049900
H	-3.64175400	1.59012600	5.02260000
C	-2.65371600	1.52349900	-0.29762600

H	-2.56998800	2.53877700	-0.69537900
H	-3.47101800	1.02438800	-0.83119700
N	-1.39404000	0.84575900	-0.59496700
H	-1.27996700	-0.09031300	-0.16889100
C	-0.44557800	1.30860700	-1.41817500
S	-0.55257200	2.70413500	-2.34146600
C	0.82259300	0.44193600	-1.39520200
C	1.55561100	0.33727900	-2.75139200
O	2.75134900	0.53654500	-2.84415800
C	0.74302300	-0.16552800	-3.92874300
H	0.27432500	-1.12601500	-3.68155100
H	-0.05444500	0.54145400	-4.16931400
H	1.40251000	-0.29239500	-4.78811300
H	0.50184900	-0.58996600	-1.19067200
C	1.75243500	0.82424100	-0.22528400
C	2.16906600	2.23014600	0.07234800
C	2.67671300	3.09359900	-0.91084100
C	2.07888900	2.69462500	1.39509300
C	3.08346600	4.38281200	-0.57114500
H	2.76848000	2.74813100	-1.93168200
C	2.48657600	3.98497200	1.73082700
H	1.68108100	2.03350000	2.15920300
C	2.99055000	4.83495300	0.74621500
H	3.47724800	5.03707300	-1.34352000
H	2.40678200	4.32500500	2.75953500
H	3.30647900	5.84220100	1.00222300
C	2.14955700	-0.14858900	0.56391900
C	2.57816000	-1.14448600	1.30883900
H	2.02190200	-1.40271300	2.21086000
C	3.75533600	-1.98690600	1.01230900
C	4.53958200	-1.79193200	-0.14067800
C	4.09715500	-3.03035300	1.89085400
C	5.63235400	-2.61356600	-0.39507000
H	4.27949900	-0.99450400	-0.83132100
C	5.19397900	-3.85374200	1.62923100
H	3.50075000	-3.18730000	2.78627800
C	5.96611300	-3.64781600	0.48677800
H	6.22900800	-2.44850500	-1.28757100
H	5.44615400	-4.65122500	2.32251700

H	6.82119000	-4.28525900	0.28248700
C	-5.89870700	-2.35784500	-0.44600300
C	-4.66446600	-2.79942800	0.03627300
C	-3.48141100	-2.53002200	-0.66207300
C	-3.56187300	-1.81083800	-1.86243800
C	-4.79160500	-1.36868400	-2.35005900
C	-5.96453100	-1.64002400	-1.64081900
H	-6.80673600	-2.58036000	0.10703800
H	-4.61951600	-3.36573100	0.96372800
H	-2.65287600	-1.59545600	-2.41781600
H	-4.83565200	-0.81724400	-3.28470900
H	-6.92290600	-1.29931400	-2.02129900
C	-2.14508800	-2.98358700	-0.11624200
H	-1.49615100	-3.30047900	-0.94005000
H	-2.30053600	-3.86844100	0.51982000
N	-1.44084600	-1.89854300	0.60192400
H	-1.99929100	-1.62164500	1.40907900
H	-0.57233800	-2.29363100	0.96951700
O	0.84870900	-3.80530700	1.39787400
H	0.74470600	-4.76433600	1.37533500
H	1.72277300	-3.64038200	1.01690500

TS1W

C	-6.47347300	-0.13403600	0.83875900
C	-5.17562500	-0.62740500	0.71491500
C	-4.89037200	-1.65486700	-0.19619000
C	-5.92837500	-2.17695700	-0.97496000
C	-7.22979400	-1.68785600	-0.84708700
C	-7.50453900	-0.66435000	0.05940700
H	-6.68208300	0.66183900	1.54792100
H	-4.37610400	-0.21202500	1.32269700
H	-5.71650900	-2.97203600	-1.68528000
H	-8.02552900	-2.10423200	-1.45789700
H	-8.51580700	-0.28095200	0.15919600
C	-3.48600600	-2.20237200	-0.31835200
H	-3.45378300	-3.04211500	-1.02323300
H	-3.12344500	-2.59256800	0.63926200
N	-2.54860500	-1.16614400	-0.75222700
H	-2.91418500	-0.33014100	-1.21208800

C	-1.22667400	-1.29326400	-0.73348100
S	-0.44499400	-2.70191900	-0.22378400
C	-0.39295900	-0.08543200	-1.18974100
C	-1.04188400	0.89105900	-2.18779900
O	-2.25428900	1.01831600	-2.32295000
C	-0.09341600	1.74096400	-3.00944100
H	0.80888200	1.19378700	-3.29502700
H	-0.62311400	2.10744600	-3.89053400
H	0.22511800	2.60227500	-2.41241800
H	0.44378900	-0.51208800	-1.74791100
C	0.23931200	0.68286300	-0.00845200
C	-0.57497800	1.22837100	1.10043600
C	-1.88981200	1.71149500	0.92182800
C	-0.04552000	1.30055700	2.40878300
C	-2.62584000	2.22817300	1.98983700
H	-2.34294600	1.71102100	-0.06123500
C	-0.77718700	1.82682000	3.46731800
H	0.95889800	0.93066800	2.58827800
C	-2.08007400	2.29235400	3.27096800
H	-3.63172100	2.59750400	1.80644600
H	-0.33056600	1.86083400	4.45757700
H	-2.65410100	2.69763400	4.09871700
C	1.60669800	0.75694700	0.04647000
C	2.63126100	1.62934900	0.18240400
H	3.60990600	1.24381000	0.46192100
C	2.59282600	3.08699000	0.01114800
C	1.40729700	3.84034600	-0.11666500
C	3.81907600	3.78374300	-0.03369400
C	1.45782400	5.21833700	-0.31853000
H	0.44861300	3.34450500	-0.03064600
C	3.86419100	5.16135900	-0.22602200
H	4.74703500	3.22780100	0.08106500
C	2.68141300	5.88883900	-0.37707500
H	0.52957400	5.77523900	-0.41221300
H	4.82462500	5.66850700	-0.25787500
H	2.71281000	6.96417200	-0.52459000
C	3.73056800	-5.20651000	0.78678300
C	3.14208600	-3.96249000	1.01138700
C	3.86071500	-2.78249300	0.77522900

C	5.18033300	-2.87518000	0.31481100
C	5.77098900	-4.11898600	0.08989000
C	5.04597000	-5.28794900	0.32525700
H	3.16251500	-6.11262200	0.97549700
H	2.11768000	-3.90314200	1.36868500
H	5.75183800	-1.96673500	0.13727500
H	6.79680800	-4.17482500	-0.26268700
H	5.50436900	-6.25739700	0.15369300
C	3.21647800	-1.42846800	0.98983100
H	3.98442300	-0.68121000	1.20660300
H	2.52664100	-1.45367400	1.83798600
N	2.43139900	-0.96347300	-0.18006500
H	2.99162100	-0.92887100	-1.03672400
H	1.63571300	-1.60870400	-0.31950200
O	3.11938500	0.30130700	-2.71124600
H	3.76737200	0.61261000	-3.35538300
H	2.99818100	1.03499500	-2.08525100

Int1W

C	6.32601300	0.22244000	-0.98059700
C	5.07138400	-0.35897400	-0.80404500
C	4.92809100	-1.51015600	-0.01590900
C	6.06195000	-2.06498800	0.58653200
C	7.31968900	-1.48701900	0.40425200
C	7.45390400	-0.34106300	-0.37905500
H	6.42376900	1.11459600	-1.59232000
H	4.19728700	0.08647000	-1.27132300
H	5.95996200	-2.95502600	1.20234900
H	8.19092300	-1.92954600	0.87835300
H	8.43078800	0.11229900	-0.51960100
C	3.57228400	-2.15832700	0.15845300
H	3.64273200	-3.03476600	0.81450500
H	3.17447300	-2.51857100	-0.79645900
N	2.59669500	-1.21499700	0.70538300
H	2.93156400	-0.44474400	1.28779500
C	1.28161500	-1.37510000	0.66704500
S	0.52940000	-2.74795100	0.01299200
C	0.39984300	-0.25483600	1.23536000
C	0.99301800	0.61809600	2.35497000

O	2.19217900	0.68467600	2.60366200
C	0.00256600	1.42946800	3.16751400
H	-0.98136200	0.95792400	3.22551800
H	0.41629300	1.58475800	4.16629400
H	-0.12777800	2.40947700	2.69748600
H	-0.39962200	-0.77917500	1.76777500
C	-0.28353000	0.60140500	0.14917200
C	0.49014400	1.48329500	-0.73002100
C	1.81737300	1.89828500	-0.45512100
C	-0.05362700	1.94065600	-1.95914900
C	2.54212200	2.69087000	-1.34578700
H	2.29813800	1.62094100	0.47197600
C	0.67132800	2.73231700	-2.84022200
H	-1.06460200	1.65313400	-2.22410800
C	1.98308700	3.11762300	-2.54914600
H	3.55480700	2.98451300	-1.07989400
H	0.20533000	3.04918900	-3.76988400
H	2.54756500	3.73871300	-3.23787800
C	-1.68691700	0.46383500	0.02149800
C	-2.73274600	1.35644700	-0.16098700
H	-3.68932200	0.92921300	-0.45872800
C	-2.78480500	2.80728800	-0.05447000
C	-1.70959400	3.64464100	0.32334800
C	-4.02890400	3.43793600	-0.30452600
C	-1.88780300	5.01942300	0.46935100
H	-0.73141700	3.21826700	0.49321000
C	-4.19776400	4.80981800	-0.16773800
H	-4.87522700	2.82496500	-0.60848200
C	-3.12504200	5.61626700	0.22542100
H	-1.03974400	5.63209900	0.76362000
H	-5.16894800	5.25370600	-0.37028300
H	-3.25109800	6.68972600	0.32980900
C	-3.40894900	-5.28615800	-0.98061500
C	-2.80369400	-4.04956500	-1.20641300
C	-3.48469300	-2.86298700	-0.90743600
C	-4.78245400	-2.93662400	-0.38237200
C	-5.38657000	-4.17191200	-0.15287200
C	-4.69898800	-5.34966900	-0.45216800
H	-2.87157300	-6.19918600	-1.21799600

H	-1.79822800	-4.00208400	-1.61335200
H	-5.32521200	-2.02072800	-0.15849200
H	-6.39373200	-4.21536800	0.25073300
H	-5.16904600	-6.31290200	-0.27777200
C	-2.84087900	-1.51715500	-1.13656100
H	-3.57263500	-0.78431500	-1.47387300
H	-2.03382400	-1.56540900	-1.86957300
N	-2.20544800	-0.98193600	0.13025200
H	-2.85746700	-1.05028200	0.92873700
H	-1.39181400	-1.62335900	0.29196900
O	-3.33571900	-0.04637800	2.53081200
H	-4.13264900	0.06116500	3.06442600
H	-3.26385300	0.76021000	1.98611500

TS2W

C	5.81997000	-0.99724300	-1.17649200
C	4.48442400	-1.32076900	-0.94096200
C	4.14816800	-2.51421500	-0.28597900
C	5.17297800	-3.37417300	0.12319000
C	6.50971400	-3.05521600	-0.12106100
C	6.83628000	-1.86451400	-0.77002400
H	6.06582400	-0.06669300	-1.67959900
H	3.70006500	-0.64074200	-1.26258400
H	4.92309300	-4.29893600	0.63692500
H	7.29385700	-3.73341900	0.20256900
H	7.87604400	-1.61189800	-0.95597300
C	2.70106100	-2.88535400	-0.04908000
H	2.62713500	-3.80258300	0.54780800
H	2.18073200	-3.09349300	-0.99151800
N	1.97646700	-1.80590200	0.62099300
H	2.51187500	-1.10533800	1.13552500
C	0.65835700	-1.77436900	0.78442400
S	-0.39573400	-2.97977900	0.25667400
C	0.08031100	-0.52366200	1.45668800
C	0.90385500	0.06079300	2.61724600
O	2.11810400	-0.04462000	2.69305600
C	0.10428900	0.77648400	3.68383300
H	-0.66287000	1.41672200	3.23868500
H	-0.41269200	0.03344800	4.30384600

H	0.77204100	1.36091700	4.31795100
H	-0.85294400	-0.84273800	1.92512500
C	-0.25045400	0.57068900	0.41471100
C	0.87779600	1.37059500	-0.15387800
C	1.65537300	2.27610900	0.58546300
C	1.19673400	1.18803200	-1.51193600
C	2.71467100	2.96400900	-0.00580300
H	1.41892400	2.47436200	1.62440000
C	2.25302100	1.87676700	-2.10689400
H	0.60159000	0.49490400	-2.09872000
C	3.02039300	2.76601900	-1.35197500
H	3.29404000	3.66550400	0.58701600
H	2.47469800	1.71965500	-3.15888900
H	3.84307600	3.30651800	-1.81109600
C	-1.51335100	0.75423400	-0.07191100
C	-2.14289200	1.94803100	-0.64320500
H	-2.54554200	1.79345600	-1.65041100
C	-1.52830200	3.29550700	-0.49306800
C	-1.37658900	3.87346700	0.78236500
C	-1.19609900	4.08615000	-1.60530300
C	-0.89025700	5.16878100	0.93777200
H	-1.68217600	3.30059100	1.65423600
C	-0.71807700	5.38855700	-1.45389100
H	-1.31091200	3.66878600	-2.60279600
C	-0.55507000	5.93620200	-0.18143000
H	-0.78961400	5.58997600	1.93497600
H	-0.46845300	5.97500300	-2.33441300
H	-0.18235300	6.94944300	-0.06185400
C	-4.83734600	-4.26548500	-1.08332100
C	-3.89879000	-3.25756700	-1.30970700
C	-4.14068600	-1.95094700	-0.87118800
C	-5.33551400	-1.66975200	-0.19333500
C	-6.26899700	-2.67785000	0.04015100
C	-6.02331700	-3.97775500	-0.40794200
H	-4.63771900	-5.27488600	-1.43016300
H	-2.97036500	-3.48595800	-1.82490300
H	-5.52437600	-0.66058600	0.16198200
H	-7.18978000	-2.44830200	0.56819500
H	-6.75275200	-4.76214200	-0.22895100

C	-3.13631700	-0.85547000	-1.14304800
H	-3.60891500	-0.00952600	-1.64334400
H	-2.31194800	-1.21790000	-1.75962600
N	-2.54220200	-0.32239000	0.14009800
H	-3.35622000	0.20360400	0.68994800
H	-2.13753200	-1.14366900	0.60799600
O	-4.06810300	1.45444400	1.05531400
H	-4.96834300	1.63355100	0.75441100
H	-3.27763200	1.89180000	0.21540500

Int2W

C	6.67012200	0.43724600	-0.75522100
C	5.37889900	-0.08452200	-0.82239500
C	5.12558000	-1.40978500	-0.44063900
C	6.19180200	-2.19855000	0.00522300
C	7.48657100	-1.68056100	0.06384700
C	7.72849700	-0.36026900	-0.31499400
H	6.85033200	1.46717000	-1.04921300
H	4.56163600	0.54366500	-1.16642100
H	6.00621800	-3.22564300	0.30857300
H	8.30287300	-2.30696300	0.41150400
H	8.73428400	0.04643600	-0.26557500
C	3.73422000	-1.99572300	-0.53534100
H	3.71577300	-3.01941900	-0.14373000
H	3.40292800	-2.06848600	-1.57912300
N	2.75741000	-1.18513700	0.19057200
H	3.08879800	-0.43609100	0.80237500
C	1.45625900	-1.46240100	0.24875900
S	0.74361500	-2.77792100	-0.52898300
C	0.58223200	-0.48230700	1.04334800
C	1.24023400	0.12861200	2.29406500
O	2.41869100	0.45342000	2.32265600
C	0.35307900	0.29006500	3.50530800
H	-0.69740200	0.44242600	3.24205000
H	0.39998700	-0.64916300	4.07394800
H	0.73933400	1.08693200	4.14359100
H	-0.27601100	-1.05257200	1.40121000
C	0.04194200	0.63377300	0.11610600
C	0.93061500	1.80951300	-0.15517500

