

Electronic Supplementary Information

Mechanistic Investigation on $N \rightarrow C^{\alpha} \rightarrow O$ Relay via Non-Brook Rearrangement: Reaction Conditions Promote Synthesis of Furo[3,2- c]pyridinones

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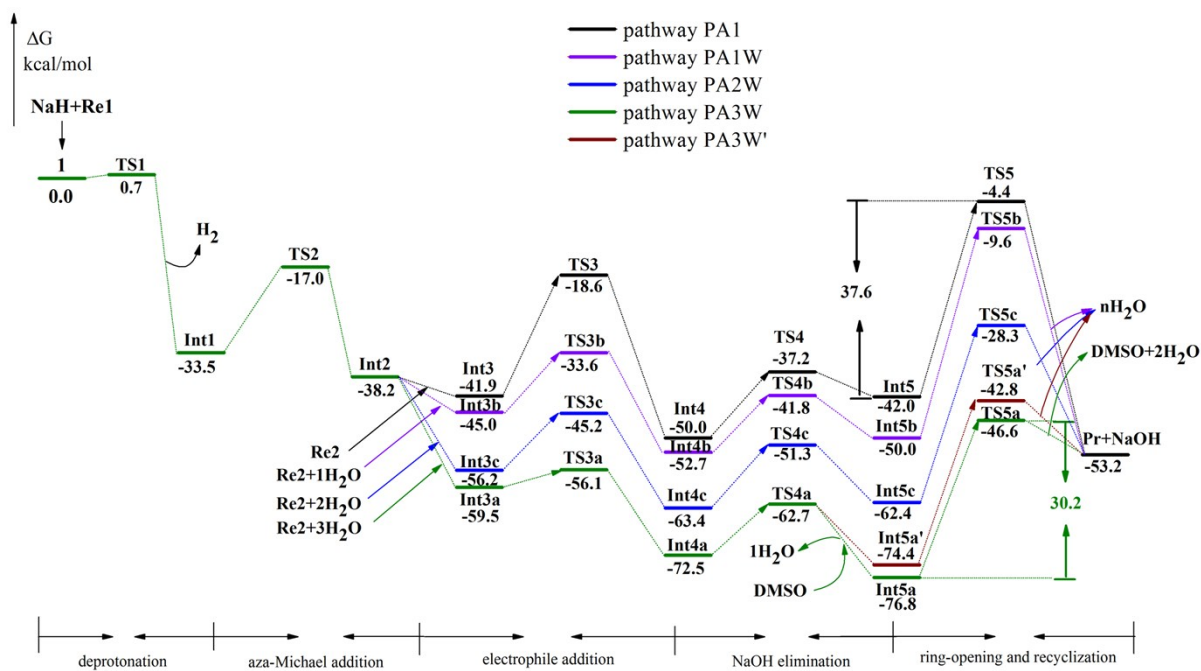


Fig. S1 DFT computed energy surfaces for Na⁺-assisted pathway PA1 (black line), H₂O-Na⁺ co-assisted PA1W (purple line), 2H₂O-Na⁺ co-assisted PA2W (blue line), 3H₂O-Na⁺ (red line) co-assisted PA3W', and 2H₂O-DMSO-Na⁺ (green line) co-assisted PA3W in the solvent phase, and free energies are given in kcal/mol.

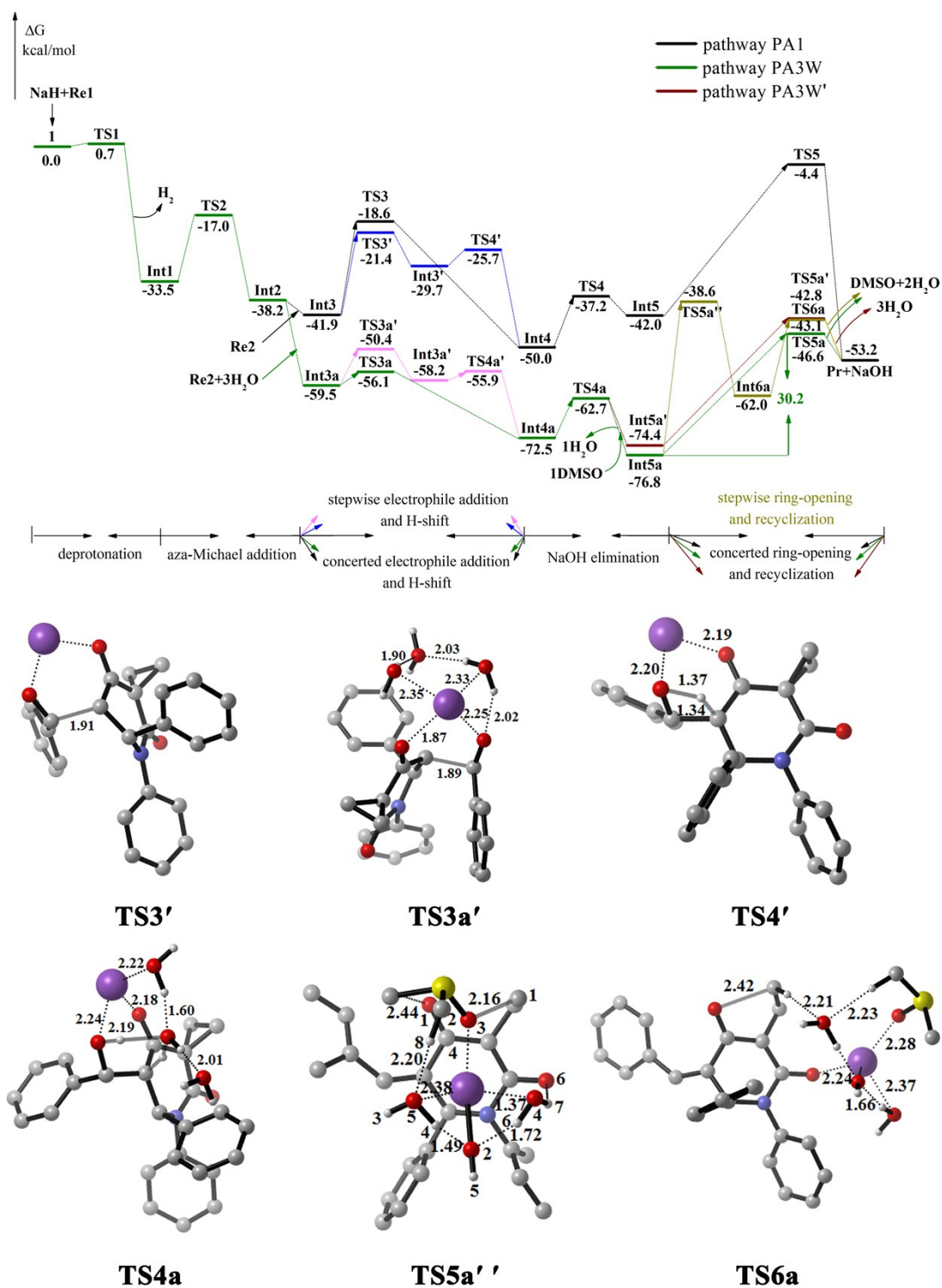


Fig. S2 DFT computed energy surfaces for the Na⁺-assisted pathway PA1 (black line), 2H₂O-DMSO-Na⁺ co-assisted PA3W (olive line), and 3H₂O-Na⁺ co-assisted PA3W' (wine line) in the solvent phase, and free energies are given in kcal/mol. And optimized geometry structures of stepwise transition states for Na⁺-assisted, 2H₂O-DMSO-Na⁺, and 3H₂O-Na⁺ co-assisted pathways PA1 and PA3W in the DMSO phase, respectively. Distances are in angstrom. N: blue, C: gray, O: red, H: white, Na: purple.

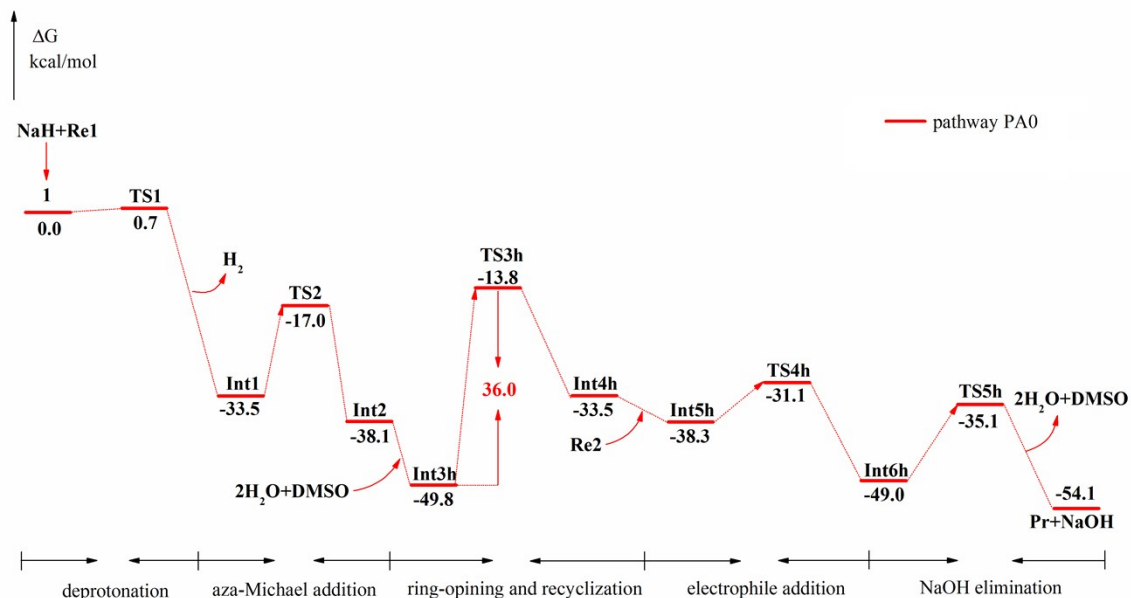


Fig. S3 DFT computed energy surfaces for the Na⁺-DMSO-2H₂O co-assisted path PA0 (red line). Activation free energies are given in kcal/mol.

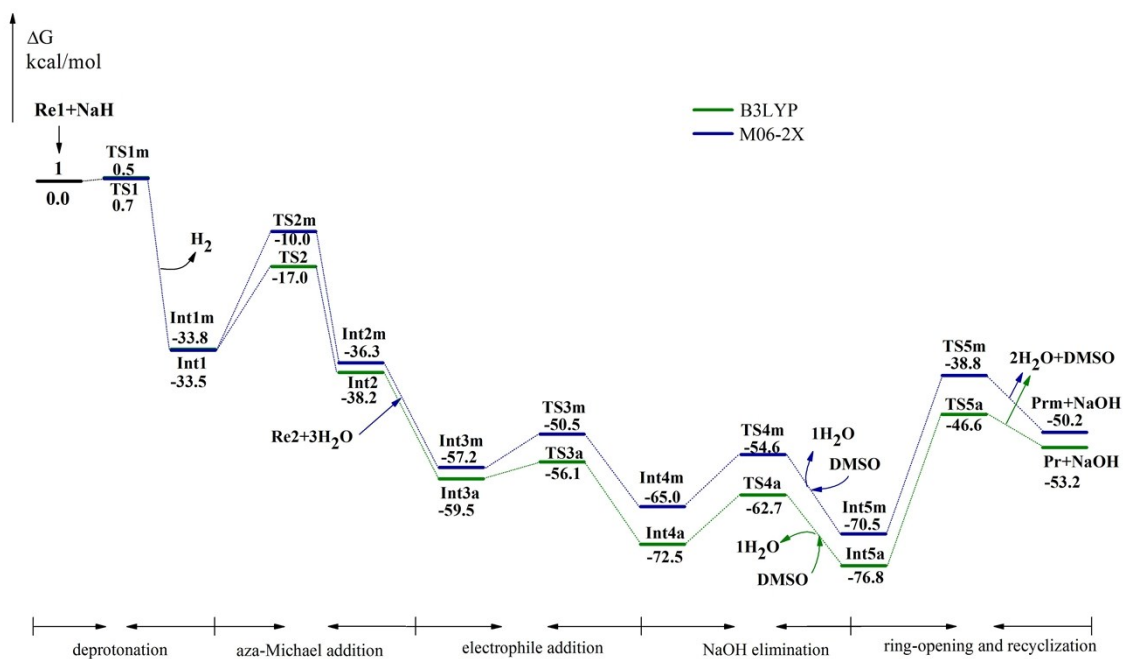


Fig. S4 The comparison of free energy profiles in 2H₂O-DMSO-assisted path PA3W at M06-2X/6-311+G(d,p) (blue line) and B3LYP-D3/6-311+G(d,p) (green line). Activation free energies are given in kcal/mol.