C	0.97503900	2.91680600	0.70623700
C	1.74644500	1.82889100	-1.29981300
C	1.80441900	4.00554900	0.43586400
H	0.34309300	2.92996600	1.58954500
C	2.57471400	2.91843600	-1.57467400
H	1.71332000	0.98524200	-1.98315100
C	2.60852100	4.00922100	-0.70435300
H	1.81795500	4.85312000	1.11487400
H	3.18698300	2.91756300	-2.47232900
H	3.25196900	4.85809400	-0.91630600
C	-1.16460300	0.49718500	-0.50147800
C	-1.74848400	1.60551000	-1.35590100
H	-0.96836900	2.35091800	-1.52620800
C	-2.97662200	2.31432300	-0.79063500
C	-3.20100900	2.43777200	0.58574500
C	-3.88859600	2.91085800	-1.67358600
C	-4.30809300	3.14071300	1.06523400
H	-2.52168100	1.97077400	1.29050200
C	-4.99025900	3.61976200	-1.19617900
H	-3.73080300	2.82053900	-2.74598700
C	-5.20420900	3.73722100	0.17848100
H	-4.46921800	3.21406400	2.13678300
H	-5.68373500	4.07483700	-1.89776700
H	-6.06506900	4.28309600	0.55336400
C	-4.39948500	-4.52493400	-1.04731600
C	-3.70596300	-3.38642500	-1.46349200
C	-3.84071400	-2.17621000	-0.77557100
C	-4.68398400	-2.12433700	0.34429700
C	-5.37652400	-3.26012100	0.76180500
C	-5.23725600	-4.46358900	0.06560900
H	-4.28369300	-5.45692700	-1.59278300
H	-3.05277700	-3.43840000	-2.33076400
H	-4.78475700	-1.19355600	0.89602100
H	-6.03127300	-3.20521400	1.62702600
H	-5.78006400	-5.34686200	0.38944400
C	-3.09016600	-0.94167300	-1.23050500
H	-3.76131000	-0.08008800	-1.21817600
H	-2.75249700	-1.08491100	-2.26719100
N	-1.95338400	-0.66374800	-0.32919700

H	-2.57581100	-0.47754100	1.50424000
H	-1.36282300	-1.49763800	-0.26796200
O	-2.76598800	-0.33364500	2.45562000
H	-2.94340600	-1.22003400	2.79469700
H	-2.00177700	1.20508500	-2.34513800

Int3-1W

C	6.68655200	0.78906900	0.20444200
C	5.52291600	0.19542600	-0.28249600
C	5.28585700	-1.17232000	-0.08305100
C	6.23684000	-1.93021500	0.60853800
C	7.40590100	-1.33832200	1.08996500
C	7.63222800	0.02334700	0.89011900
H	6.85690300	1.84990800	0.04518000
H	4.79288200	0.79547700	-0.81935500
H	6.06097800	-2.99057700	0.77004300
H	8.13573100	-1.94034600	1.62339600
H	8.53997600	0.48634700	1.26599000
C	4.02751600	-1.81844200	-0.61741500
H	4.04870200	-2.90456700	-0.47253500
H	3.92508800	-1.65682900	-1.69728400
N	2.83615500	-1.27245800	0.03382200
H	2.95223900	-0.63797500	0.82687400
C	1.58973200	-1.62071900	-0.26620000
S	1.20712600	-2.75438800	-1.45958800
C	0.47847500	-0.90247200	0.50322600
C	0.79347100	-0.47655100	1.94323300
O	1.90019800	-0.10172900	2.30942700
C	-0.37996600	-0.51881400	2.89761000
H	-0.56449900	-1.56460200	3.17428400
H	-0.15063000	0.05248100	3.79850400
H	-1.29525700	-0.15282200	2.42289700
H	-0.33827300	-1.61621700	0.57136300
C	-0.01506600	0.36166600	-0.23396500
C	1.02740500	1.37361500	-0.60647300
C	1.47274700	2.35910700	0.28991800
C	1.59719300	1.34680800	-1.89263500
C	2.44240600	3.29017600	-0.08639100
H	1.05473300	2.40020200	1.29027900

C	2.56324900	2.27903800	-2.27337700
H	1.26909000	0.58485700	-2.59352100
C	2.98916100	3.25552900	-1.36973600
H	2.76512900	4.04642600	0.62341000
H	2.97967100	2.24500700	-3.27635400
H	3.73733400	3.98556100	-1.66532900
C	-1.33141900	0.52886500	-0.56638500
C	-1.80730800	1.81071700	-1.23118700
H	-0.93250200	2.40122300	-1.51033100
C	-2.72778400	2.67420500	-0.37653900
C	-2.49728100	2.85170800	0.99392500
C	-3.79992400	3.35771700	-0.96503900
C	-3.31438000	3.68905000	1.75321500
H	-1.67025100	2.32889400	1.46475400
C	-4.61833000	4.19851600	-0.20895700
H	-3.99343000	3.23230900	-2.02794200
C	-4.37854200	4.36644300	1.15496400
H	-3.11931500	3.81280700	2.81485100
H	-5.44425200	4.71837800	-0.68615200
H	-5.01552900	5.01706900	1.74690000
C	-5.70621200	-3.61447400	-0.75345700
C	-4.87163100	-2.61625300	-1.26545600
C	-4.48638900	-1.52927400	-0.47187500
C	-4.94986000	-1.45995400	0.84893600
C	-5.78204600	-2.45313000	1.36146000
C	-6.16247100	-3.53437200	0.56178400
H	-5.99834800	-4.45008800	-1.38300900
H	-4.52366700	-2.67674400	-2.29419000
H	-4.64696000	-0.62339400	1.47199000
H	-6.13524600	-2.38560600	2.38641700
H	-6.81014400	-4.30839400	0.96275200
C	-3.58177200	-0.44680800	-1.02402400
H	-4.08886600	0.52006600	-0.94700200
H	-3.40929700	-0.63747300	-2.09560300
N	-2.32742700	-0.39323200	-0.26500000
H	-0.93597800	-3.38009300	-0.55467500
H	-2.00614600	-1.33700700	-0.04873100
O	-1.67260200	-3.31667400	0.08704100
H	-2.46370700	-3.62055500	-0.37774200

H	-2.31965600	1.57024700	-2.17030700
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TS3-1W

C	-6.19759700	-1.08349100	1.22842600
C	-5.35332400	-2.04363400	0.66256500
C	-4.34262100	-1.67169100	-0.22882000
C	-4.19566300	-0.30832300	-0.55182200
C	-5.03162200	0.65287400	0.02240100
C	-6.03432300	0.26560400	0.91766500
H	-6.97822300	-1.39247000	1.91759800
H	-5.48069600	-3.09224700	0.91979200
H	-3.44063300	-0.01663600	-1.27814600
H	-4.90337400	1.69955700	-0.23812200
H	-6.68682600	1.01135600	1.36170200
C	-3.36600500	-2.69411100	-0.78685300
H	-3.22116100	-2.56179600	-1.86070900
H	-3.73331600	-3.70907000	-0.60464500
N	-2.06176900	-2.55119900	-0.14443900
H	-2.01209100	-2.76780900	0.85096600
C	-1.00330600	-1.86536700	-0.63483500
S	-0.95598000	-1.36811900	-2.26361500
C	0.07928100	-1.51205300	0.32578500
C	0.05296300	-2.02624400	1.68532900
O	-1.04108500	-2.25646800	2.29743400
C	1.31553200	-2.17281800	2.50538100
H	1.95770700	-1.29357900	2.41763100
H	1.03221000	-2.33224800	3.54654100
H	1.90198600	-3.02494300	2.14923300
H	-0.80772500	-0.28785500	0.87007900
C	1.41972100	-1.05742100	-0.21458400
C	2.47889400	-2.09944500	-0.36956100
C	3.80087800	-1.92880500	0.08397700
C	2.14980200	-3.33684400	-0.95675500
C	4.75474200	-2.93653900	-0.06552700
H	4.08151800	-1.00864700	0.58653900
C	3.10161300	-4.34387200	-1.10408400
H	1.14087500	-3.49644800	-1.32174500
C	4.41183400	-4.14984100	-0.66156100
H	5.76527700	-2.77381400	0.29930900

H	2.81869700	-5.28290900	-1.57193600
H	5.15273900	-4.93604000	-0.77412200
C	1.58934200	0.24500400	-0.58329200
C	2.88503100	0.81517400	-1.12154500
H	3.52295100	-0.01289400	-1.44354200
C	3.69338000	1.70315600	-0.17945100
C	3.48824400	1.71725200	1.20576800
C	4.70786100	2.51585700	-0.70746600
C	4.27577600	2.51526700	2.04014700
H	2.69762900	1.10582200	1.63076000
C	5.49756600	3.30998100	0.12165200
H	4.87968700	2.52178100	-1.78138600
C	5.28462200	3.31270000	1.50250500
H	4.09666900	2.51204500	3.11177500
H	6.27793100	3.93041200	-0.31009600
H	5.89706400	3.93340700	2.14984100
C	-2.74518700	4.33407500	-1.52182000
C	-1.50382500	3.72150200	-1.71354900
C	-0.78804800	3.19725900	-0.63220300
C	-1.34401400	3.29290900	0.65211200
C	-2.58140000	3.90406200	0.84853300
C	-3.28630300	4.42872800	-0.23973500
H	-3.28521600	4.73814900	-2.37324800
H	-1.08591700	3.65034300	-2.71454300
H	-0.80058800	2.88071500	1.49710700
H	-2.99335700	3.98014600	1.85101500
H	-4.24597100	4.91419600	-0.08610600
C	0.55673700	2.52812800	-0.83985300
H	1.29221100	2.96002100	-0.15442500
H	0.90573000	2.74946300	-1.86104100
N	0.45209300	1.09145400	-0.57054300
H	-1.79966200	-0.79368900	2.00763800
H	-0.27032700	0.67058300	-1.16075800
O	-1.69842800	0.08729600	1.51933600
H	-2.48492000	0.22333100	0.95234800
H	2.66513500	1.38905900	-2.03032700

Int3W

C	7.00664000	0.67568000	-0.39732200
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C	5.83767800	0.25683100	-1.03496500
C	5.01212000	-0.70918400	-0.44936400
C	5.37305000	-1.24931300	0.79424800
C	6.53783800	-0.82568600	1.43375600
C	7.35907800	0.13501300	0.83923200
H	7.63920900	1.42397300	-0.86607300
H	5.56284700	0.68286700	-1.99631500
H	4.73711900	-1.99635200	1.26356600
H	6.80876600	-1.25148400	2.39578000
H	8.26855500	0.45895700	1.33693500
C	3.75609800	-1.17435200	-1.15135900
H	3.73218400	-2.26655000	-1.24572500
H	3.70541700	-0.77693900	-2.17093400
N	2.55656000	-0.75609100	-0.42322600
H	2.67353600	-0.20029100	0.42109700
C	1.32050200	-1.14765400	-0.72252200
S	0.95863600	-2.17949800	-2.00320200
C	0.19305100	-0.57976400	0.14369800
C	0.49117300	-0.43369100	1.64073900
O	1.61410700	-0.18151800	2.08030800
C	-0.68034100	-0.63270600	2.56325500
H	-1.60395800	-0.24420300	2.12815300
H	-0.80580000	-1.71787000	2.66300200
H	-0.47376900	-0.19199300	3.54014400
H	-0.62356900	-1.29090700	0.08472600
C	-0.33466800	0.77089800	-0.38587700
C	0.67259600	1.82516800	-0.72177300
C	1.29173600	2.59885300	0.27394400
C	1.03476900	2.04811800	-2.06081300
C	2.23744100	3.56941500	-0.06050200
H	1.03298200	2.44064900	1.31614900
C	1.97758100	3.02050100	-2.39505100
H	0.57263200	1.44635900	-2.83749800
C	2.58243800	3.78417200	-1.39541500
H	2.70188800	4.15980400	0.72403700
H	2.23962300	3.18008700	-3.43715300
H	3.31672200	4.54132700	-1.65442700
C	-1.66578100	0.95955500	-0.55513800
C	-2.26711100	2.29429400	-0.97749500

H	-2.79268400	2.15054600	-1.93091100
C	-3.24754800	2.84611800	0.04597700
C	-2.78031200	3.39929500	1.24764300
C	-4.62951700	2.80238200	-0.17560100
C	-3.67020700	3.89738200	2.19713400
H	-1.70995600	3.44292500	1.43158600
C	-5.52503800	3.29753300	0.77620600
H	-5.00852500	2.38984500	-1.10773100
C	-5.04743700	3.84607000	1.96523500
H	-3.29015800	4.32800900	3.11922100
H	-6.59330700	3.25663200	0.58408300
H	-5.74068700	4.23400800	2.70564900
C	-4.28856000	-4.09454700	0.41802900
C	-3.39190200	-3.11669600	-0.00873100
C	-3.78923100	-2.14406200	-0.93848800
C	-5.10028000	-2.17505100	-1.42584600
C	-6.00106800	-3.15387400	-0.99941200
C	-5.59619200	-4.11561000	-0.07493100
H	-3.96431700	-4.84545900	1.13277500
H	-2.37619900	-3.11599600	0.37778700
H	-5.41724200	-1.42963800	-2.15187600
H	-7.01434800	-3.16465500	-1.39102400
H	-6.29235800	-4.88033700	0.25758400
C	-2.82398600	-1.07033300	-1.39117400
H	-3.21115000	-0.59116300	-2.30507000
H	-1.85716300	-1.51093200	-1.65257200
N	-2.60524700	-0.08116700	-0.30520300
H	-3.50259200	0.31883300	-0.04302000
H	-1.47296200	3.02165400	-1.15594000
O	2.78285500	-2.78316300	2.54573200
H	2.85706700	-3.06695000	3.46562400
H	2.53269600	-1.84378200	2.58741100
O	0.30785700	-3.50370100	1.30046900
H	1.19831700	-3.44749900	1.69565700
H	0.46761200	-3.59217300	0.34953300

TS3W

C	7.53987900	-0.05413500	0.94386100
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C	6.48984500	0.21813300	0.06506100
C	5.41087700	-0.66442800	-0.05391700
C	5.39777500	-1.82902700	0.72830500
C	6.44326000	-2.09870900	1.61041300
C	7.51798900	-1.21306300	1.71945500
H	8.37163700	0.63987300	1.02313600
H	6.50816600	1.12342100	-0.53625500
H	4.56345500	-2.52118800	0.64511600
H	6.42254900	-3.00401900	2.21046500
H	8.33337000	-1.42661400	2.40444600
C	4.28164000	-0.37645100	-1.01785700
H	4.11992100	-1.21235100	-1.70835100
H	4.51527900	0.49344700	-1.64171000
N	3.02737600	-0.13582400	-0.30232400
H	3.06242300	-0.09293400	0.71355200
C	1.81119600	-0.14283100	-0.85260400
S	1.60643200	-0.43069300	-2.52845500
C	0.62261500	0.03229800	0.03898500
C	0.75474000	-0.17571800	1.46392900
O	1.71604700	-0.82247300	1.98174900
C	-0.33716400	0.27709400	2.41308300
H	-0.65331500	1.30648700	2.23270300
H	-1.22255600	-0.35271500	2.27457100
H	0.02718600	0.16370500	3.43511400
H	0.09527400	-1.42391700	-0.27246400
C	-0.39450200	1.03017500	-0.46588800
C	0.17376900	2.35264400	-0.89068800
C	0.95888300	3.10591500	-0.00242300
C	-0.02860900	2.85760900	-2.18502100
C	1.49297400	4.33739400	-0.38192900
H	1.15078800	2.72529500	0.99690800
C	0.50974700	4.08560400	-2.56863000
H	-0.59412700	2.26457300	-2.89632100
C	1.26884900	4.83342200	-1.66718600
H	2.08677900	4.90794600	0.32683500
H	0.34511700	4.45254000	-3.57777200
H	1.68976900	5.78897800	-1.96620500
C	-1.73080100	0.80907300	-0.46758000
C	-2.77860900	1.89171600	-0.71876500