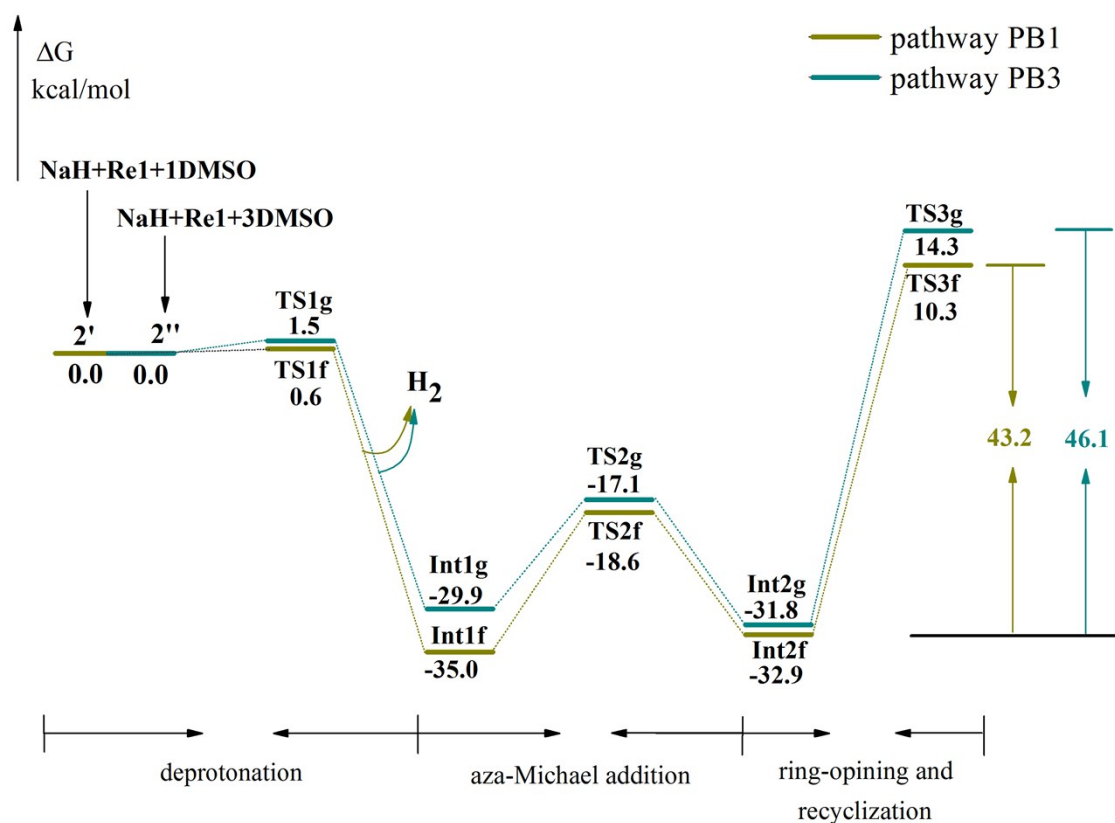


Fig. S5 DFT computed energy surfaces for the Na^+ -DMSO co-assisted path PB1 (dark yellow) and Na^+ -3DMSO co-assisted path PB3 (dark cyan). Activation free energies are given in kcal/mol.

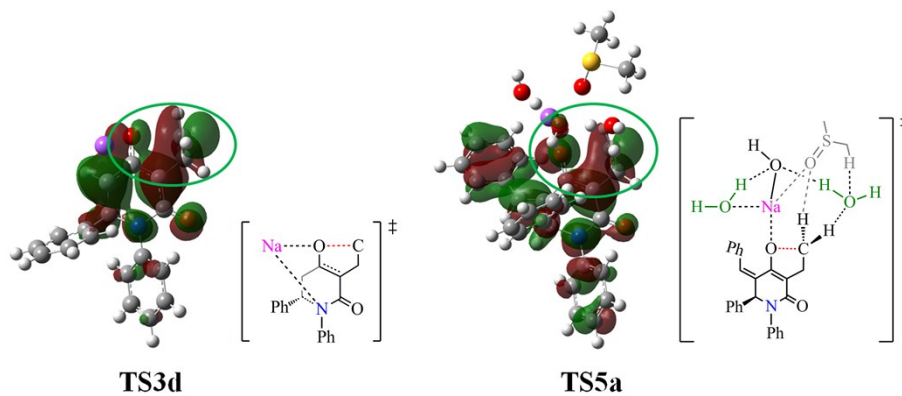


Fig. S6 Secondary orbital interactions in HOMOs of **TS3d** and **TS5a** for the concerted ring-opening and recyclization transition state (green ellipse) process.

As illustrated in **Fig. S6**, the electron delocalization of the reaction sites and the whole molecular fragments in HOMO of **TS5a** are higher than that in **TS3d**. Therefore, the cooperation of electrostatic and HBs interactions effectively stabilize the structure of **TS5a** and reduce the energy barrier of the rate-determining step.

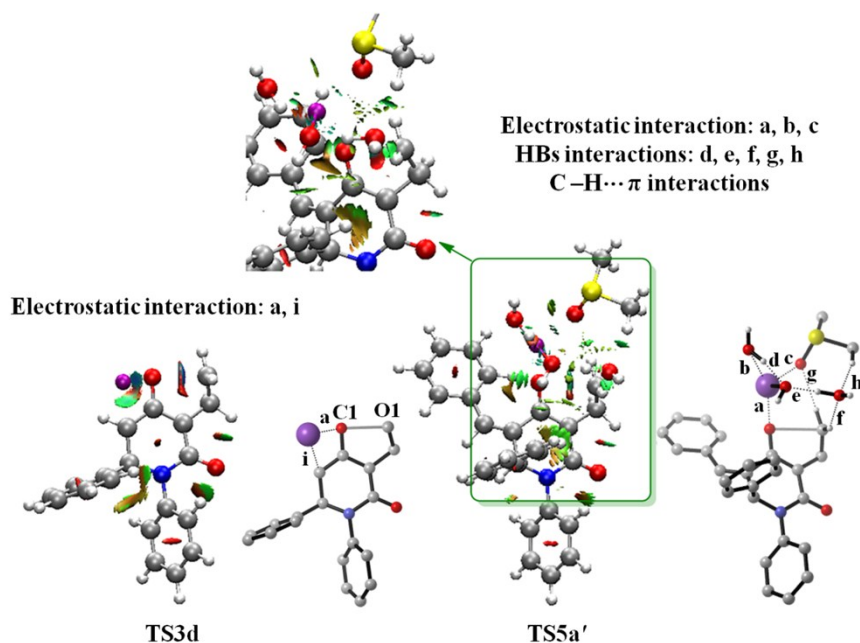


Fig. S7 Non-covalent interactions analysis (blue, strong interaction; green, weak interaction; and red, strong repulsion) for concerted ring-opening and recyclization transition states **TS3d** and **TS5a** under Na^+ -assisted and $2\text{H}_2\text{O}$ -DMSO- Na^+ co-assisted conditions.

To unravel the non-covalent interactions of transition states **TS5a** and **TS3d**, we employed the Multiwfn^{17, 26} and VMD¹⁸ to conduct electron densities and reduced density gradient RDG²⁷ isosurface for the rate-determining step structures. As shown in Fig. S7, it is clear that both TSs have strong interactions between the reaction sites C1 and O1 represented by the deep blue color. Moreover, in **TS5a**, triple electrostatic interactions (a, b, and c) and five HBs interactions (d, e, g, h, and f) shown in green color further stabilize the **TS5a** structure as compared to $\text{Na}^+\cdots\text{O}$ electrostatic interaction in transition state **TS3d**.