H	-3.44820700	1.57111800	-1.52702500
C	-3.61006800	2.17963800	0.52258400
C	-3.11686100	3.03480600	1.51986700
C	-4.86577300	1.58837900	0.71413800
C	-3.85675300	3.28978400	2.67339700
H	-2.14824700	3.50826400	1.38060700
C	-5.60819100	1.83818600	1.87150300
H	-5.27440200	0.93729600	-0.05528300
C	-5.10534700	2.68915100	2.85466400
H	-3.46120200	3.96081500	3.43071700
H	-6.58072200	1.37130700	1.99916000
H	-5.68232000	2.88817400	3.75298400
C	-3.86725200	-4.42279200	0.48207700
C	-3.13643500	-3.28744900	0.13269400
C	-3.56409200	-2.45629400	-0.91206800
C	-4.74106500	-2.79044100	-1.59335100
C	-5.46973500	-3.93062100	-1.25119100
C	-5.03515300	-4.75042500	-0.20960900
H	-3.52367700	-5.05521100	1.29619400
H	-2.22800700	-3.03391000	0.66751300
H	-5.08968900	-2.15128900	-2.40114000
H	-6.37965800	-4.17262000	-1.79303700
H	-5.60285500	-5.63524700	0.06353400
C	-2.77277700	-1.23019500	-1.31925100
H	-3.40677800	-0.60479100	-1.96859000
H	-1.90923500	-1.52046900	-1.92782100
N	-2.26164300	-0.49126100	-0.14281700
H	-3.04308700	-0.37067200	0.50183300
H	-2.29966600	2.81208900	-1.05239500
O	2.03113900	-3.18534900	0.86186800
H	1.84634600	-3.84624800	1.54160400
H	2.05364500	-2.30322600	1.33749000
O	0.12427400	-2.48193100	-0.69476900
H	0.86880100	-2.91512600	-0.13255000
H	0.52342700	-2.24473700	-1.57344000

Int4W

C	7.59636800	-0.09880000	0.85111400
C	6.53397600	0.12064000	-0.02775400

C	5.46183400	-0.77646300	-0.08810800
C	5.46673000	-1.90138000	0.75034700
C	6.52601300	-2.11828600	1.63072400
C	7.59349500	-1.21863900	1.68280500
H	8.42382100	0.60401400	0.88496700
H	6.53836900	0.99361200	-0.67562200
H	4.63485900	-2.59995600	0.70709700
H	6.52204300	-2.99362100	2.27407900
H	8.41950500	-1.39166300	2.36658300
C	4.31046300	-0.54473100	-1.04056400
H	4.07142900	-1.45085900	-1.60705300
H	4.56071600	0.22594200	-1.77885900
N	3.10546100	-0.14322800	-0.31167100
H	3.21889500	0.08380300	0.66905900
C	1.86310700	-0.14295800	-0.81640900
S	1.56968600	-0.53092600	-2.43996400
C	0.75991900	0.23534400	0.10890800
C	0.76749100	-0.06594000	1.44475800
O	1.70843800	-0.82711100	2.05595200
C	-0.24088300	0.41384100	2.44981700
H	-0.87927100	1.21254000	2.07855000
H	-0.87317900	-0.42457500	2.76655700
H	0.29594400	0.75366500	3.34181800
H	-0.59105400	-2.06030900	-0.26432600
C	-0.32584000	1.09038800	-0.46466800
C	0.13327400	2.44948300	-0.90255700
C	0.83582600	3.28626000	-0.02066200
C	-0.08098400	2.89826400	-2.21597200
C	1.27402700	4.54749300	-0.42512600
H	1.03722400	2.94449300	0.99033000
C	0.36338200	4.15546400	-2.62374100
H	-0.57913800	2.23989700	-2.92023900
C	1.03755000	4.98768100	-1.72832000
H	1.80465000	5.18412100	0.27733300
H	0.19291800	4.48010700	-3.64624300
H	1.38494000	5.96628100	-2.04654100
C	-1.62721700	0.71986000	-0.52722900
C	-2.76547900	1.71849500	-0.74364900
H	-3.48220800	1.33648100	-1.47828000

C	-3.49901100	2.01362300	0.55887200
C	-3.04318300	3.03307300	1.40911500
C	-4.62259900	1.27388800	0.95149400
C	-3.69027200	3.30245700	2.61467800
H	-2.17692500	3.62096000	1.11691100
C	-5.27006000	1.53861100	2.16097100
H	-5.00499300	0.48948300	0.30382500
C	-4.80587800	2.55358300	2.99660000
H	-3.32582700	4.10093500	3.25488200
H	-6.14067400	0.95398100	2.44441600
H	-5.31080600	2.76400400	3.93478500
C	-4.07855200	-4.62666800	-0.16205700
C	-3.18566600	-3.63532600	-0.56963700
C	-3.65932000	-2.39173800	-1.01397000
C	-5.04383100	-2.17571900	-1.05180000
C	-5.93798700	-3.16771800	-0.64579800
C	-5.45549800	-4.39649200	-0.19537900
H	-3.69747400	-5.58653800	0.17533300
H	-2.11624500	-3.82196800	-0.56037000
H	-5.42700000	-1.22693400	-1.42090200
H	-7.00746300	-2.98222700	-0.68787100
H	-6.14731000	-5.17246100	0.11945600
C	-2.70962700	-1.29288700	-1.44300400
H	-3.27281800	-0.55836300	-2.03103500
H	-1.92798000	-1.68713600	-2.09762100
N	-2.02907600	-0.65254700	-0.26799200
H	-2.69419400	-0.65851600	0.50650400
H	-2.37252500	2.65097400	-1.14738700
O	2.16584100	-3.10866600	0.82646300
H	2.00108100	-3.76801700	1.51263300
H	1.98616300	-1.62178900	1.51184700
O	-0.03727500	-2.78639200	-0.63675200
H	1.34497300	-3.10511800	0.25944600
H	0.35443400	-2.36088000	-1.42510600

TS4W

C	-7.53503600	-0.94425700	-1.03597100
C	-6.60354300	-0.12437700	-0.39508100
C	-5.48735800	-0.67311200	0.24714300

C	-5.32431400	-2.06591300	0.23620600
C	-6.25061300	-2.88789900	-0.40311100
C	-7.35952400	-2.32777800	-1.04262900
H	-8.39745500	-0.50170200	-1.52626000
H	-6.74672500	0.95345600	-0.38634800
H	-4.46683400	-2.50662700	0.73905700
H	-6.11112600	-3.96511400	-0.39912100
H	-8.08361300	-2.96764900	-1.53852000
C	-4.47023400	0.21964700	0.92331800
H	-4.17408700	-0.18040900	1.89597200
H	-4.88856700	1.21432100	1.11364300
N	-3.25486500	0.31179700	0.09213500
H	-3.50725400	0.56987100	-0.85972800
C	-2.12888100	1.09579800	0.54389200
S	-2.20359800	1.92684900	2.01477300
C	-1.00930500	1.02725400	-0.31350800
C	-0.70261500	-0.15991600	-1.11491900
O	-1.50815000	-1.23869600	-1.05634000
C	-0.08865300	-0.03838700	-2.49576700
H	0.67889600	0.73279100	-2.53528500
H	0.32855100	-0.99365600	-2.82316400
H	-0.89406200	0.23528400	-3.18526900
H	3.05686700	-2.74362300	-1.20847400
C	0.25961100	1.70323300	0.03130100
C	0.35470700	3.17399600	0.19271200
C	-0.23690600	4.00475300	-0.77253500
C	1.03765900	3.77513500	1.26178000
C	-0.12191400	5.39066500	-0.68961600
H	-0.79266900	3.54871100	-1.58616200
C	1.14943500	5.16191800	1.34724600
H	1.44100900	3.15125500	2.05254800
C	0.57660200	5.97541500	0.36841600
H	-0.58283000	6.01581000	-1.44924900
H	1.67122900	5.60804400	2.18909400
H	0.66110100	7.05604900	0.43745400
C	1.31425600	0.84802500	0.11680100
C	2.77181400	1.16168400	0.36137200
H	3.07886200	0.79769700	1.34902500
C	3.72699700	0.59038200	-0.67679900

C	3.66596000	1.01484900	-2.01223600
C	4.68428600	-0.37046900	-0.32497400
C	4.52646900	0.48263200	-2.97382000
H	2.94128300	1.77377000	-2.29549300
C	5.55479500	-0.90005400	-1.28173800
H	4.74489800	-0.70941500	0.70567000
C	5.47413000	-0.48147100	-2.61226300
H	4.46650900	0.82674000	-4.00241300
H	6.29495400	-1.63893000	-0.98759800
H	6.14996400	-0.89030100	-3.35758300
C	3.27731500	-3.98978600	1.74339600
C	2.16978400	-3.33089300	1.20493900
C	1.77517500	-2.07927800	1.70651200
C	2.48472700	-1.52562200	2.77991500
C	3.58974300	-2.18721900	3.31988600
C	3.99509800	-3.41637900	2.79587400
H	3.56670300	-4.96243800	1.35498800
H	1.57787200	-3.78938200	0.41407400
H	2.15989600	-0.57964000	3.20553700
H	4.12563800	-1.74843100	4.15665900
H	4.85124700	-3.93360200	3.21900600
C	0.59035700	-1.36478200	1.09313000
H	0.10654300	-0.69520000	1.80756600
H	-0.14376200	-2.10107100	0.75422800
N	0.92006600	-0.54396300	-0.11326400
H	1.55779800	-1.05583500	-0.73339600
H	2.87782800	2.25015900	0.38538000
O	0.07471900	-3.79153400	-1.44229200
H	-0.58840500	-3.08455600	-1.42272500
H	-2.26752600	-1.00183200	-0.43960500
O	2.55038400	-2.36747900	-1.94251500
H	0.81825300	-3.40982500	-1.93321600
H	3.19441600	-1.84423700	-2.44280900

Int5W

C	7.37024900	-1.28376300	1.22939500
C	6.53712800	-0.30656400	0.67991100
C	5.48556900	-0.65747900	-0.17487400
C	5.28691600	-2.01415400	-0.47050200

C	6.11488200	-2.99283900	0.07626500
C	7.15996000	-2.62946000	0.92973000
H	8.18366500	-0.99242500	1.88788600
H	6.70763200	0.74224700	0.91054600
H	4.47942400	-2.30147500	-1.13958600
H	5.94862300	-4.03866800	-0.16586600
H	7.80755100	-3.39139100	1.35380600
C	4.57538400	0.40380700	-0.75334400
H	4.39863800	0.23654600	-1.81900900
H	5.02748800	1.39745400	-0.66831300
N	3.26341600	0.35966400	-0.07726800
H	3.40736600	0.42406200	0.92964600
C	2.22175800	1.29758000	-0.48667100
S	2.58263700	2.55568600	-1.56226100
C	0.97130700	0.97418300	0.05177700
C	0.60817300	-0.38952600	0.62558100
O	1.42599000	-1.45111300	0.27049200
C	0.38363100	-0.40979800	2.14390800
H	-0.32719600	0.35355700	2.46320600
H	0.03896200	-1.39431700	2.47355800
H	1.34557900	-0.20916000	2.62180400
H	-2.89670200	-2.85834200	1.09993900
C	-0.28409100	1.67419700	-0.11333800
C	-0.43785500	3.14711200	-0.18937700
C	0.19023700	3.96109600	0.76622700
C	-1.24152900	3.75398600	-1.16508700
C	0.00751000	5.34052200	0.75369700
H	0.82958300	3.49864300	1.51139100
C	-1.41716600	5.13784800	-1.18344900
H	-1.69950500	3.14036100	-1.93479700
C	-0.79774500	5.93494100	-0.22137400
H	0.50088000	5.95581800	1.50060800
H	-2.03166100	5.59247500	-1.95524300
H	-0.93303700	7.01252200	-0.23521800
C	-1.34874900	0.81525200	-0.08378400
C	-2.82967300	1.07103300	-0.05804200
H	-3.30655700	0.77024400	-0.99792800
C	-3.59534400	0.41465000	1.08329300
C	-3.28846100	0.70741600	2.42012100

C	-4.62660700	-0.49683800	0.81945700
C	-3.97840600	0.09047600	3.46507900
H	-2.50548300	1.42841300	2.63895500
C	-5.32648600	-1.11160700	1.86195200
H	-4.88076800	-0.72914500	-0.21155100
C	-4.99882600	-0.82716600	3.18957500
H	-3.72865000	0.33228300	4.49421000
H	-6.12585900	-1.81196100	1.63657800
H	-5.53945700	-1.30352300	4.00198200
C	-3.61864100	-3.63290800	-1.98878300
C	-2.41506000	-3.09353400	-1.53089600
C	-2.02156600	-1.80365600	-1.92591400
C	-2.82964400	-1.09112700	-2.82102900
C	-4.03031300	-1.63427800	-3.28225400
C	-4.43287100	-2.90202400	-2.85777200
H	-3.90949500	-4.63503200	-1.68626200
H	-1.74717100	-3.67385500	-0.89558100
H	-2.51059600	-0.11121800	-3.16610000
H	-4.64439900	-1.07224300	-3.97972600
H	-5.36430100	-3.32713000	-3.22002900
C	-0.71610100	-1.23771500	-1.42546000
H	-0.31315600	-0.46889900	-2.08553700
H	0.02067000	-2.03006100	-1.30912800
N	-0.82259900	-0.58379300	-0.04804000
H	-1.38322700	-1.20232100	0.56323200
H	-2.94780800	2.15742200	0.00936400
O	0.03616400	-4.00037800	0.61187200
H	0.70271400	-3.29402500	0.57440400
H	2.28599000	-1.01892700	-0.03635900
O	-2.22160600	-2.54435100	1.71836100
H	-0.56822700	-3.71528200	1.31255200
H	-2.71921300	-2.07595400	2.40599500

TS5W

C	7.51909500	-0.37497800	1.08656700
C	6.38350400	0.37001500	1.41363400
C	5.43219500	0.69229400	0.44052000
C	5.63695300	0.24651300	-0.87309100
C	6.76745100	-0.49846200	-1.20256200