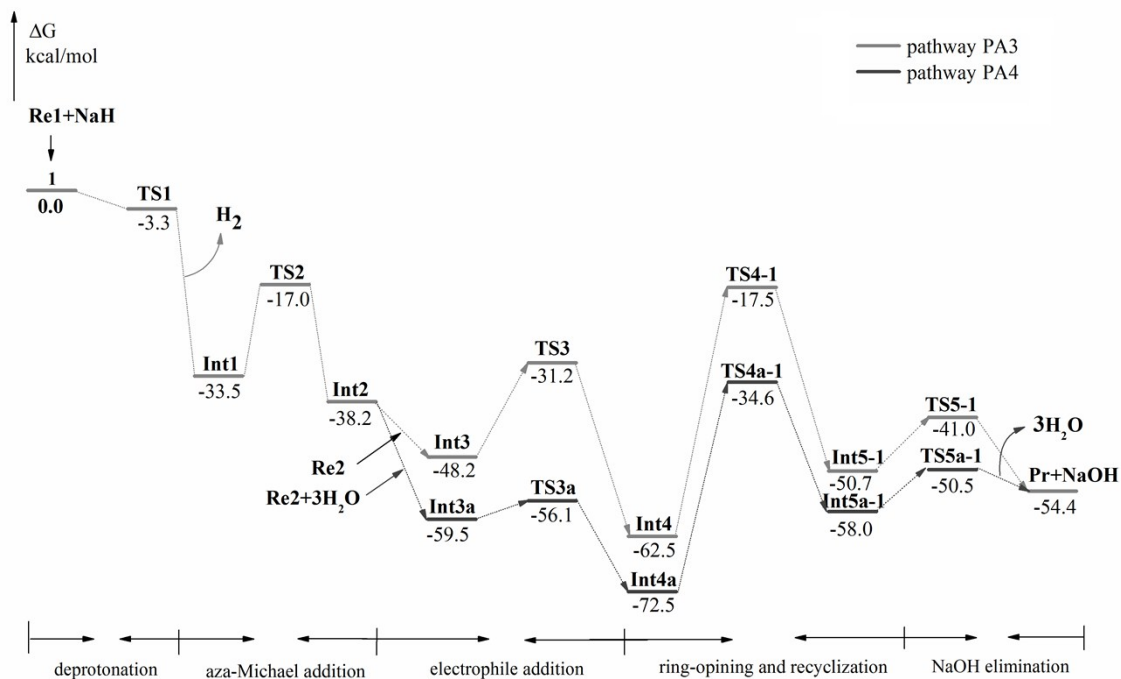


Fig. S8 DFT computed energy surfaces for the Na^+ -assisted pathway PA3 (gray line) and $3\text{H}_2\text{O}$ - Na^+ co-assisted path PA4 (dark gray line). Activation free energies are given in kcal/mol.

Additionally, we also investigated the effect of the sequence of NaOH elimination and concerted ring-opening and recyclization processes on the energy profile (Figure S4). The computational results indicated that the high activation energy barriers of **TS4'** (45.01/-17.50 kcal/mol) and **TS4b'** (41.38/-22.06 kcal/mol) are kinetically inaccessible and can be excluded.

Table S1. Selected donor-acceptor bond orbital interaction and second-order perturbation stabilization energies (E(2), kcal/mol) for transition state **TS5a''**

TSs	donor	acceptor	interaction	E(2)
TS5a	LP O1	LP* Na	n→n*	15.4
	BD C4–O1	LP* Na	π→n*	3.33
	LP O3	LP* Na	n→n*	17.5
	LP O5	LP* Na	n→n*	13.16
	BD O5–H4	LP* O2	σ→n*	60.46
	BD O4–H6	LP* O2	σ→n*	86.01
	LP O3	BD* C1–H1	n→σ*	3.31
	LP O4	BD* C1–H2	n→σ*	4.94
	LP O4	BD* C2–H8	n→σ*	7.76
	TS5a''	LP O4	LP* Na	n→n*
LP O3		LP* Na	n→n*	15.5
LP O5		LP* Na	n→n*	10.16
BD O5–H4		LP* O2	σ→n*	51.24
BD O4–H6		LP* O2	σ→n*	22.45
LP O5		BD* C2–H8	n→σ*	5.38
BD O4–H7		LP* O6	σ→n*	42.31

Table S2. DFT calculated free energy profiles of solvation effects and gas phase of TSs and intermediates in path PA3W

TSs	gas phase	solvation effects	$\Delta G/\text{kcal/mol}$
1	0	0	0
TS1	2.5	0.7	1.8
Int1	-33.1	-33.5	2.4
TS2	1.8	-17.0	18.8
Int2	-19.7	-38.2	18.5
Int3a	-50.4	-59.5	9.1
TS3a	-39.7	-56.1	16.4
Int4a	-48.9	-72.5	23.6
TS4a	-28.4	-62.7	34.3
Int5a	-61.1	-76.8	15.7
TS5a	-25.7	-46.6	21.6
Pr	-34.2	-53.2	19.0

Table S3. DFT calculated $\Delta\Delta G^\ddagger$ values of solvation effects and gas phase of key TSs (**TS5**, **TS5a**, **TS3d**, **TS5e**, **TS5a'**, and **TS3e'**) and intermediates (**Int5**, **Int5a**, **Int2**, **Int5e**, **Int5a'**, **Int2e**) in the solvent phase

TSs	solvation effects	gas phase	$\Delta\Delta G^\ddagger$
TS5	37.6	42.4	4.8
TS5a	30.2	35.4	5.2
TS3d	49.2	55.7	6.5
TS5e	35.9	40.7	4.8
TS5a'	31.6	36.5	4.9
TS3e'	36.2	40.9	4.7

Table S4. DFT calculated $\Delta\Delta G^\ddagger$ values of optimization and single point calculation of key TSs (TS5, TS5a, TS3d, TS5e, TS5a', and TS3e') and intermediates (Int5, Int5a, Int2, Int5e, Int5a', Int2e) in the solvent phase

TSs Method	optimization	single point	$\Delta\Delta G^\ddagger$
TS5	36.1	37.6	1.5
TS5a	28.3	30.2	1.9
TS3d	46.7	49.2	2.5
TS5e	33.8	35.9	2.1
TS5a'	30.3	31.6	1.3
TS3e'	35.2	36.2	1.0

Table S5. NBO charges of selected atoms in key transition states in PA3W and PB0

TSs	N1	C1	O1	Na1	O2
TS1	-0.675	-0.328	-0.675	0.841
TS2	-0.646	-0.497	-0.747	0.898
TS3a/TS3d	-0.492/-0.509	-0.545/-0.531	-0.744/-0.782	0.897/0.916	-0.844/.....
TS4a/TS4d	-0.489/-0.522	-0.238/ -0.622	-0.765/-0.607	0.866/0.844	-1.100 /-0.912
TS5a/TS5d	-0.493/-0.503	-0.071/-0.269	-0.693/-0.585	0.854/0.873	-1.256 / -1.065

Table S6. Properties of electron density at bond critical points for TSs obtained from AIM analysis, all quantities are in atomic unit

Specise	Hydrogen bonds	$\rho(r)$	$\nabla^2\rho(r)$	Distance (Å)
TS3d	Na...C4–O1	0.1819	0.1006	2.476
	Na...O1	0.2862	0.1949	2.195
TS5a	Na...O1	0.2207	0.1540	2.249
	Na...O5	0.1806	0.1211	2.331
	Na...O3	0.2098	0.1346	2.311
	H4...O2-H5	0.6625	0.1545	1.565
	H6...O2-H5	0.7472	0.1546	1.508
	C1-H1...O3	0.1264	0.4150	2.307
	C1-H2...O4	0.1490	0.5034	2.237
	C2-H8...O4	0.1794	0.5789	2.164
	O2-H5...Ph	0.3937	0.1093	2.957

To further shed light on the hydrogen bonding and electrostatic interactions in transition states **TS3d** and **TS5a**, topological analysis based on Bader's theory of atoms in molecules (AIM) was carried out. The AIM theory allows one to identify and characterize a bonding interaction between atoms through an analysis of the charge density ρ . In AIM topological analysis, hydrogen bond is characterized by a bond critical point (bcp) between the interacting hydrogen and hydrogen acceptor. The calculated electron density (ρ_{BCP}), Laplacian of electron density ($\nabla^2\rho_{BCP}$), and hydrogen bond distances at the critical points of the hydrogen bonds are listed in Table S2. Two and three electrostatic interactions are considered respectively in **TS3d** and **TS5a**, five HBs interactions are considered in **TS5a**. The sum of corresponding ρ and $\nabla^2\rho$ values in **TS5a** are 2.4756 and 2.2161, respectively, which is 2.0075 and 1.9206 larger than those in **TS3d** (0.4681 and 0.2955). Thus, the results of NBO and the AIM topological analyses clearly confirm that two molecules of water and solvent DMSO can intensively stabilize the structure of the transition state **TS5a** by HBs and electrostatic interactions.