C	7.71395900	-0.81202400	-0.22294100
H	8.24658900	-0.61703000	1.85641800
H	6.23353500	0.70522800	2.43725900
H	4.89862400	0.48930900	-1.63174000
H	6.91441600	-0.83277600	-2.22606900
H	8.59471500	-1.39359600	-0.48016800
C	4.22089900	1.53533600	0.79013300
H	4.29075900	2.51866500	0.31701200
H	4.20018000	1.71133000	1.87713400
N	2.98286900	0.92742500	0.33023000
H	2.82897600	-0.01800100	0.65008200
C	1.86876900	1.60622400	-0.11460200
S	2.06267300	3.30152600	-0.55752100
C	0.64277600	0.96356900	-0.23268000
C	-0.62482700	1.61542800	-0.76904700
O	-0.76563700	3.00442800	-0.47263000
C	-0.74446100	1.41010500	-2.28937200
H	-0.70662800	0.34931000	-2.54071600
H	-1.67341300	1.81835400	-2.69525500
H	0.10682800	1.91473300	-2.75330900
H	-4.61389800	1.26197400	-1.18751300
C	0.22170100	-0.40538200	0.04135200
C	1.11500900	-1.58889800	0.13965400
C	2.03561000	-1.87366600	-0.88539000
C	1.05247200	-2.45986300	1.24031800
C	2.85582100	-2.99795300	-0.81520100
H	2.10243700	-1.19945000	-1.73355600
C	1.87483400	-3.58541000	1.31012900
H	0.36033500	-2.24116000	2.04800700
C	2.77739000	-3.85880800	0.28209400
H	3.56091500	-3.20001900	-1.61597600
H	1.81375800	-4.24442200	2.17149500
H	3.42109200	-4.73162900	0.33807900
C	-1.14357500	-0.49120900	0.07351700
C	-2.04083500	-1.69826400	0.11245100
H	-2.62453600	-1.72475400	1.03961200
C	-3.00864800	-1.80601300	-1.05979600
C	-2.53670800	-2.02901800	-2.36064600
C	-4.39130900	-1.69736500	-0.86294200

C	-3.41877900	-2.13165000	-3.43537300
H	-1.46693400	-2.12898900	-2.52603000
C	-5.27936400	-1.79712600	-1.93827100
H	-4.77442000	-1.54301900	0.14291300
C	-4.79515700	-2.01146600	-3.22886300
H	-3.03277900	-2.30992800	-4.43514100
H	-6.34954900	-1.71943200	-1.76429400
H	-5.48291600	-2.09287400	-4.06553800
C	-5.29961100	0.30901800	2.76529100
C	-4.34715700	0.94992400	1.97283100
C	-2.97638500	0.73749000	2.17835800
C	-2.58380000	-0.11365100	3.21973700
C	-3.53245100	-0.75710100	4.01615800
C	-4.89375000	-0.55185800	3.78747700
H	-6.35703900	0.49025000	2.59438400
H	-4.66571300	1.63412900	1.19098100
H	-1.52451600	-0.26966400	3.40427000
H	-3.20830200	-1.41368200	4.81834900
H	-5.63328300	-1.04824600	4.40872600
C	-1.94640200	1.45586200	1.33918600
H	-0.98080800	1.47933700	1.85408000
H	-2.25859800	2.49041200	1.19250500
N	-1.73266100	0.85749000	-0.03870500
H	-2.96292400	1.12138400	-0.81859600
H	-1.39780200	-2.58424400	0.12945000
O	-2.87566300	3.85763300	-1.32091700
H	-1.84776300	3.55993100	-0.97560600
H	0.22696300	3.39038600	-0.52080400
O	-3.74340200	1.61747500	-1.40068800
H	-2.81449400	4.24772000	-2.20380000
H	-3.43172700	2.86565500	-1.37489100

Int6W

C	6.38987800	0.92684000	1.19556800
C	5.70372900	0.26304000	0.17718300
C	4.76845800	-0.73267200	0.48040600
C	4.52647300	-1.05427900	1.82383000
C	5.20947500	-0.38931400	2.84134600
C	6.14338200	0.60153800	2.52966300

H	7.11692700	1.69449000	0.94656200
H	5.89711500	0.51685600	-0.86191600
H	3.80153200	-1.82838500	2.06247800
H	5.01664900	-0.64812600	3.87847700
H	6.67835800	1.11509600	3.32339800
C	4.02222000	-1.45674200	-0.61730200
H	3.93608800	-2.52427500	-0.39491200
H	4.55358800	-1.38240700	-1.57413400
N	2.66963800	-0.91518400	-0.76975300
H	2.49062900	-0.02778000	-0.31696700
C	1.68388900	-1.49125200	-1.48770300
S	1.93542800	-2.99241100	-2.23324900
C	0.41274200	-0.75195500	-1.53565500
C	-0.85565900	-1.30369200	-1.76345700
O	-0.89990100	-2.82826500	2.69938900
C	-1.28296800	-2.69878900	-2.09792600
H	-1.14989900	-2.90603800	-3.16542400
H	-0.65946700	-3.42443400	-1.57493400
H	-2.32615100	-2.87383400	-1.82943100
H	-0.30899000	-1.12636900	2.22980100
C	0.21336300	0.65847400	-1.25163800
C	1.24539700	1.71961200	-1.08811400
C	1.45348700	2.35973700	0.14574500
C	2.02763400	2.11364400	-2.18864500
C	2.40860200	3.37179000	0.26988200
H	0.88327900	2.04401200	1.01387700
C	2.98105000	3.12173300	-2.06128400
H	1.87678600	1.62331800	-3.14580900
C	3.17250300	3.75624300	-0.83120500
H	2.55780200	3.85239300	1.23215200
H	3.57255900	3.41548900	-2.92373500
H	3.91563600	4.54202800	-0.73259300
C	-1.14519300	0.90308900	-1.30829300
C	-1.85783300	2.22088500	-1.21260900
H	-2.39667400	2.42321000	-2.14846800
C	-2.81953600	2.41877500	-0.04536000
C	-2.52985100	1.94538900	1.24093700
C	-4.00034200	3.14613600	-0.24044500
C	-3.39833100	2.20090200	2.30253600

H	-1.62969900	1.36464900	1.41979800
C	-4.86971500	3.40322100	0.82021000
H	-4.23879300	3.52085200	-1.23352500
C	-4.56984200	2.93103800	2.09800400
H	-3.15891000	1.82298200	3.29227500
H	-5.78063700	3.96905400	0.64638600
H	-5.24509700	3.12561900	2.92600000
C	-4.08001800	-2.23853800	1.51624800
C	-3.33794700	-1.66090200	0.48348800
C	-3.97708400	-1.05870900	-0.60213400
C	-5.37819100	-1.03731200	-0.63408000
C	-6.12112700	-1.61039000	0.39552100
C	-5.47265200	-2.21585900	1.47516700
H	-3.54799000	-2.70597000	2.33827800
H	-2.25606500	-1.69040100	0.53804300
H	-5.89121900	-0.56684800	-1.47011300
H	-7.20632000	-1.58305100	0.35606000
H	-6.05212400	-2.66499500	2.27651000
C	-3.22550200	-0.45258400	-1.78181800
H	-3.63863000	0.53418700	-1.99955600
H	-3.39456600	-1.06055700	-2.67718700
N	-1.78161000	-0.29518500	-1.61526400
H	-0.05255500	-0.33009200	0.92484100
H	-1.07559500	2.98627900	-1.15689500
O	1.55184300	-3.02989400	1.49259100
H	-0.09586600	-3.18991300	2.25962100
H	-0.75177200	-2.98250300	3.64093300
O	0.30900800	-0.48877000	1.80935500
H	1.64270100	-3.30051100	0.56470100
H	1.40379700	-2.06201300	1.46343000

Com1F

C	-7.40863700	-1.53241500	0.78921000
C	-6.04345000	-1.63505700	0.52587700
C	-5.59026700	-1.98808700	-0.75347400
C	-6.53017500	-2.23855800	-1.75908300
C	-7.89758900	-2.14114600	-1.49568100
C	-8.33919500	-1.78652600	-0.22105400
H	-7.74752500	-1.25989100	1.78453500

H	-5.32195800	-1.43844600	1.31470400
H	-6.18873700	-2.51368200	-2.75365700
H	-8.61538300	-2.34109200	-2.28578500
H	-9.40258600	-1.71025500	-0.01406000
C	-4.10945400	-2.09556800	-1.03814400
H	-3.92774600	-2.57873400	-2.00534400
H	-3.59896200	-2.71053200	-0.28831800
N	-3.47877500	-0.77400000	-1.03633000
H	-4.07571200	0.05286900	-1.02261700
C	-2.16827300	-0.57110800	-1.15061100
S	-1.05156300	-1.81387100	-1.33020800
C	-1.68771100	0.88719000	-1.09959500
C	-2.66826300	1.97027400	-1.58408400
O	-3.88092000	1.89662500	-1.43384000
C	-2.03955000	3.15723800	-2.27551200
H	-1.16034600	3.51527000	-1.73264700
H	-1.69784300	2.84632600	-3.27080100
H	-2.77517200	3.95502600	-2.38383600
H	-0.82410800	0.92991000	-1.76448200
C	-1.13023000	1.26515900	0.30434800
C	-1.86338400	0.92846100	1.56406600
C	-3.24406500	1.13632000	1.71747800
C	-1.14152700	0.41408800	2.65446100
C	-3.87705700	0.83546800	2.92475900
H	-3.82669700	1.55250500	0.90449700
C	-1.77510900	0.11657000	3.85868700
H	-0.07411700	0.25046400	2.54541000
C	-3.14866300	0.32311700	3.99878500
H	-4.94367300	1.01563500	3.02591700
H	-1.19560800	-0.28273700	4.68596300
H	-3.64502500	0.09008100	4.93618300
C	0.04920500	1.84911800	0.35200500
C	1.23815500	2.40809600	0.38117100
H	2.11713100	1.75636000	0.40343600
C	1.53144400	3.85432200	0.35261200
C	0.53158500	4.83582000	0.46569700
C	2.86824100	4.26280800	0.21483900
C	0.86030300	6.18782800	0.42699200
H	-0.50195800	4.52933300	0.60197400

C	3.19402500	5.61807200	0.17789500
H	3.64018800	3.50218300	0.13461700
C	2.19294300	6.58505800	0.28113600
H	0.07746000	6.93545800	0.51895400
H	4.23208100	5.91952800	0.06956400
H	2.44732800	7.64056600	0.25436000
C	5.82466200	-1.92386500	-3.80032800
C	5.50486900	-0.75605200	-3.10738300
C	4.18074600	-0.46949100	-2.74821900
C	3.17957500	-1.38121500	-3.11209700
C	3.49455700	-2.55119000	-3.80580300
C	4.81896600	-2.82697700	-4.15028700
H	6.85686100	-2.12639300	-4.07259200
H	6.29308700	-0.05345400	-2.84411200
H	2.14389400	-1.17120300	-2.85332400
H	2.70400500	-3.24312400	-4.08293300
H	5.06503800	-3.73524700	-4.69280300
C	3.84596400	0.77506700	-1.94256900
H	2.81054600	1.07120700	-2.14614200
H	4.48030300	1.60722200	-2.27083600
N	3.98807300	0.63816400	-0.48225300
H	3.43171700	-0.16564000	-0.16293200
H	4.95590000	0.41052200	-0.26025900
C	5.07054100	-3.96641100	3.46486700
C	3.85215600	-3.84306100	2.79187300
C	3.39032700	-2.59398100	2.36527400
C	4.17897400	-1.46297300	2.62358100
C	5.39470800	-1.58164500	3.29416100
C	5.84508600	-2.83541200	3.71771300
H	5.41300400	-4.94568100	3.78743900
H	3.25238800	-4.72865000	2.59507100
H	3.83392600	-0.48823800	2.29024800
H	5.99192000	-0.69535500	3.49039600
H	6.79282300	-2.92739200	4.24049700
C	2.06537500	-2.45941200	1.64150200
H	1.39799000	-1.80841000	2.22020000
H	1.57627800	-3.44565500	1.60584600
N	2.22813600	-1.83977800	0.31677800
H	2.70947100	-2.48437600	-0.30761200

H	1.31130300	-1.66757900	-0.09840500
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TS1F

C	-6.47192700	-2.94564800	0.87575700
C	-5.09927200	-3.11072800	0.68492200
C	-4.40892100	-2.32382900	-0.24311500
C	-5.11189100	-1.35615800	-0.97488400
C	-6.48235300	-1.18782400	-0.77791400
C	-7.16704600	-1.98248100	0.14426900
H	-6.99413800	-3.56339300	1.60073400
H	-4.56016100	-3.85744400	1.26321000
H	-4.58163800	-0.72676100	-1.68427400
H	-7.01633100	-0.43333100	-1.34838200
H	-8.23431200	-1.84829900	0.29475800
C	-2.92897800	-2.55124200	-0.48091400
H	-2.75324200	-3.09371400	-1.41495500
H	-2.50773900	-3.15667300	0.33197800
N	-2.19454600	-1.29268100	-0.58760300
H	-2.43776000	-0.57664400	0.09198300
C	-1.34154200	-0.95727200	-1.55579000
S	-0.82877600	-2.00896400	-2.77495200
C	-0.84525000	0.49357500	-1.57021200
C	-1.81399200	1.37258200	-2.40773600
O	-3.00945800	1.15499300	-2.48310200
C	-1.16567800	2.51922400	-3.15523200
H	-0.41259600	3.02378500	-2.54527300
H	-0.66197900	2.11291200	-4.04147500
H	-1.93099500	3.22566700	-3.47953400
H	0.05840500	0.45877800	-2.17814200
C	-0.42787900	1.17574200	-0.25254400
C	-1.34180600	1.44836500	0.87588800
C	-2.75083600	1.51246000	0.73595500
C	-0.83647700	1.66219800	2.18386500
C	-3.58636700	1.74589800	1.83210100
H	-3.20928900	1.40368700	-0.23928300
C	-1.67262400	1.90745500	3.26512900
H	0.23689600	1.64205700	2.33930800
C	-3.06207300	1.94532000	3.10591200
H	-4.66071100	1.77792500	1.67201800

H	-1.23431100	2.06357700	4.24755000
H	-3.71367900	2.13015600	3.95414300
C	0.89989800	1.52204100	-0.15001300
C	1.72064000	2.54917100	0.15399500
H	2.75685300	2.33190800	0.41108400
C	1.39704600	3.97863400	0.17861400
C	0.09716700	4.50222700	0.02374100
C	2.45358700	4.89450900	0.36480200
C	-0.12104300	5.87825500	0.02544700
H	-0.74151300	3.82601900	-0.08305700
C	2.23019600	6.26780700	0.37551700
H	3.46436600	4.51451500	0.49499600
C	0.93873900	6.77033600	0.20096000
H	-1.13265100	6.25545700	-0.09675600
H	3.06579400	6.94751000	0.51843000
H	0.75997700	7.84140700	0.21112900
C	6.26154100	-1.48018000	-1.38027400
C	5.23426200	-0.53806100	-1.32558700
C	3.98011600	-0.81413100	-1.88633000
C	3.77853600	-2.05048000	-2.51657100
C	4.80608400	-2.99284500	-2.57457100
C	6.04894100	-2.71097100	-2.00372700
H	7.22932000	-1.25039500	-0.94424600
H	5.41066600	0.42425600	-0.84974700
H	2.81323300	-2.26666800	-2.96836200
H	4.63888400	-3.94321100	-3.07327300
H	6.84964000	-3.44296300	-2.05154100
C	2.85233400	0.18961000	-1.78822300
H	2.14321500	0.04151100	-2.60668600
H	3.22899700	1.21539600	-1.85266600
N	2.08740200	0.08699600	-0.51988700
H	1.62024700	-0.84051000	-0.42228900
H	2.73085400	0.13143600	0.27062800
C	3.78021000	-3.08331200	3.73258800
C	2.85998500	-3.53727000	2.78557700
C	1.81744800	-2.71314900	2.34655300
C	1.70805200	-1.42207300	2.88245800
C	2.62421600	-0.96611500	3.83055300
C	3.66508300	-1.79536100	4.25589900

H	4.58181700	-3.73691500	4.06440600
H	2.94938900	-4.54538700	2.38697200
H	0.89144400	-0.77792200	2.56557400
H	2.52015400	0.03263800	4.24517800
H	4.37612800	-1.44192600	4.99691600
C	0.85308600	-3.18968500	1.28136400
H	-0.13992800	-2.76753800	1.46765700
H	0.75599800	-4.28467400	1.34189500
N	1.27835300	-2.72821800	-0.05509400
H	2.15732700	-3.17488500	-0.31165800
H	0.59373800	-2.99009400	-0.76622100

Int1F

C	-6.82680000	-2.20661900	1.41601700
C	-5.46209400	-2.49419000	1.46402800
C	-4.61533200	-2.11109500	0.41821500
C	-5.15237400	-1.42253100	-0.67822700
C	-6.51551000	-1.12951500	-0.72099600
C	-7.35692300	-1.52219600	0.32212100
H	-7.47155300	-2.50931900	2.23615700
H	-5.05152600	-3.02041100	2.32270800
H	-4.50281000	-1.10269500	-1.48806200
H	-6.92029200	-0.59234300	-1.57384900
H	-8.41763900	-1.29145600	0.28468900
C	-3.14574700	-2.48676000	0.46180000
H	-2.94135900	-3.35440600	-0.17247700
H	-2.85858400	-2.74740800	1.48782100
N	-2.27935300	-1.41209400	-0.01611900
H	-2.41251200	-0.50032200	0.41708500
C	-1.44752500	-1.47343700	-1.05400900
S	-1.13349800	-2.88172100	-1.94129600
C	-0.75646800	-0.16780500	-1.47618400
C	-1.56105800	0.48943900	-2.63288000
O	-2.76223300	0.34678700	-2.77078400
C	-0.74863100	1.32565200	-3.60337000
H	0.02631200	1.90411500	-3.09552600
H	-0.26010100	0.65030500	-4.31788000
H	-1.41464300	1.98841000	-4.15781700
H	0.14145500	-0.51916700	-1.98252800

C	-0.30578400	0.87262300	-0.43421400
C	-1.25320200	1.59566600	0.42552900
C	-2.65192700	1.65384400	0.17622200
C	-0.82156800	2.24119800	1.61705500
C	-3.53808000	2.26521500	1.06646100
H	-3.06372000	1.23271500	-0.73170300
C	-1.70871100	2.85031900	2.49390100
H	0.23685700	2.26227200	1.84761900
C	-3.08363600	2.86735300	2.23665800
H	-4.59770100	2.27018000	0.82455500
H	-1.31899500	3.32127800	3.39297300
H	-3.77390800	3.34734500	2.92325700
C	1.08054400	1.16693500	-0.39421500
C	1.82731500	2.31261400	-0.18590500
H	2.87176100	2.15955500	0.09410700
C	1.47636600	3.71732200	-0.29002500
C	0.23751900	4.21569300	-0.75515200
C	2.46358700	4.67377500	0.05083900
C	0.01914600	5.58516800	-0.88897100
H	-0.55323400	3.52674900	-1.01943200
C	2.23673800	6.03874400	-0.07357300
H	3.42807100	4.32440800	0.41391300
C	1.00806100	6.50878800	-0.54739700
H	-0.94326200	5.93244900	-1.25544400
H	3.02103300	6.74021000	0.19890300
H	0.82498500	7.57488600	-0.64312300
C	6.06345400	-1.98559900	-1.37933600
C	5.10932000	-0.96853800	-1.41655500
C	3.80790700	-1.22943800	-1.86567600
C	3.47877200	-2.52609600	-2.28684200
C	4.43361200	-3.54260100	-2.25181100
C	5.72641800	-3.27437800	-1.79601700
H	7.06975000	-1.76988600	-1.03332500
H	5.38039300	0.03746400	-1.10435700
H	2.47291300	-2.73571900	-2.64358100
H	4.17015300	-4.54118500	-2.58733800
H	6.47008900	-4.06524300	-1.77289600
C	2.76948800	-0.13614000	-1.87813400
H	2.01933200	-0.31442900	-2.64977100

H	3.20636600	0.84910300	-2.05142900
N	2.03462100	-0.03690500	-0.56000300
H	1.60070900	-0.97071500	-0.28171400
H	2.74383300	0.08727700	0.16798100
C	4.06995100	-1.93376100	4.02043300
C	3.08476500	-2.60447900	3.29331200
C	2.01617200	-1.90454900	2.72042000
C	1.94697700	-0.51494400	2.89809500
C	2.93092500	0.15833200	3.62412900
C	3.99647600	-0.54995700	4.18467400
H	4.88997000	-2.49220100	4.46255000
H	3.14245100	-3.68433000	3.17574700
H	1.10927000	0.03779500	2.47990200
H	2.85845000	1.23350700	3.75996700
H	4.75906900	-0.02708000	4.75429200
C	0.98005900	-2.62579300	1.88564800
H	0.01217700	-2.12396600	1.97637400
H	0.85382000	-3.65227100	2.25856700
N	1.34856700	-2.59815900	0.45115400
H	2.20524000	-3.13027800	0.30408100
H	0.62115400	-3.04139600	-0.11563100

TS2F

C	-7.13835900	-1.97703500	1.43782800
C	-5.77843500	-2.21942900	1.63358300
C	-4.86101600	-2.01100100	0.59759000
C	-5.32217000	-1.54220500	-0.64005700
C	-6.68161600	-1.29279300	-0.83081200
C	-7.59346100	-1.51225400	0.20340800
H	-7.83874400	-2.14256500	2.25145700
H	-5.42703400	-2.57298600	2.60014500
H	-4.61570900	-1.35596600	-1.44394700
H	-7.02772700	-0.92518100	-1.79250700
H	-8.65083600	-1.31667600	0.05031200
C	-3.39708200	-2.34334200	0.81227800
H	-3.14799000	-3.32681300	0.40358900
H	-3.17282800	-2.36654400	1.88621700
N	-2.51138700	-1.38145300	0.16088500
H	-2.72534400	-0.39685200	0.32049100

C	-1.49917100	-1.65603100	-0.64927000
S	-1.00990300	-3.24842300	-1.02283800
C	-0.77356500	-0.47315100	-1.30743300
C	-1.57558500	0.00019300	-2.55161400
O	-2.76988900	-0.20170000	-2.69132500
C	-0.77896400	0.74300600	-3.60891500
H	-0.02659700	1.40134100	-3.16998100
H	-0.26447500	0.00710300	-4.24057300
H	-1.46239400	1.31350800	-4.23987700
H	0.11736500	-0.92785900	-1.73787100
C	-0.28888300	0.70544500	-0.43904200
C	-1.23214200	1.51204300	0.34969500
C	-2.60451200	1.67882400	0.01840000
C	-0.81982500	2.14054500	1.55505100
C	-3.49252500	2.36724300	0.85158200
H	-2.99005500	1.29408600	-0.91843100
C	-1.70191700	2.83382600	2.37110700
H	0.22307300	2.07913800	1.84449300
C	-3.05739400	2.94867800	2.03844800
H	-4.53283100	2.45495900	0.54872500
H	-1.32874900	3.28730100	3.28613900
H	-3.74511400	3.48907500	2.68134500
C	1.09016500	1.06043700	-0.51944600
C	1.73981900	2.28348300	-0.39755500
H	2.81436100	2.22118500	-0.21161700
C	1.28027200	3.65750100	-0.49939500
C	0.02733000	4.06598900	-1.01301000
C	2.17733500	4.68747900	-0.12383900
C	-0.29369100	5.41436800	-1.14623200
H	-0.69387700	3.32051800	-1.32027900
C	1.85039800	6.03231700	-0.25037800
H	3.15290200	4.41138000	0.27158700
C	0.60643600	6.41075700	-0.76338900
H	-1.26494900	5.68814300	-1.55034600
H	2.56906000	6.78986500	0.05230500
H	0.34461400	7.46019000	-0.86118300
C	6.06593500	-1.87705400	-1.92295200
C	5.06141400	-0.90817600	-1.94211200
C	3.72014200	-1.27186800	-2.11866900

C	3.40391600	-2.62917600	-2.28236300
C	4.40688400	-3.59928800	-2.26342300
C	5.74026800	-3.22479800	-2.08161400
H	7.10182700	-1.57872200	-1.79134400
H	5.32132200	0.14178200	-1.82934200
H	2.36761600	-2.92378000	-2.43518000
H	4.14867900	-4.64524600	-2.40163000
H	6.52161000	-3.97890000	-2.07248400
C	2.62856100	-0.22679500	-2.09115100
H	1.80646600	-0.52150900	-2.74616300
H	2.99607200	0.74406000	-2.44115500
N	2.08476700	-0.06295400	-0.70332500
H	1.78558400	-1.26061800	-0.00902100
H	2.89249300	0.22174300	-0.14512000
C	4.33282600	-1.74959600	4.27687300
C	3.20673300	-2.21548200	3.59755200
C	2.41953600	-1.34125700	2.83664200
C	2.77615900	0.01342200	2.77295000
C	3.90243400	0.47954000	3.45201400
C	4.68316200	-0.40064800	4.20357200
H	4.93075700	-2.43730500	4.86736300
H	2.93078100	-3.26529900	3.66784300
H	2.16864600	0.70680600	2.19640800
H	4.16337100	1.53227800	3.40003900
H	5.55629000	-0.03553400	4.73595000
C	1.22304000	-1.86379700	2.07633600
H	0.44107000	-1.10450500	1.99137100
H	0.80031700	-2.74123700	2.57466700
N	1.58921500	-2.23757600	0.67274400
H	2.41596300	-2.83557300	0.65221000
H	0.80969400	-2.74207400	0.20583000

Int2F'

C	-7.25741500	-1.83065300	1.44640100
C	-5.90171600	-2.07088100	1.67047400
C	-4.97007400	-1.91650800	0.63741000
C	-5.41340600	-1.50424500	-0.62652300
C	-6.76891900	-1.25567500	-0.84557500
C	-7.69464000	-1.42139900	0.18597300

H	-7.96881800	-1.95457600	2.25785100
H	-5.56449500	-2.38103600	2.65671800
H	-4.69633700	-1.36166500	-1.42981900
H	-7.10079800	-0.93159100	-1.82772000
H	-8.74886900	-1.22765200	0.01058900
C	-3.51291300	-2.25172500	0.88716800
H	-3.27574500	-3.26594500	0.55337200
H	-3.29590100	-2.20464300	1.96207700
N	-2.61032500	-1.35042700	0.17478700
H	-2.85105100	-0.36022300	0.20828700
C	-1.53119400	-1.68768100	-0.51405800
S	-0.99276000	-3.30683100	-0.64370900
C	-0.78636700	-0.57400000	-1.26220400
C	-1.59042900	-0.13969100	-2.51776500
O	-2.79520100	-0.29744700	-2.62894000
C	-0.78689900	0.51604200	-3.62665600
H	0.00609300	1.15835900	-3.23874200
H	-0.32404200	-0.27102000	-4.23617500
H	-1.46002100	1.08853700	-4.26698200
H	0.09176700	-1.07361800	-1.66839900
C	-0.26515600	0.64065600	-0.46418700
C	-1.18268400	1.48960100	0.31210300
C	-2.54498300	1.70963000	-0.02525200
C	-0.74776000	2.11103900	1.51229000
C	-3.40795200	2.43835800	0.80047600
H	-2.93917700	1.34014300	-0.96524400
C	-1.60266200	2.84620600	2.32075000
H	0.29152500	2.00796200	1.80423500
C	-2.95228600	3.01052400	1.98390900
H	-4.44290800	2.56733100	0.49394100
H	-1.21447900	3.29203100	3.23332900
H	-3.61954400	3.58189200	2.62160900
C	1.11401300	0.98518500	-0.59975500
C	1.75908000	2.21583500	-0.53308000
H	2.83993800	2.16260700	-0.38431300
C	1.29024800	3.58638400	-0.65025500
C	0.03634400	3.98029700	-1.17243700
C	2.17927900	4.62708500	-0.28625500
C	-0.29556500	5.32441900	-1.31929800

H	-0.67677300	3.22577600	-1.47668400
C	1.84244900	5.96828000	-0.42759600
H	3.15618600	4.36246000	0.11380600
C	0.59615900	6.33191000	-0.94510500
H	-1.26779200	5.58649300	-1.72886700
H	2.55512400	6.73438500	-0.13229700
H	0.32630400	7.37822200	-1.05411400
C	6.02778500	-2.02604200	-2.08407600
C	5.02369700	-1.05669400	-2.11951800
C	3.67374900	-1.42594100	-2.17232300
C	3.34834400	-2.79087000	-2.19379500
C	4.35012700	-3.76141900	-2.15810400
C	5.69298700	-3.38055900	-2.10127500
H	7.07016300	-1.72293100	-2.05001600
H	5.29038400	-0.00238400	-2.11661100
H	2.30425300	-3.09218300	-2.25167900
H	4.08325400	-4.81403600	-2.18664300
H	6.47336000	-4.13545500	-2.07969300
C	2.58433400	-0.37786200	-2.16226300
H	1.74036500	-0.71065200	-2.76976800
H	2.94095600	0.56805500	-2.58746100
N	2.09766300	-0.14217400	-0.76780000
H	1.81428900	-1.36584500	0.12955100
H	2.92928700	0.17228700	-0.26412200
C	4.38754800	-1.44389600	4.41014000
C	3.23562900	-1.92208200	3.78510300
C	2.49973500	-1.10104000	2.92045500
C	2.93354500	0.21347000	2.69599500
C	4.08573400	0.69124100	3.32119900
C	4.81498000	-0.13585400	4.17748000
H	4.94522400	-2.08903900	5.08233800
H	2.89889500	-2.93794200	3.97978700
H	2.36811500	0.86695000	2.03571500
H	4.40741100	1.71313400	3.14465200
H	5.70832700	0.23964600	4.66731700
C	1.27318100	-1.64230900	2.22516100
H	0.52831800	-0.86213800	2.04751800
H	0.81062200	-2.43990200	2.81254600
N	1.60995200	-2.19718600	0.87116700

H	2.41596000	-2.82218800	0.91067000
H	0.79981300	-2.71702100	0.46244100

Int2F

C	6.27187800	-1.93025600	-1.32493800
C	5.18514700	-1.05772900	-1.24745800
C	4.01553400	-1.30975200	-1.97353700
C	3.95190900	-2.45731900	-2.77659800
C	5.03294900	-3.33485600	-2.84683200
C	6.19778900	-3.07201500	-2.12286800
H	7.17303700	-1.71988700	-0.75623900
H	5.24524900	-0.17340000	-0.61832300
H	3.04931800	-2.66661500	-3.34457000
H	4.96704900	-4.22205300	-3.46988500
H	7.04093800	-3.75423100	-2.17991200
C	2.86074200	-0.33514200	-1.91386900
H	2.72928900	0.18758400	-2.86933100
H	3.03840900	0.43224600	-1.15219100
N	1.60038900	-1.01111000	-1.60256300
H	1.62886800	-1.98084600	-1.28614800
C	0.39422200	-0.47445600	-1.75148900
S	0.11550100	1.07510800	-2.37390900
C	-0.79371300	-1.31515100	-1.27379700
C	-0.67651100	-2.83213600	-1.48229300
O	0.38257500	-3.43756200	-1.42386900
C	-1.97544200	-3.55426900	-1.76813100
H	-2.78362000	-3.17716200	-1.13494300
H	-2.26547900	-3.36432000	-2.80912700
H	-1.84389000	-4.62769200	-1.62640200
H	-1.65366600	-0.99085200	-1.86468800
C	-1.12153400	-1.02016300	0.20839000
C	-0.31621400	-1.73428800	1.25260000
C	-0.75800900	-2.94189500	1.81922200
C	0.91842200	-1.21537500	1.68346800
C	-0.00125800	-3.60723800	2.78400600
H	-1.71290700	-3.35629700	1.50863500
C	1.67775000	-1.88255700	2.64635400
H	1.28497000	-0.28172200	1.26530000
C	1.22194200	-3.08009100	3.19896800