S1. The B3LYP/6-31+G** optimized coordinates between benzaldehyde and 1-cinnamoylcyclopropanecarboxamides in gas phase.

1

C	-5.30399000	-1.83920200	-1.50412600
C	-4.04025400	-1.26784700	-1.35632600
C	-3.75619400	-0.40263500	-0.28224700

C	-4.78616200	-0.11712800	0.63703000
C	-6.04813000	-0.68477200	0.48770800
C	-6.31229200	-1.54941700	-0.58215000
H	-5.50040000	-2.50811300	-2.33658300
H	-3.25614700	-1.49827500	-2.07259900
H	-4.60235200	0.55737000	1.46742500
H	-6.83108700	-0.45203700	1.20343500
H	-7.29834300	-1.99025700	-0.69467500
C	-2.41183200	0.16703100	-0.18271200
C	-1.89726200	0.87216900	0.84906900
H	-1.75854200	-0.05378000	-1.02317200
H	-2.46655300	1.03578400	1.76071000
C	-0.48858400	1.28581000	0.94360000
O	0.04543100	1.31011400	2.06746300
C	0.30311500	1.75677500	-0.24112700
C	-0.35008100	2.24275000	-1.53913600
C	0.07366700	3.24863700	-0.52828500
H	-1.41077700	2.07797900	-1.68424300
H	0.26269300	2.13383900	-2.42812200
H	0.98653300	3.80867500	-0.70018400
H	-0.69705200	3.74518600	0.05404400
C	1.76268700	1.32096600	-0.42172700
O	2.55690700	2.10470000	-0.94509700
N	2.06975400	0.04228400	-0.06755200
H	1.34048000	-0.57454500	0.35282600
C	3.32885000	-0.59577200	-0.21722300
C	3.35147400	-1.99358900	-0.04900400
C	4.52680400	0.08280300	-0.50137200
C	4.55005500	-2.69605800	-0.15976300
H	2.42541900	-2.50954100	0.18351900
C	5.71860500	-0.63935000	-0.61110100
H	4.51692600	1.15317600	-0.64579800
C	5.74391000	-2.02527900	-0.44337100
H	4.54665000	-3.77474800	-0.02837300
H	6.63668400	-0.10260700	-0.83461700
H	6.67647300	-2.57454400	-0.53489300
Na	0.62153500	-0.66668700	2.94181500
H	0.49919700	-1.74986100	1.30885000
TS1			
C	4.76663700	-2.24626200	0.64902500
C	3.62610100	-1.45987800	0.80821700
C	3.33900800	-0.41094000	-0.08827300
C	4.23835800	-0.16793900	-1.14755100

C	5.37839400	-0.95046400	-1.30276300
C	5.64624100	-1.99347900	-0.40648600
H	4.96790400	-3.05417200	1.34603900
H	2.93692500	-1.65862400	1.62426600
H	4.04837600	0.64034000	-1.84645700
H	6.06289700	-0.74950200	-2.12165700
H	6.53672100	-2.60243300	-0.53226600
C	2.12453100	0.37007100	0.13410300
C	1.61193200	1.32356600	-0.68336900
H	1.57500600	0.12151300	1.04025500
H	2.08822500	1.59563300	-1.62141700
C	0.38587800	2.06366200	-0.41036500
O	0.01499600	2.93652800	-1.22536500
C	-0.41985600	1.78532300	0.84050400
C	0.08785600	2.35855300	2.14205100
C	-1.15413200	2.93333300	1.50744700
H	0.99055000	2.96242100	2.11549000
H	-0.01253200	1.71948700	3.01374200
H	-2.11780900	2.71505700	1.95627300
H	-1.06701500	3.93082000	1.07863900
C	-1.05235400	0.36845400	0.90786200
O	-0.53411300	-0.47061700	1.66478400
N	-2.09580100	0.20959900	0.07567100
H	-2.80196600	1.24468600	-0.33322500
C	-2.81037600	-0.99924400	-0.06543100
C	-3.63509000	-1.10746600	-1.20448300
C	-2.78393300	-2.07381100	0.84683300
C	-4.40801900	-2.24566600	-1.42627100
H	-3.66189900	-0.28534100	-1.91211200
C	-3.56015800	-3.21135400	0.61108600
H	-2.14942600	-2.01095600	1.71973800
C	-4.37500300	-3.30998900	-0.51962900
H	-5.03390800	-2.30317200	-2.31308000
H	-3.52293800	-4.03083300	1.32449300
H	-4.97299700	-4.20019300	-0.69266600
Na	-2.14924200	3.32948500	-1.31113700
H	-3.43701300	1.98762400	-0.62363700

Int1

C	4.87541700	-2.16168200	0.74711800
C	3.72644900	-1.37974900	0.86180500
C	3.41299300	-0.40598200	-0.10744600
C	4.29333500	-0.23584300	-1.19627600
C	5.44138600	-1.01427300	-1.30806300

C	5.73667200	-1.98087500	-0.33781900
H	5.09729200	-2.91028300	1.50177000
H	3.05233100	-1.52361800	1.70166900
H	4.08099000	0.51132600	-1.95431400
H	6.11031500	-0.86985400	-2.15141000
H	6.63322200	-2.58694400	-0.42988100
C	2.19354600	0.37870200	0.07359400
C	1.66451800	1.27805400	-0.79252500
H	1.64885900	0.17779000	0.99458700
H	2.12071500	1.49616900	-1.75438700
C	0.40751200	1.97875200	-0.54999900
O	-0.09022000	2.68772600	-1.45188800
C	-0.31428000	1.80628800	0.76630300
C	0.27199900	2.39776500	2.01492300
C	-0.95945100	3.02737100	1.39896100
H	1.20639900	2.94679900	1.93735500
H	0.15596000	1.80836500	2.91945100
H	-1.90785700	2.88512000	1.91095500
H	-0.83909100	3.99250600	0.91004300
C	-1.06515200	0.43906300	0.88697800
O	-0.62883700	-0.38659300	1.71157000
N	-2.09826400	0.37134800	0.03463100
C	-2.93539100	-0.75023300	-0.05146400
C	-3.94841700	-0.70830700	-1.03783500
C	-2.87190400	-1.91070900	0.75669400
C	-4.84973100	-1.75431600	-1.21922900
H	-4.01930600	0.16914900	-1.68124000
C	-3.78052800	-2.95511000	0.57009500
H	-2.10789700	-1.97331700	1.51891800
C	-4.77376100	-2.89365900	-0.41125800
H	-5.61101400	-1.68038000	-1.99175000
H	-3.70678800	-3.83297900	1.20754200
H	-5.47332300	-3.71359600	-0.54483600
Na	-2.28652400	2.28760900	-1.16379000