H	-0.36836900	-4.53619000	3.21105700
H	2.62658100	-1.46145000	2.96687400
H	1.81383200	-3.59713700	3.94871100
C	-2.06230800	-0.07930500	0.52692500
C	-2.46223800	0.16394100	1.97068600
H	-2.39327000	1.23601500	2.19139600
C	-3.85167800	-0.32602900	2.36668600
C	-4.43051000	-1.46150800	1.78662200
C	-4.55875200	0.33708500	3.37935700
C	-5.67831100	-1.92308100	2.20821200
H	-3.89950300	-1.98169400	0.99535100
C	-5.80432100	-0.12354900	3.80596900
H	-4.12648300	1.22236700	3.83991100
C	-6.36977800	-1.25750600	3.22084100
H	-6.11089200	-2.80454800	1.74309100
H	-6.33430600	0.40652300	4.59220500
H	-7.34129100	-1.61593500	3.54794100
C	-5.05219400	3.89531300	-2.98329700
C	-4.30348200	3.51357900	-1.86740600
C	-4.38344400	2.21175100	-1.36514700
C	-5.22371900	1.29047900	-2.00561400
C	-5.97028600	1.66725200	-3.11978600
C	-5.88720500	2.97288200	-3.61182600
H	-4.97693400	4.91038000	-3.36248200
H	-3.64808400	4.23379100	-1.38404400
H	-5.28262500	0.27517700	-1.62382800
H	-6.61958900	0.94407400	-3.60527800
H	-6.46855500	3.26615600	-4.48116600
C	-3.59193700	1.80068400	-0.13907000
H	-4.28563000	1.50245800	0.65211100
H	-3.03184600	2.67250400	0.23554000
N	-2.71354000	0.67166600	-0.44449900
H	-1.72754400	-0.32663400	2.61401300
H	-2.14149300	0.85424800	-1.26720300
C	6.09606900	4.54193700	2.13360900
C	4.96709200	4.50133000	1.31534300
C	4.27734200	3.30166500	1.09959700
C	4.73691700	2.14139400	1.73522000
C	5.86335300	2.18023200	2.55900900

C	6.54906400	3.37915200	2.75932900
H	6.61701000	5.48267700	2.28870600
H	4.61485200	5.41307600	0.83781300
H	4.19219300	1.21501900	1.58491200
H	6.20457100	1.27151200	3.04767900
H	7.42456600	3.40910100	3.40156900
C	3.08205200	3.27144600	0.16266200
H	3.43671100	3.08673600	-0.86059600
H	2.62812700	4.27659800	0.14321400
N	2.13448000	2.20122600	0.48493500
H	1.64177600	2.41960000	1.34790300
H	1.43675600	2.12039200	-0.25390500

Int3F

C	-4.82206600	-4.55823300	-2.78421500
C	-3.70283900	-3.77331200	-3.06646300
C	-3.30166000	-2.76030700	-2.18868900
C	-4.03980400	-2.55132200	-1.01517800
C	-5.15272300	-3.33971200	-0.72712400
C	-5.54891600	-4.34395900	-1.61295500
H	-5.12044100	-5.34036700	-3.47636400
H	-3.13514900	-3.94849300	-3.97692100
H	-3.74216200	-1.77507700	-0.31600600
H	-5.70722700	-3.16362600	0.18977800
H	-6.41723600	-4.95714600	-1.39002200
C	-2.11492400	-1.88323600	-2.52463900
H	-2.42815200	-0.86217600	-2.77177100
H	-1.59275600	-2.26651900	-3.40987000
N	-1.17813700	-1.79451500	-1.40650800
H	-1.22689200	-2.50165300	-0.66962200
C	-0.32438500	-0.79602700	-1.19816700
S	-0.15729600	0.53342300	-2.23236200
C	0.58314200	-0.92195400	0.02789800
C	-0.01412500	-1.63107300	1.25167300
O	-0.81162800	-2.55524600	1.16622000
C	0.44241300	-1.10945200	2.59120900
H	1.49410000	-0.81001500	2.57359800
H	-0.16472000	-0.21851000	2.79413100
H	0.26207200	-1.85430500	3.36788200

H	0.79963500	0.09722100	0.35182800
C	1.92970100	-1.58071100	-0.34538700
C	1.95189900	-3.06871900	-0.52039700
C	2.12351600	-3.94694100	0.56215900
C	1.78071100	-3.62782300	-1.79965700
C	2.13089700	-5.32940800	0.37574300
H	2.26219800	-3.54204700	1.56022800
C	1.78795300	-5.01011200	-1.98985000
H	1.64871400	-2.96312600	-2.64861600
C	1.96200100	-5.86571600	-0.90123700
H	2.27042400	-5.98698400	1.22893900
H	1.65842900	-5.41791400	-2.98847300
H	1.96727600	-6.94202500	-1.04678300
C	3.01907400	-0.79890600	-0.61386700
C	4.38797300	-1.41186300	-0.84776300
H	4.82637900	-0.99744800	-1.76319400
C	5.38389700	-1.23973400	0.29576200
C	4.98588800	-1.33341000	1.63555000
C	6.74242200	-1.03658500	0.01751700
C	5.91895600	-1.22699200	2.66725500
H	3.93678200	-1.49123900	1.86626500
C	7.67869300	-0.93219500	1.04700400
H	7.06968000	-0.96128700	-1.01686800
C	7.26946000	-1.02627200	2.37759000
H	5.58976400	-1.30109200	3.70000400
H	8.72650100	-0.77380100	0.80819100
H	7.99527400	-0.94176500	3.18095000
C	3.50934200	5.26640900	-1.01295300
C	3.74080500	3.95897800	-1.44967300
C	3.74769200	2.89392100	-0.54482200
C	3.51015300	3.15865400	0.81229900
C	3.27693700	4.46126100	1.25152700
C	3.27652700	5.52074700	0.33806200
H	3.50838000	6.08246100	-1.72974600
H	3.91613400	3.76483600	-2.50478600
H	3.51213000	2.33338000	1.51870300
H	3.10439800	4.65351600	2.30683300
H	3.09859600	6.53592700	0.68050600
C	4.02620300	1.47606700	-1.00755800

H	4.93999300	1.11918000	-0.52506300
H	4.21519100	1.48184900	-2.09285500
N	2.92496800	0.58966600	-0.64200800
H	4.25372400	-2.48100500	-1.02996400
H	2.03354900	0.91825900	-1.00930700
C	-6.32827900	-0.34067100	3.58180000
C	-5.41715100	0.66020100	3.24570800
C	-4.12262100	0.34321900	2.81180200
C	-3.76433600	-1.00751600	2.70985100
C	-4.67773700	-2.01212500	3.04009600
C	-5.96125400	-1.68405600	3.47937700
H	-7.32670200	-0.07194400	3.91572700
H	-5.71418700	1.70415000	3.31810500
H	-2.77035500	-1.27398800	2.36829200
H	-4.37895700	-3.05338500	2.95569600
H	-6.66954500	-2.46609700	3.73815800
C	-3.14251500	1.45785500	2.49138300
H	-2.61255100	1.74131900	3.41222500
H	-3.72156500	2.34967600	2.19657700
N	-2.12645900	1.06776800	1.50690500
H	-2.58746300	0.79721000	0.63966200
H	-1.54614800	1.87909000	1.26614000
C	-4.28239000	4.50375600	-1.08934900
C	-3.04586000	4.20464900	-0.51372500
C	-1.97422100	5.09834700	-0.62194400
C	-2.16976100	6.29508200	-1.32457600
C	-3.40570300	6.60023400	-1.89281900
C	-4.46895000	5.70264300	-1.77752900
H	-5.10169200	3.79566300	-0.99995800
H	-2.90183900	3.27020700	0.01666300
H	-1.34239200	6.99367700	-1.42868800
H	-3.53590800	7.53336100	-2.43391700
H	-5.43116100	5.93356300	-2.22548100
C	-0.62652300	4.82337500	0.01917700
H	-0.59340200	5.31726900	1.00079700
H	0.15276400	5.31101400	-0.58797200
N	-0.36782100	3.39467300	0.24376400
H	-0.33850900	2.89708600	-0.64702400
H	0.56183300	3.29484700	0.64691900

TS3F

C	4.70359400	4.45998900	-1.12451000
C	3.36469300	4.52346400	-1.51102500
C	2.33864700	4.23219100	-0.60213000
C	2.68432500	3.86883900	0.70544100
C	4.02468500	3.80429000	1.09433400
C	5.03917700	4.10017900	0.18229800
H	5.48441800	4.68629400	-1.84498800
H	3.11084200	4.80121500	-2.53112700
H	1.90562300	3.63862300	1.42681100
H	4.27431200	3.53016800	2.11575600
H	6.08067600	4.05124200	0.48598200
C	0.88959700	4.37799200	-1.04897900
H	0.78586200	4.09748100	-2.09903900
H	0.59136000	5.43131500	-0.95520000
N	-0.04581000	3.58036700	-0.27818400
H	-0.19687300	3.80288900	0.71538000
C	-0.70549200	2.49007100	-0.69510800
S	-0.59592100	1.93573900	-2.30988500
C	-1.47018700	1.73018000	0.35275100
C	-1.50428900	2.26047900	1.74059700
O	-0.78219600	3.18243200	2.16766100
C	-2.35737400	1.54192200	2.77592400
H	-2.62197200	0.52448200	2.48347300
H	-1.81614200	1.54677800	3.72543700
H	-3.28994000	2.09596200	2.91937200
H	-0.40585000	0.85166500	0.71265500
C	-2.77612900	1.06563800	-0.08469100
C	-3.99513600	1.90294600	0.16624900
C	-5.11798400	1.43439200	0.87512600
C	-4.02549900	3.23816000	-0.28125100
C	-6.22672600	2.25085500	1.10396400
H	-5.11650300	0.42024200	1.26387900
C	-5.12990500	4.05605100	-0.04951600
H	-3.17788000	3.63030100	-0.83394700
C	-6.23917200	3.56747600	0.64374400
H	-7.07666500	1.85711400	1.65486800
H	-5.12544800	5.07837100	-0.41769000

H	-7.09885900	4.20567700	0.82613200
C	-2.86356500	-0.13544000	-0.72719700
C	-4.18056800	-0.71205400	-1.20999700
H	-4.11610400	-0.88756000	-2.29096300
C	-4.63676600	-2.00192100	-0.53757700
C	-4.20749400	-2.36828300	0.74449100
C	-5.55083000	-2.83850200	-1.19515500
C	-4.68185800	-3.53205600	1.35398700
H	-3.48799400	-1.74071600	1.26107200
C	-6.02874400	-3.99944400	-0.58873800
H	-5.89274300	-2.57266400	-2.19283700
C	-5.59543900	-4.35143700	0.69127300
H	-4.33428700	-3.79813300	2.34852100
H	-6.73711100	-4.63125700	-1.11726700
H	-5.96348900	-5.25712600	1.16433500
C	1.54253400	-3.37047200	-3.35777100
C	0.39361300	-2.57541700	-3.28834300
C	-0.48843200	-2.68428600	-2.20730000
C	-0.19864400	-3.61060000	-1.19464800
C	0.94924000	-4.39942700	-1.25560800
C	1.82558500	-4.28046200	-2.33857900
H	2.20969200	-3.28112800	-4.21075200
H	0.17579700	-1.86754200	-4.08399200
H	-0.88998700	-3.71724200	-0.36312900
H	1.15739100	-5.11295100	-0.46366900
H	2.71628700	-4.89960900	-2.39010700
C	-1.75049000	-1.84923300	-2.14449900
H	-2.60160900	-2.52325400	-2.01945300
H	-1.88267000	-1.32425900	-3.10287800
N	-1.72174200	-0.91346700	-1.00956300
H	-4.96205000	0.03929000	-1.08706800
H	-0.92548700	-0.29153400	-1.13256200
C	3.48669600	-3.02775400	2.58704900
C	2.44988100	-2.42253500	1.87868300
C	1.38619300	-1.80959500	2.55675200
C	1.38432700	-1.82024900	3.95706700
C	2.41916900	-2.43008700	4.66866600
C	3.47319500	-3.03460900	3.98402900
H	4.30737300	-3.48755400	2.04547300

H	2.46948900	-2.42117100	0.79285200
H	0.56359800	-1.35110800	4.49470600
H	2.40036600	-2.43191800	5.75471700
H	4.28036000	-3.50882200	4.53487000
C	0.26277200	-1.13855300	1.79643400
H	-0.55018200	-0.88890000	2.48494500
H	-0.15640700	-1.79272000	1.02878200
N	0.66362400	0.11272500	1.10185900
H	1.18533100	0.71248100	1.74189800
H	1.28991000	-0.06408200	0.28385000
C	5.97294400	-2.51691200	-0.98562400
C	5.01454700	-1.70206800	-1.58894800
C	4.63191600	-0.48684800	-1.00431100
C	5.23598200	-0.10402600	0.19921900
C	6.20012000	-0.91224800	0.80337700
C	6.57116000	-2.12142300	0.21291200
H	6.26240600	-3.45249800	-1.45601700
H	4.56172100	-2.00891800	-2.52895900
H	4.95380400	0.84036100	0.65666300
H	6.66371400	-0.59659900	1.73367400
H	7.32727000	-2.74749000	0.67815300
C	3.58593700	0.38506800	-1.66560200
H	3.80299300	0.44450800	-2.74386600
H	3.65146300	1.40392700	-1.27419200
N	2.21315900	-0.10583200	-1.41062300
H	1.54842300	0.51438300	-1.88297200
H	2.09462200	-1.02131800	-1.84271400

Int4F

C	4.74871200	4.14955000	-1.12491400
C	3.40796500	4.08148100	-1.50971600
C	2.38844200	3.92588300	-0.56083700
C	2.74892100	3.84809000	0.79378400
C	4.08989800	3.90952100	1.18131100
C	5.09574200	4.05869800	0.22388800
H	5.52043000	4.26978800	-1.87983600
H	3.14641200	4.15264000	-2.56255600
H	1.98408900	3.74945200	1.55945800
H	4.34762800	3.85664600	2.23571900