TS2

C	3.33220300	-1.51179600	-1.54963500
C	1.98942200	-1.13301700	-1.56491000
C	1.10876500	-1.53935600	-0.54825000
C	1.62061500	-2.32835200	0.49674400
C	2.96137000	-2.71108500	0.51489800
C	3.82276700	-2.30368800	-0.50891400
H	3.99368500	-1.18776900	-2.34760300
H	1.61403700	-0.51456300	-2.37526100

H	0.96504400	-2.65810900	1.29677700
H	3.33540400	-3.32816400	1.32695200
H	4.86723500	-2.60124800	-0.49387300
C	-0.31490900	-1.12647600	-0.61609900
C	-1.34178500	-1.89691600	0.02275700
H	-0.55569300	-0.68300000	-1.58057200
H	-1.10023600	-2.78544900	0.59963400
C	-2.58626300	-1.28422100	0.21643100
O	-3.42639200	-1.63414600	1.11226200
C	-2.78089400	0.06265100	-0.47715800
C	-3.47688900	0.11742700	-1.84415400
C	-4.19012800	0.58971000	-0.61709700
H	-3.75649300	-0.83842000	-2.27788900
H	-3.11934300	0.86551400	-2.54572200
H	-4.31512100	1.66043500	-0.49611300
H	-4.95947600	-0.04516000	-0.18999300
C	-1.68943900	1.10301300	-0.24602400
O	-1.91883400	2.29605000	-0.45560900
N	-0.49772200	0.59724400	0.26199900
C	0.63988900	1.44027800	0.32652600
C	1.52217400	1.27836100	1.40894400
C	0.97292400	2.37724200	-0.67047800
C	2.69517300	2.02773300	1.50497600
H	1.28783300	0.54316200	2.17565300
C	2.14582200	3.12615600	-0.57119100
H	0.29857100	2.53352000	-1.50328600
C	3.01280500	2.95957300	0.51347700
H	3.35952100	1.88195400	2.35216500
H	2.38135300	3.84983000	-1.34683000
H	3.92254800	3.54827800	0.58501100
Na	-1.69406600	-0.47274200	2.27169900

Int2

C	-1.39092100	3.83534000	-0.36921500
C	-1.03196300	2.62991700	-0.98560100
C	-0.33051800	1.64451600	-0.28385300
C	-0.00289700	1.88433400	1.06047600
C	-0.36839000	3.07785400	1.68339900
C	-1.05963500	4.06417100	0.96675200
H	-1.93836000	4.58694600	-0.93144900
H	-1.30798100	2.45199900	-2.02266400
H	0.52637500	1.11907800	1.62365800
H	-0.12355100	3.23839200	2.73027200

H	-1.34588500	4.99309200	1.45150100
C	0.13375900	0.36333400	-0.99679900
C	1.61901800	0.40630000	-1.24183200
H	-0.39035000	0.34265500	-1.96256300
H	1.93604200	1.06887500	-2.04934700
C	2.54544100	-0.42936200	-0.65325800
O	3.83272300	-0.28127800	-0.76564700
C	2.03530400	-1.54737400	0.20763900
C	2.87040900	-2.83084100	0.21899300
C	2.87187000	-1.96003200	1.42484600
H	3.74581800	-2.80772200	-0.42058600
H	2.30423500	-3.75466900	0.26351200
H	2.31091700	-2.29366200	2.29163000
H	3.75620700	-1.35724900	1.60584100
C	0.55414200	-1.75626900	0.34710700
O	0.10631700	-2.71483000	0.97852500
N	-0.28986900	-0.84459100	-0.25856100
C	-1.70830700	-1.08589100	-0.19581500
C	-2.39921300	-0.98896700	1.01569300
C	-2.40277400	-1.40930100	-1.36592200
C	-3.77670100	-1.21060200	1.05335200
H	-1.85307300	-0.75665800	1.92287900
C	-3.78311100	-1.62202000	-1.32788600
H	-1.85922700	-1.50950400	-2.30103200
C	-4.47375700	-1.52271000	-0.11758400
H	-4.30564100	-1.13938900	1.99941900
H	-4.31377000	-1.87635000	-2.24098900
H	-5.54605200	-1.69290500	-0.08564100
Na	3.59186500	1.81942700	-0.40095400

Int3

C	3.52026000	-1.97250100	-3.06297200
C	2.65591300	-1.01660700	-2.51551500
C	2.13066300	-1.17496200	-1.22933600
C	2.48743100	-2.31502700	-0.49401500
C	3.35641800	-3.26508500	-1.02921100
C	3.87559800	-3.09855300	-2.31971600
H	3.91866000	-1.83092200	-4.06409400
H	2.39305800	-0.13382100	-3.09438700
H	2.07321600	-2.45743600	0.50056100
H	3.62784100	-4.13948400	-0.44337500
H	4.55015500	-3.84070700	-2.73757900
C	1.16142100	-0.13286600	-0.64681800
C	-0.19254500	-0.72096000	-0.36727200

H	1.06303300	0.64947100	-1.41329400
H	-0.72842000	-1.09374600	-1.23659800
C	-0.70756200	-0.93315800	0.87423900
O	-1.85708900	-1.51463100	1.11638300
C	0.07671400	-0.45109700	2.06492100
C	-0.69857900	-0.08209900	3.32740600
C	0.10514600	-1.33838400	3.31383900
H	-1.77615000	-0.17202700	3.24410900
H	-0.30831700	0.75702900	3.89271400
H	1.03647800	-1.34872100	3.87083300
H	-0.42285400	-2.28262500	3.22604200
C	1.32162400	0.36135700	1.83970100
O	1.92452600	0.87673600	2.78500700
N	1.75258800	0.52875500	0.54098900
C	2.91297800	1.34537900	0.30605200
C	4.17697400	0.94534900	0.75070100
C	2.77553100	2.54669500	-0.39678000
C	5.29307400	1.74146800	0.48992300
H	4.27604600	0.01958000	1.30585300
C	3.89517200	3.33855100	-0.66492200
H	1.78903200	2.86330100	-0.72336700
C	5.15780000	2.93753700	-0.22155400
H	6.27090700	1.42526500	0.84195400
H	3.77779900	4.27077000	-1.21049900
H	6.02915200	3.55343900	-0.42513400
Na	-3.49462100	-2.69014500	0.73527300
C	-5.90982700	1.55067700	-1.35831900
C	-5.16537600	0.49782200	-0.78907000
C	-3.84143000	0.72242900	-0.35584600
C	-3.28581600	1.99181200	-0.49316700
C	-4.03286000	3.03421200	-1.05668400
C	-5.34542300	2.81599100	-1.49195100
H	-6.92895500	1.36849000	-1.69132000
H	-3.24602200	-0.07458500	0.08788100
H	-2.26630100	2.16141300	-0.16296700
H	-3.58912600	4.02053000	-1.15853800
H	-5.91886400	3.62701500	-1.92978600
C	-5.81578700	-0.80504800	-0.67026600
O	-5.32239600	-1.82948000	-0.19157200
H	-6.85306400	-0.85049500	-1.05268900
TS3			
C	2.15443400	3.77597700	-0.08859300
C	1.55103600	2.62351200	0.42641000