H	6.13707400	4.11213400	0.52732300
C	0.94060400	3.90115900	-1.02323600
H	0.86943500	3.54383600	-2.05308300
H	0.55072000	4.93229600	-1.02461600
N	0.08483800	3.05752800	-0.21250500
H	0.10928500	3.15006800	0.80268600
C	-0.90960200	2.24334300	-0.65802500
S	-1.11082900	1.94546500	-2.33765500
C	-1.75990600	1.64336500	0.36538100
C	-1.37508900	1.59893000	1.71728300
O	-0.22333000	1.99049900	2.17535100
C	-2.31663200	1.00751600	2.75475800
H	-2.45843700	-0.06617400	2.58531700
H	-1.88119800	1.15745300	3.74472800
H	-3.30566100	1.47273900	2.71696800
H	0.97143500	1.20529600	1.52569000
C	-3.12780200	1.13546900	-0.01664100
C	-4.25573800	2.09718900	0.15239200
C	-5.42814100	1.76623300	0.85903000
C	-4.15393600	3.40735100	-0.35512500
C	-6.46225000	2.68954600	1.02641000
H	-5.52575000	0.77496200	1.29192000
C	-5.18358200	4.32951200	-0.18583900
H	-3.26382400	3.68858600	-0.90761600
C	-6.34623300	3.97712800	0.50493700
H	-7.35343300	2.40157600	1.57788100
H	-5.08043300	5.32887800	-0.60052300
H	-7.14694500	4.69902600	0.63845100
C	-3.29665800	-0.13541000	-0.47364400
C	-4.59003500	-0.67561300	-1.04286700
H	-4.43360100	-0.90066000	-2.10651900
C	-5.16185800	-1.91350700	-0.36670200
C	-4.98655800	-2.15711500	1.00225200
C	-5.92759900	-2.82385500	-1.10861700
C	-5.56767700	-3.27015200	1.61175800
H	-4.38234000	-1.47222000	1.58900600
C	-6.51059900	-3.93736100	-0.50305600
H	-6.07206500	-2.65351200	-2.17319500
C	-6.33305500	-4.16466700	0.86250000

H	-5.41919500	-3.43964500	2.67482800
H	-7.10107700	-4.62801200	-1.09879000
H	-6.78343300	-5.03188600	1.33675400
C	1.04111500	-4.22195800	-2.06105800
C	0.00386000	-3.31783900	-2.30610600
C	-0.85081300	-2.90783400	-1.27383100
C	-0.63952400	-3.42021800	0.01487200
C	0.40042500	-4.31792100	0.26273000
C	1.24505000	-4.72277400	-0.77425400
H	1.68523900	-4.53804500	-2.87697600
H	-0.15271600	-2.93286300	-3.31102200
H	-1.30741400	-3.11115200	0.81277800
H	0.54594800	-4.71072300	1.26524700
H	2.04959000	-5.42646100	-0.58186800
C	-2.00684100	-1.96951600	-1.56180100
H	-2.91446000	-2.57126800	-1.68750900
H	-1.82779900	-1.45057400	-2.51691000
N	-2.21860100	-1.03833600	-0.45632200
H	-5.33667500	0.12148900	-1.02439600
H	-1.36711800	-0.53154700	-0.23381200
C	4.84415100	-2.75167300	2.01859300
C	3.61590900	-2.18241700	1.68422200
C	2.98728300	-1.28905400	2.56176800
C	3.60868600	-0.98007400	3.77921300
C	4.83676000	-1.55066900	4.11490800
C	5.45618500	-2.43785100	3.23371000
H	5.32237700	-3.43775300	1.32699500
H	3.14366800	-2.43598500	0.73946500
H	3.12214600	-0.29764000	4.47204400
H	5.30425700	-1.30769000	5.06446300
H	6.41039100	-2.88616700	3.49445600
C	1.66421800	-0.65560200	2.20942400
H	1.14356000	-0.30872200	3.10470900
H	1.01086300	-1.36136100	1.68978200
N	1.79763000	0.54202400	1.30974000
H	2.65659300	1.05728700	1.50911900
H	1.80275100	0.27583800	0.26736500
C	5.38098700	-2.55433800	-2.16394200
C	4.21215300	-1.85182100	-2.45885700

C	4.03008800	-0.53726900	-2.00725600
C	5.04917500	0.05974100	-1.25399400
C	6.22166100	-0.63826200	-0.96058000
C	6.39129800	-1.94675800	-1.41530300
H	5.50921000	-3.56919400	-2.52980200
H	3.43550900	-2.32497300	-3.05476000
H	4.93033400	1.08404500	-0.90977900
H	7.00528100	-0.15751300	-0.38213000
H	7.30776800	-2.48689700	-1.19574000
C	2.76117500	0.21739000	-2.33926300
H	2.48700200	0.02504900	-3.38608300
H	2.93658300	1.29252400	-2.24692000
N	1.64042100	-0.12533100	-1.42652300
H	0.81307100	0.40161900	-1.74024200
H	1.40276100	-1.11063100	-1.54748000

Int5F

C	3.18165000	6.25155700	0.28040300
C	2.76854400	5.03146600	-0.25826100
C	1.41415100	4.77912600	-0.50198600
C	0.47587800	5.77415500	-0.19083600
C	0.88507300	6.99022800	0.35369300
C	2.24037800	7.23302200	0.58970300
H	4.23731200	6.43159700	0.46173200
H	3.50561200	4.26806700	-0.49476800
H	-0.57891600	5.59141700	-0.37787900
H	0.14671200	7.75089800	0.59009400
H	2.55904000	8.18153300	1.01183000
C	0.97276800	3.46801900	-1.11524300
H	1.83772600	2.80813900	-1.26739300
H	0.52646300	3.61708800	-2.10463600
N	-0.02145100	2.80613500	-0.27769000
H	-0.02700700	3.04722400	0.70753700
C	-0.82477900	1.79538800	-0.66623100
S	-0.80453000	1.23453700	-2.26624900
C	-1.75034000	1.25756300	0.37179900
C	-1.44389600	1.27106700	1.70751100
O	-0.25204600	1.65919100	2.22412700
C	-2.40013100	0.86919200	2.79567400

H	-2.06346400	-0.06521400	3.26119700
H	-2.37514300	1.63593500	3.57736800
H	-3.42187200	0.74782000	2.44198000
H	0.56306500	1.23123700	1.75534000
C	-3.08733800	0.72638200	-0.08144200
C	-4.22425500	1.68581000	-0.04465300
C	-5.47227800	1.35195500	0.51753400
C	-4.06574200	2.99854200	-0.53136100
C	-6.52033700	2.27242100	0.55925400
H	-5.61829900	0.36222700	0.94023700
C	-5.10938900	3.91941700	-0.48406700
H	-3.11627200	3.28995700	-0.96829600
C	-6.34624300	3.56195000	0.05817000
H	-7.47044600	1.98140800	0.99910200
H	-4.95838500	4.92071000	-0.87865300
H	-7.15911600	4.28129400	0.09537300
C	-3.19254700	-0.56728600	-0.50140300
C	-4.42058600	-1.13978500	-1.17482000
H	-4.14727500	-1.42347500	-2.19996500
C	-5.06826500	-2.33901300	-0.49702200
C	-4.97760700	-2.55215300	0.88487700
C	-5.82294600	-3.24158900	-1.25983000
C	-5.62971700	-3.63015900	1.48658200
H	-4.37930700	-1.87705100	1.48869300
C	-6.47706200	-4.31847100	-0.66182000
H	-5.90132300	-3.09458600	-2.33471400
C	-6.38329100	-4.51659100	0.71684700
H	-5.54521400	-3.77815600	2.55971200
H	-7.05691200	-5.00425400	-1.27325200
H	-6.88879900	-5.35615900	1.18507700
C	1.49516200	-4.36936300	-1.51650500
C	0.41314400	-3.56375800	-1.88208800
C	-0.61284600	-3.28296900	-0.97127000
C	-0.53165800	-3.82238000	0.32062200
C	0.54945200	-4.62357600	0.68978300
C	1.56672200	-4.90072700	-0.22759600
H	2.27948500	-4.58091100	-2.23778400
H	0.36017500	-3.15231000	-2.88709400
H	-1.32562600	-3.60772600	1.02931900

H	0.59547900	-5.03848300	1.69276100
H	2.40467300	-5.52964100	0.05865800
C	-1.79957500	-2.43626500	-1.38558500
H	-2.66825300	-3.08838300	-1.53321700
H	-1.58271300	-1.95137600	-2.34961100
N	-2.12466200	-1.45757100	-0.34669100
H	-5.16123400	-0.34460100	-1.28438800
H	-1.29259400	-0.96991300	-0.03362500
C	5.11576200	-2.82976300	2.34300600
C	3.85201900	-2.33519000	2.01652100
C	3.27799600	-1.29554800	2.75986100
C	3.99661700	-0.76666600	3.84144700
C	5.26135900	-1.25608200	4.16840300
C	5.82444000	-2.29024600	3.41833200
H	5.54500300	-3.63873200	1.75910100
H	3.30231700	-2.76267000	1.18233000
H	3.55590800	0.02954500	4.43758800
H	5.80233300	-0.83761200	5.01228900
H	6.80569900	-2.67860100	3.67527400
C	1.92079400	-0.72773200	2.39779000
H	1.40053200	-0.40754800	3.30720700
H	1.30132600	-1.49731600	1.92672600
N	1.95189600	0.43530100	1.47422300
H	2.69049500	1.07399300	1.76764900
H	2.18196600	0.14024300	0.51160400
C	6.71991500	-1.49938000	-3.25179700
C	5.42753000	-1.00005300	-3.42025200
C	4.66938000	-0.57782500	-2.32103400
C	5.23220600	-0.67949900	-1.04233900
C	6.52094200	-1.18449200	-0.86924200
C	7.27137100	-1.59320200	-1.97355400
H	7.29140900	-1.82112100	-4.11792100
H	5.00071100	-0.93680100	-4.41857800
H	4.65114600	-0.37184100	-0.17993600
H	6.93466600	-1.26159800	0.13213600
H	8.27521100	-1.98570300	-1.83847800
C	3.28689100	0.00761900	-2.53190500
H	2.94874600	-0.24831700	-3.54810700
H	3.35071900	1.10423100	-2.50678500

N	2.32209600	-0.39275400	-1.49314300
H	1.41605200	0.02330700	-1.72452700
H	2.18598800	-1.40237800	-1.53222100

TS5F

C	-7.22765800	-2.98565900	-3.04738400
C	-6.60764200	-2.87549600	-1.80023600
C	-6.13449200	-1.64199200	-1.33954500
C	-6.29362000	-0.51526000	-2.16062800
C	-6.90902000	-0.62104900	-3.40650700
C	-7.37858600	-1.85888100	-3.85461700
H	-7.58975900	-3.95203100	-3.38693300
H	-6.49116700	-3.75672200	-1.17427200
H	-5.93317700	0.44829700	-1.81102600
H	-7.02837600	0.26243300	-4.02769400
H	-7.85990700	-1.94166200	-4.82486300
C	-5.47170200	-1.52101200	0.01649000
H	-5.52891800	-2.47831200	0.55391500
H	-5.98933000	-0.79384500	0.64993200
N	-4.09086700	-1.07455300	-0.12216200
H	-3.58717800	-1.50617000	-0.88494200
C	-3.30927500	-0.64052800	0.93460400
S	-3.97351700	-0.52581800	2.49623800
C	-1.95887900	-0.30484800	0.60527400
C	-1.55324400	0.35378000	-0.64619800
O	-0.56106700	-0.19887800	-1.40264200
C	-2.53000100	1.06131200	-1.56053700
H	-1.98688000	1.73562000	-2.22550800
H	-3.03869800	0.32453400	-2.18445500
H	-3.28878100	1.60982000	-1.00299200
H	-0.06713700	-0.94552700	-0.92266000
C	-0.91044800	-0.12861000	1.59739800
C	-0.67811400	-1.10269100	2.69535000
C	-0.25291200	-0.72171000	3.97808400
C	-0.85083200	-2.47475200	2.43902600
C	0.01261400	-1.67602700	4.95987600
H	-0.16115600	0.33032300	4.22226400
C	-0.58508000	-3.42914500	3.41837400
H	-1.21528200	-2.77497800	1.46245600

C	-0.14594900	-3.03417200	4.68440200
H	0.33066800	-1.35423400	5.94746500
H	-0.73730700	-4.48243800	3.19866900
H	0.05400400	-3.77619400	5.45193300
C	-0.08529200	0.93610400	1.34593200
C	1.28543000	1.24228100	1.88608100
H	2.01898300	1.19209700	1.06294700
C	1.50702400	2.56708300	2.61282900
C	0.60430900	3.04116200	3.57655300
C	2.66528600	3.31473400	2.36495400
C	0.85739100	4.22321600	4.27321700
H	-0.31164200	2.48882800	3.76664800
C	2.92137300	4.49909300	3.05946300
H	3.38107500	2.95935900	1.62674100
C	2.01765400	4.95716100	4.01780000
H	0.14449900	4.57212400	5.01484100
H	3.82630700	5.06236900	2.84958900
H	2.21264100	5.87844300	4.55859500
C	0.43760400	5.50706600	-1.89771300
C	0.26266100	4.55373200	-0.89549900
C	-1.01344200	4.04943100	-0.59992300
C	-2.11113600	4.54073500	-1.31612100
C	-1.93961900	5.50150300	-2.31427100
C	-0.66435400	5.98191500	-2.61216400
H	1.43138400	5.88960300	-2.11161000
H	1.12038200	4.21613400	-0.31773500
H	-3.10705000	4.17226000	-1.08790800
H	-2.80302000	5.87318300	-2.85816100
H	-0.53001200	6.72796700	-3.38975100
C	-1.17880100	3.02511700	0.49997300
H	-2.23140100	2.82054600	0.71407400
H	-0.72827900	3.39719800	1.42245900
N	-0.54390200	1.70308300	0.17820400
H	1.55547500	0.42685400	2.56675600
H	0.19437000	1.82390500	-0.51639300
C	4.68331000	-4.99077800	-0.93948400
C	3.47703300	-4.38655300	-1.29862000
C	2.47504200	-4.16282100	-0.34558300
C	2.70644700	-4.56099200	0.97868500

C	3.91096700	-5.16362400	1.34123500
C	4.90311400	-5.38019100	0.38258600
H	5.44699100	-5.16261100	-1.69280100
H	3.30946700	-4.08806000	-2.33082600
H	1.93715900	-4.39525600	1.72985500
H	4.07339900	-5.46909100	2.37091400
H	5.83927500	-5.85368900	0.66366100
C	1.18521700	-3.45807300	-0.72036200
H	0.34513200	-3.89973600	-0.17512200
H	0.98102300	-3.58992000	-1.78794400
N	1.18787600	-2.00588000	-0.44460200
H	1.38104800	-1.84968300	0.54299300
H	1.92931900	-1.55116200	-0.98968600
C	7.01892400	0.90015200	-3.56666300
C	5.67120100	1.25626700	-3.49739200
C	4.76258100	0.49016300	-2.75761600
C	5.23057300	-0.65237500	-2.09483100
C	6.57587700	-1.01334300	-2.16684600
C	7.47567200	-0.23754300	-2.90065700
H	7.70847800	1.50661700	-4.14699200
H	5.31960800	2.13909800	-4.02655600
H	4.53405200	-1.26342900	-1.53042800
H	6.91982600	-1.90373800	-1.64804300
H	8.52297400	-0.51996000	-2.95638300
C	3.30915700	0.91487000	-2.66090400
H	3.10283400	1.64669500	-3.45882500
H	3.15026900	1.44871900	-1.71258800
N	2.39283200	-0.23309200	-2.66686400
H	1.42660400	0.07876900	-2.57294300
H	2.46227800	-0.71866600	-3.55869000

Int6F

C	-5.89804300	-3.37014000	-3.52293700
C	-5.51394400	-3.17724300	-2.19351700
C	-5.47538000	-1.89473500	-1.63582100
C	-5.83195900	-0.80307600	-2.44229200
C	-6.21341400	-0.99050700	-3.76939300
C	-6.24696900	-2.27701600	-4.31493000
H	-5.92340400	-4.37398400	-3.93773500