C	1.25722300	1.53679800	-0.40241100
C	1.58392000	1.61927300	-1.76273200
C	2.19186100	2.76222000	-2.28062300
C	2.47764100	3.84737500	-1.44404200
H	2.37329100	4.61141100	0.57040700
H	1.31269200	2.56865900	1.48609600
H	1.35821100	0.78322900	-2.41944300
H	2.43854500	2.81048100	-3.33762900
H	2.94752400	4.73941000	-1.84827500
C	0.58745600	0.28111100	0.16921000
C	-0.78077400	0.03151400	-0.46875200
H	0.42735000	0.47701000	1.24045400
H	-1.09365200	0.64354200	-1.62144900
C	-1.20091400	-1.30221900	-0.82313100
O	-2.38616600	-1.59964300	-1.13771300
C	-0.15028200	-2.35287200	-0.95900900
C	-0.62469100	-3.80963800	-0.82889100
C	-0.25967100	-3.29657600	-2.16927200
H	-1.67785200	-3.92277900	-0.59652000
H	0.07492100	-4.47360600	-0.33380300
H	0.68855600	-3.60869200	-2.59369000
H	-1.06063400	-3.06240400	-2.86277100
C	1.24206700	-2.10368200	-0.45930500
O	2.09555600	-2.99023900	-0.51606700
N	1.51647200	-0.87276000	0.08873100
C	2.79586400	-0.70646500	0.73626500
C	3.95969500	-0.53343800	-0.01641800
C	2.86202100	-0.71185900	2.13224300
C	5.18588700	-0.36351300	0.62783300
H	3.89850200	-0.54062900	-1.09879300
C	4.08932700	-0.53373400	2.77580100
H	1.95637200	-0.86741900	2.71170900
C	5.25380200	-0.35885400	2.02418700
H	6.08864300	-0.23327100	0.03818300
H	4.13493200	-0.54103500	3.86106200
H	6.20908600	-0.22357100	2.52306000
Na	-3.79895300	-0.07277100	-1.82320500
C	-2.93808000	-0.13409500	1.79595900
C	-3.02864500	0.77990700	0.73596600
C	-4.24189100	1.46671300	0.55194400
C	-5.33738400	1.23213700	1.39210800
C	-5.23434300	0.31101300	2.43728000
C	-4.02760800	-0.36700300	2.63789200
H	-2.01276500	-0.68064500	1.95415100

H	-4.30521800	2.21021600	-0.23966500
H	-6.26302600	1.78064300	1.23809100
H	-6.08115200	0.12670300	3.09187600
H	-3.93706700	-1.08576300	3.44765800
C	-1.84829100	1.10334000	-0.17378000
O	-2.21994900	1.42080000	-1.52803500
H	-1.33758800	1.96929500	0.28110000

Int4

C	2.08785300	3.80954200	0.21936600
C	1.59229800	2.59312800	0.70474000
C	1.21731600	1.56746000	-0.17013700
C	1.35459200	1.78198000	-1.55181600
C	1.85838900	2.98793000	-2.04037600
C	2.22343700	4.01020100	-1.15467400
H	2.37265500	4.59309800	0.91611200
H	1.50560600	2.43768400	1.77780500
H	1.06731700	0.99524400	-2.24489200
H	1.96764100	3.13240400	-3.11199700
H	2.61189000	4.95037300	-1.53557100
C	0.63909700	0.24458400	0.37000300
C	-0.76974700	-0.00691100	-0.12835800
H	0.61377900	0.35269400	1.46332100
H	-1.48123000	2.23320700	-1.10189400
C	-1.04847000	-0.91876500	-1.12918800
O	-2.20090200	-1.06557200	-1.70062800
C	0.05573000	-1.83023500	-1.59320500
C	-0.36392900	-3.18913100	-2.15426400
C	0.12929900	-2.14618700	-3.09392300
H	-1.43137200	-3.37750100	-2.12915500
H	0.30097300	-4.01403500	-1.92375500
H	1.12675000	-2.26406600	-3.50514000
H	-0.60159000	-1.63288500	-3.71067000
C	1.37494300	-1.83042600	-0.87863900
O	2.24817300	-2.65964600	-1.14121000
N	1.56189400	-0.87809500	0.10118800
C	2.80338600	-0.87141400	0.82860000
C	4.01029800	-0.56991300	0.19022300
C	2.79365800	-1.14934800	2.19924800
C	5.19861100	-0.54527400	0.92186100
H	4.01246100	-0.36894600	-0.87505300
C	3.98298000	-1.11543900	2.93176500
H	1.85598800	-1.40499900	2.68462700
C	5.18884100	-0.81310600	2.29409800

H	6.13340900	-0.31515300	0.41876000
H	3.96719300	-1.33658300	3.99525300
H	6.11523200	-0.79146500	2.86087000
Na	-3.71732100	0.41372300	-1.64971700
C	-3.12729900	-0.95197600	1.46481100
C	-3.07614900	0.36995800	1.00070300
C	-4.21232400	1.18403800	1.16978000
C	-5.37130500	0.68173800	1.77376800
C	-5.40847000	-0.63846300	2.22946200
C	-4.28037900	-1.45006600	2.07542300
H	-2.25820800	-1.58634600	1.32719000
H	-4.17737800	2.21957400	0.84388200
H	-6.23549300	1.32817900	1.90122200
H	-6.30435700	-1.02948900	2.70302800
H	-4.29968800	-2.47900800	2.42317700
C	-1.80082700	0.95123500	0.38202400
O	-2.28163900	1.90515800	-0.66562500
H	-1.34032200	1.58338800	1.15339500

TS4

C	-1.60441000	3.91231300	-0.73522900
C	-1.23353100	2.60661500	-1.06888800
C	-1.19360100	1.59856200	-0.09754600
C	-1.54611000	1.92328900	1.21993400
C	-1.92094200	3.22538000	1.55692500
C	-1.94859100	4.22637800	0.58102300
H	-1.62983400	4.67880000	-1.50449900
H	-0.97385500	2.37018300	-2.09790400
H	-1.53802800	1.15798700	1.98990900
H	-2.19528900	3.45727700	2.58235700
H	-2.24201700	5.23847100	0.84388900
C	-0.73332500	0.19040100	-0.49662700
C	0.71828300	-0.09228000	-0.11733000
H	-0.80248100	0.13470600	-1.58570100
H	1.68848400	3.04509700	-0.68638100
C	0.95975500	-0.52193300	1.24596100
O	2.02102400	-0.28393100	1.87170900
C	-0.13865800	-1.26983600	1.92126200
C	0.31070800	-2.37753500	2.89189900
C	-0.25908200	-1.13335600	3.45142300
H	1.38419500	-2.51912500	2.95536500
H	-0.31455900	-3.26328000	2.88043000
H	-1.27265900	-1.16717500	3.83699500