H	-5.24358000	-4.03251300	-1.57897900
H	-5.81359200	0.19662700	-2.01638700
H	-6.49138100	-0.13464100	-4.37834700
H	-6.54650500	-2.42417900	-5.34863600
C	-5.06218600	-1.68429300	-0.19454800
H	-4.98491400	-2.65263300	0.32116800
H	-5.81234300	-1.11079800	0.35828100
N	-3.81148400	-0.94121900	-0.11653600
H	-3.09716600	-1.23441700	-0.77088400
C	-3.35518500	-0.30390800	1.02549800
S	-4.30199200	-0.29227700	2.43641700
C	-2.08227000	0.33198600	0.89445200
C	-1.52296300	0.84716300	-0.41306500
O	-0.72949500	-0.06168700	-1.12858000
C	-2.46264900	1.50155400	-1.41637400
H	-1.90275400	1.91493100	-2.25738700
H	-3.13867500	0.73800100	-1.79707200
H	-3.07552100	2.27767400	-0.95797300
H	-0.34464100	-0.76943600	-0.52304700
C	-1.10831700	0.56676000	1.90580400
C	-1.03423300	-0.12644200	3.21749300
C	-0.78993500	0.58120300	4.40248300
C	-1.13999800	-1.52530500	3.28484700
C	-0.64758500	-0.08725600	5.61933900
H	-0.74490000	1.66489500	4.36979100
C	-0.99199100	-2.19403600	4.49688800
H	-1.36134100	-2.07663000	2.37746000
C	-0.74239400	-1.47733200	5.67043100
H	-0.47058700	0.48095700	6.52814400
H	-1.08833600	-3.27586300	4.53071500
H	-0.63485900	-1.99876000	6.61718000
C	-0.09807100	1.41601600	1.49699900
C	1.34280100	1.48708400	1.90693300
H	1.97887300	0.94749400	1.17912400
C	1.96520100	2.86642500	2.10930800
C	1.41559900	3.78753200	3.01375500
C	3.12656400	3.23042100	1.41734300
C	2.00961700	5.03222400	3.21789200
H	0.51222500	3.52225200	3.55573500

C	3.72491500	4.47790400	1.61693400
H	3.57778800	2.52209000	0.72523300
C	3.16726100	5.38343800	2.51812700
H	1.57011200	5.72914900	3.92593100
H	4.62660700	4.73781100	1.06953000
H	3.62881000	6.35357000	2.67635300
C	0.86668200	5.08144500	-2.73163300
C	0.64169200	4.33750000	-1.57393300
C	-0.65726100	4.17438300	-1.06910200
C	-1.71954000	4.80040200	-1.73169500
C	-1.49474000	5.55653200	-2.88259900
C	-0.20234600	5.69142800	-3.39051700
H	1.87803000	5.19809900	-3.10968000
H	1.48760400	3.90773100	-1.04153100
H	-2.72898300	4.69802700	-1.34391400
H	-2.33029800	6.03700300	-3.38271600
H	-0.02743200	6.27610800	-4.28864600
C	-0.87621500	3.39789200	0.20964500
H	-1.91625800	3.40627300	0.53685300
H	-0.27432200	3.82750000	1.01086600
N	-0.45968000	1.93415600	0.14619300
H	1.42450500	0.92338500	2.84289600
H	0.32062200	1.84523100	-0.51160600
C	3.63303300	-5.56724400	-0.04189400
C	2.52445400	-4.81042300	-0.42458600
C	1.64438100	-4.29089200	0.53400800
C	1.89818300	-4.54987000	1.88794200
C	3.00573800	-5.30500700	2.27449000
C	3.87638500	-5.81604900	1.31001400
H	4.30104800	-5.96807500	-0.79905400
H	2.33767200	-4.62152000	-1.47910400
H	1.22308300	-4.15496000	2.64416600
H	3.18604500	-5.49918700	3.32791000
H	4.73587800	-6.40832800	1.61003500
C	0.47218300	-3.42004500	0.12369500
H	-0.37258800	-3.58790700	0.79952600
H	0.13565400	-3.69173800	-0.88224400
N	0.76785300	-1.97189400	0.11405400
H	1.10962100	-1.69147400	1.03151000

H	1.50689900	-1.77642000	-0.57099300
C	6.68067100	-0.79087700	-3.81627400
C	5.42307500	-0.18956100	-3.74515400
C	4.46181200	-0.63994900	-2.83263300
C	4.78260700	-1.71776400	-1.99646300
C	6.03669300	-2.32369600	-2.06903800
C	6.99134000	-1.86140100	-2.97733000
H	7.41292700	-0.42815400	-4.53203800
H	5.18395500	0.63834600	-4.40880500
H	4.04146800	-2.08618800	-1.29499400
H	6.26634300	-3.15927800	-1.41380000
H	7.96741700	-2.33449300	-3.03361500
C	3.11400600	0.05109400	-2.74036400
H	2.97179300	0.66677200	-3.64356100
H	3.12512500	0.75368200	-1.89412200
N	2.01797800	-0.89520300	-2.49681300
H	1.13138100	-0.40029300	-2.39900300
H	1.92423500	-1.52060000	-3.29424300

TS6F

C	-4.47187600	-2.44078800	3.30990500
C	-3.31690700	-3.02061400	2.77963900
C	-2.06110000	-2.75879600	3.34021500
C	-1.98557600	-1.90696900	4.45169100
C	-3.13583600	-1.32630200	4.98357500
C	-4.38307700	-1.59069100	4.41193700
H	-5.43783900	-2.65577900	2.86242800
H	-3.39132700	-3.68945000	1.92597000
H	-1.01780700	-1.70779100	4.90514600
H	-3.06125000	-0.67255900	5.84791800
H	-5.27981000	-1.14049500	4.82762600
C	-0.80708700	-3.36987800	2.75507900
H	-1.05721600	-4.22122600	2.10833800
H	-0.15034900	-3.76572200	3.53652400
N	-0.04780400	-2.37368500	2.00458800
H	-0.56408200	-1.59953500	1.60215800
C	1.24717100	-2.52525900	1.60723700
S	2.12588800	-3.92393100	1.92204900
C	1.78551200	-1.36253000	0.91115200

C	1.50351300	-0.03684200	1.25966000
O	0.00000900	0.74561600	0.32717200
C	1.19513800	0.47526300	2.63685500
H	0.71233100	1.44970600	2.60261200
H	0.52880200	-0.22811400	3.13407600
H	2.10915700	0.54280800	3.23828600
H	-0.32747800	0.06859900	-0.30263800
C	2.61767700	-1.36455200	-0.28349800
C	2.88693400	-2.54368200	-1.14209400
C	4.18634300	-2.90181100	-1.52585400
C	1.80655300	-3.29246300	-1.63688200
C	4.40237300	-3.98483800	-2.37903100
H	5.03262400	-2.34416600	-1.13929500
C	2.02324000	-4.36804400	-2.49346600
H	0.79660000	-3.01364400	-1.35262000
C	3.32273000	-4.72088600	-2.86525900
H	5.41684700	-4.25475000	-2.65778700
H	1.17680100	-4.93556900	-2.86938900
H	3.49097200	-5.56528500	-3.52732300
C	2.98572000	-0.09729100	-0.61620500
C	3.60444100	0.44769400	-1.86640400
H	2.94892900	1.21254500	-2.30929500
C	5.01981000	1.02238100	-1.78229100
C	5.98597700	0.48763900	-0.91925600
C	5.39071300	2.08028400	-2.62275400
C	7.28739700	0.99123500	-0.90338100
H	5.70942500	-0.31862100	-0.24595500
C	6.69134300	2.58578900	-2.60999200
H	4.65340100	2.51034500	-3.29694800
C	7.64600500	2.04130700	-1.75000500
H	8.02112500	0.56243100	-0.22667300
H	6.95661600	3.40741900	-3.26921600
H	8.65817900	2.43444600	-1.73646600
C	1.17493500	5.02080400	1.22666400
C	1.72255800	3.83620600	0.73607800
C	2.62027100	3.09167600	1.51302700
C	2.96924900	3.56776400	2.78200000
C	2.43114600	4.75915800	3.26977200
C	1.52895400	5.48700500	2.49422900

H	0.47498100	5.58203500	0.61503500
H	1.43704400	3.49182300	-0.25373900
H	3.66722900	3.00192800	3.39353800
H	2.71311300	5.11319700	4.25683000
H	1.10400100	6.41136400	2.87365900
C	3.28599400	1.84448100	0.97280500
H	3.85798700	1.32749400	1.74666300
H	3.98879800	2.11645600	0.18335200
N	2.35431100	0.83643900	0.35185500
H	3.61693000	-0.38080200	-2.58492700
H	1.45555800	1.25635500	-0.08325500
C	-6.21407700	-1.12239700	-2.26174600
C	-4.98705700	-1.06276700	-1.60306500
C	-4.00765100	-2.04465700	-1.82032400
C	-4.29199200	-3.08557800	-2.71106700
C	-5.52133200	-3.14967900	-3.37208700
C	-6.48566300	-2.16753000	-3.14938100
H	-6.96082400	-0.35441800	-2.07961500
H	-4.77943300	-0.24342900	-0.91888200
H	-3.54432300	-3.85539900	-2.88866100
H	-5.72319900	-3.96612400	-4.05990400
H	-7.44238800	-2.21465200	-3.66155000
C	-2.66513600	-1.96088600	-1.11239600
H	-2.09178900	-2.87340600	-1.31333000
H	-2.82598000	-1.92524500	-0.02827400
N	-1.83251500	-0.79704400	-1.46243800
H	-1.71711600	-0.75978500	-2.47371400
H	-2.32154500	0.06144200	-1.18663400
C	-5.63621400	5.37693500	-1.27285200
C	-4.45573900	4.91318000	-0.68723700
C	-3.92316700	3.66574200	-1.02989400
C	-4.60616800	2.88328000	-1.97210800
C	-5.78518800	3.34137100	-2.55783200
C	-6.30493900	4.59139600	-2.21085000
H	-6.03416000	6.34789700	-0.99113000
H	-3.94196700	5.52780600	0.04854200
H	-4.20987400	1.90793200	-2.23570800
H	-6.29931300	2.72226000	-3.28803300
H	-7.22438400	4.94729600	-2.66688300

C	-2.62764200	3.17793600	-0.40981500
H	-2.31329700	3.90213200	0.36108300
H	-1.83503300	3.18515700	-1.17039200
N	-2.72110500	1.79981600	0.08425000
H	-1.79248700	1.49440700	0.40570100
H	-3.35730200	1.76320800	0.87783700

Int7F

C	3.06358100	-3.34094200	-1.46304900
C	1.94521300	-2.77200100	-2.07266800
C	2.08501200	-1.66505000	-2.92344600
C	3.36578500	-1.15001200	-3.15349500
C	4.48861700	-1.72111100	-2.54623100
C	4.33875100	-2.81660500	-1.69499000
H	2.94193900	-4.20222600	-0.81225300
H	0.95693700	-3.19067800	-1.90553700
H	3.48688200	-0.29904500	-3.81993800
H	5.47628000	-1.31180500	-2.74002400
H	5.20819100	-3.26476100	-1.22307100
C	0.87261100	-1.05905100	-3.60517900
H	0.40193800	-1.79267600	-4.26719100
H	1.18465900	-0.19846200	-4.20845200
N	-0.15857400	-0.61747800	-2.67322700
H	0.07555100	0.17859600	-2.06539400
C	-1.36434500	-1.20336400	-2.51515000
S	-1.86736000	-2.59822600	-3.30292300
C	-2.25591800	-0.46409100	-1.58714900
C	-2.69723000	0.83159300	-1.80204500
O	0.70138900	1.57504700	-0.98117100
C	-2.45305700	1.76106400	-2.94881500
H	-2.03316100	2.72203500	-2.62784800
H	-1.75125800	1.30717700	-3.64908900
H	-3.37737000	1.97629000	-3.49996200
H	0.95298800	1.22476300	-0.07854100
C	-2.88838200	-0.95113400	-0.38775500
C	-2.66090400	-2.25429500	0.27039500
C	-3.72464300	-3.03073200	0.75953700
C	-1.35348300	-2.74023800	0.44898500
C	-3.48859000	-4.23866100	1.41736300

H	-4.74584100	-2.69753500	0.60312600
C	-1.11799100	-3.94947500	1.09914600
H	-0.51805700	-2.15657000	0.07602700
C	-2.18542800	-4.70373100	1.59129600
H	-4.32875200	-4.82244900	1.78299000
H	-0.09803900	-4.30216800	1.22554700
H	-2.00267500	-5.64632100	2.09899800
C	-3.68261000	0.07889300	0.09526400
C	-4.49698900	0.16177700	1.35240000
H	-4.20194400	1.04056300	1.94206300
C	-6.01328500	0.18724200	1.17121900
C	-6.63692500	-0.43266400	0.08036200
C	-6.81787500	0.81237000	2.13400600
C	-8.02807900	-0.43741100	-0.03679600
H	-6.02763400	-0.90636800	-0.68396100
C	-8.20803800	0.80944000	2.01864600
H	-6.34929400	1.30310600	2.98425400
C	-8.81899300	0.18201400	0.93147100
H	-8.49261900	-0.92440700	-0.88952100
H	-8.81309900	1.29994500	2.77603600
H	-9.90102200	0.18014300	0.83810800
C	-1.12167900	3.96202700	1.30877800
C	-1.99796900	3.03464200	0.73790500
C	-3.13861400	3.46608300	0.04919500
C	-3.38432800	4.84059600	-0.05496800
C	-2.51303700	5.76605200	0.51952600
C	-1.37620300	5.32973100	1.20250300
H	-0.24076500	3.61070600	1.83867600
H	-1.79515100	1.97144100	0.82468900
H	-4.26284800	5.19005400	-0.59251200
H	-2.71818600	6.82858300	0.42680400
H	-0.69461400	6.04966000	1.64531500
C	-4.12389800	2.47781700	-0.56434200
H	-4.48744300	2.86987500	-1.51968000
H	-5.00500200	2.37598800	0.07552200
N	-3.57373400	1.15013800	-0.78175300
H	-4.22931400	-0.70657300	1.96484200
H	0.05124800	2.26935300	-0.81123800
C	5.22575900	-1.64343600	3.29486900

C	4.26204800	-1.31987900	2.33992400
C	2.91804800	-1.15382500	2.70522200
C	2.56328800	-1.32777800	4.04875700
C	3.52516600	-1.65153000	5.00766000
C	4.85987900	-1.80865100	4.63294600
H	6.26113100	-1.77454500	2.99288600
H	4.55124100	-1.19884800	1.29898300
H	1.52260800	-1.21667900	4.34545900
H	3.23081600	-1.78651200	6.04463100
H	5.60918800	-2.06448500	5.37641800
C	1.88260300	-0.75260400	1.67202700
H	0.88533000	-1.06021300	2.00348600
H	2.07793800	-1.26896900	0.72643800
N	1.84413400	0.69692300	1.37502900
H	1.72542500	1.21490800	2.24413600
H	2.74213400	0.99342200	0.97098600
C	8.61516800	2.06458200	-0.83517600
C	7.35079100	2.41748900	-1.31178200
C	6.20679200	2.22017700	-0.53035900
C	6.35459500	1.65037000	0.74195000
C	7.61499900	1.29348400	1.21940900
C	8.75101700	1.50055600	0.43316300
H	9.49087500	2.22461800	-1.45788700
H	7.25105400	2.85024000	-2.30460400
H	5.47306800	1.47838300	1.35065000
H	7.70966000	0.85376600	2.20854800
H	9.73262800	1.22171900	0.80539800
C	4.84068200	2.63571200	-1.04343700
H	4.92888500	2.88132900	-2.11478800
H	4.53401500	3.56530800	-0.54437800
N	3.81264000	1.62806900	-0.75648900
H	2.89585800	1.93660700	-1.08366100
H	4.01953300	0.76876500	-1.26283600