H	0.41894600	-0.41413600	3.89932200
C	-1.43003000	-1.54245300	1.19296000
O	-2.25442500	-2.33367400	1.64999000
N	-1.63638200	-0.86502700	0.01497800
C	-2.86444300	-1.07402300	-0.70877800
C	-4.08521300	-0.62988600	-0.19346500
C	-2.82000400	-1.70761600	-1.95467100
C	-5.25811400	-0.81929700	-0.92654200
H	-4.11223400	-0.14936200	0.77807100
C	-3.99414500	-1.88788500	-2.68944600
H	-1.86917500	-2.06731600	-2.33773200
C	-5.21560600	-1.44377200	-2.17640300
H	-6.20524200	-0.47595800	-0.52089700
H	-3.95436000	-2.38281300	-3.65541200
H	-6.12966300	-1.58722600	-2.74514600
Na	3.19014700	1.48814100	1.11660300
C	3.37335700	-1.61630100	-0.62043500
C	3.09456600	-0.30653100	-1.05732600
C	4.13154400	0.43251900	-1.66239200
C	5.40930900	-0.11561100	-1.79639700
C	5.67540000	-1.41197100	-1.34531500
C	4.64978500	-2.16090300	-0.75988700
H	2.57973200	-2.21709000	-0.18977000
H	3.91261700	1.44843900	-1.97543400
H	6.19716100	0.47214600	-2.25943800
H	6.66820900	-1.83860400	-1.45695500
H	4.84001500	-3.17513000	-0.42046100
C	1.71142600	0.23650300	-1.01258700
O	2.45693300	2.46757700	-0.60006100
H	1.39487600	0.69533800	-1.94394100

Int5

C	-0.43396000	3.95178700	-1.10333300
C	-0.15432000	2.58202700	-1.08119100
C	-1.11010500	1.68259000	-0.57880100
C	-2.33574300	2.17544100	-0.11183400
C	-2.60802000	3.54623200	-0.13938800
C	-1.65678800	4.44036900	-0.63567100
H	0.31843100	4.63331100	-1.49031300
H	0.82161300	2.25113900	-1.45282100
H	-3.08567800	1.49365700	0.27276200
H	-3.56387600	3.91070400	0.22666000
H	-1.86701300	5.50612100	-0.65670600

C	-0.80486300	0.17434600	-0.61026000
C	0.61407400	-0.14848700	-0.17238700
H	-0.92722100	-0.16926600	-1.63915300
H	3.17269000	2.80812500	-2.50032800
C	0.83840900	0.15897000	1.25976900
O	1.90128400	0.63172000	1.69005600
C	-0.32698000	-0.07574700	2.14568600
C	0.00312500	-0.44337400	3.60523900
C	-0.52617600	0.90379000	3.32679000
H	1.06266700	-0.54308100	3.81575300
H	-0.66678100	-1.17971200	4.03470800
H	-1.56260700	1.11273500	3.56940300
H	0.15613100	1.74734400	3.33635000
C	-1.58497100	-0.69886600	1.58144300
O	-2.40268000	-1.23375200	2.32642000
N	-1.74252400	-0.63141300	0.21241700
C	-2.83021000	-1.31414700	-0.43563500
C	-4.15112400	-1.15643200	0.00166500
C	-2.55953600	-2.15287600	-1.52508200
C	-5.18651300	-1.82203100	-0.65679600
H	-4.36354600	-0.53345900	0.86123700
C	-3.60092900	-2.80667700	-2.18624300
H	-1.53471100	-2.30923100	-1.84744200
C	-4.91929900	-2.64318500	-1.75510200
H	-6.20697700	-1.69369500	-0.30802400
H	-3.37652600	-3.45275700	-3.02983800
H	-5.72930100	-3.15489900	-2.26607700
Na	3.27871900	1.64890300	0.14659000
C	3.08451500	-2.09284900	0.31225100
C	2.89112300	-1.14856300	-0.71291400
C	3.99101600	-0.75958900	-1.50324400
C	5.25782300	-1.29128600	-1.24741000
C	5.44109800	-2.22726000	-0.22464000
C	4.34976200	-2.62805000	0.55334400
H	2.23602100	-2.42472800	0.90344500
H	3.84150800	0.01691700	-2.25186200
H	6.10235900	-0.97288000	-1.85202100
H	6.42555800	-2.64680400	-0.03793300
H	4.48203600	-3.36343100	1.34167200
C	1.54645500	-0.61803000	-1.02726100
O	2.97030800	2.14719100	-1.83151400
H	1.27849900	-0.64406000	-2.08254100

TS5

C	-0.39378100	3.93452000	-1.01251900
C	-0.16290200	2.55667100	-1.06405500
C	-1.09425500	1.66860600	-0.49964300
C	-2.24698300	2.18350000	0.10730300
C	-2.47229700	3.56284500	0.15310200
C	-1.54604500	4.44451000	-0.40812000
H	0.34267200	4.60355100	-1.44861800
H	0.76553800	2.21476200	-1.53152100
H	-2.97747400	1.51227600	0.54380800
H	-3.37394000	3.94307800	0.62552500
H	-1.72069300	5.51641300	-0.37422400
C	-0.84052500	0.15102400	-0.60490800
C	0.58221000	-0.22455100	-0.21734200
H	-0.98776500	-0.13960600	-1.64648800
H	3.19998200	2.92279800	-2.49194300
C	0.80386700	-0.01784300	1.24182100
O	1.85170000	0.53621100	1.70359900
C	-0.25527900	-0.43861100	2.05692400
C	0.61681700	0.61151100	3.82582000
C	0.02332300	-0.66648200	3.54238500
H	0.00989400	1.50702100	3.73217300
H	1.65509100	0.73663900	4.10888700
H	0.65143200	-1.53178500	3.76528800
H	-0.98731200	-0.79968400	3.95903200
C	-1.59290400	-0.80975500	1.56319600
O	-2.44839200	-1.27667000	2.32350200
N	-1.79875600	-0.64781800	0.19845200
C	-2.94755800	-1.21591500	-0.44658900
C	-4.23908400	-1.03323000	0.06684500
C	-2.77419200	-1.97012900	-1.61654900
C	-5.33680700	-1.58738400	-0.59388300
H	-4.37896400	-0.47817600	0.98522800
C	-3.87757500	-2.51113800	-2.27804300
H	-1.77533100	-2.15057800	-2.00130900
C	-5.16485500	-2.32181700	-1.76979400
H	-6.33214400	-1.43881300	-0.18535700
H	-3.72594000	-3.09202900	-3.18310700
H	-6.02332500	-2.74658000	-2.28138000
Na	3.09768000	1.62937900	0.09683700
C	3.08989500	-2.11965400	0.14869700
C	2.86004300	-1.14847000	-0.84352200
C	3.94027800	-0.70757100	-1.63392900
C	5.22157700	-1.22012700	-1.41393500

C	5.44000600	-2.18611200	-0.42660200
C	4.36968400	-2.63493000	0.35445200
H	2.25655800	-2.48768100	0.74008100
H	3.76706500	0.09457900	-2.35027500
H	6.05061100	-0.86114100	-2.01727900
H	6.43596700	-2.59027700	-0.26841700
H	4.53020000	-3.39278300	1.11606700
C	1.49954700	-0.63379500	-1.11345300
O	2.95969600	2.22431300	-1.87611000
H	1.21742800	-0.59531800	-2.16442000

Pr+NaOH

C	-0.43217500	3.92566400	-1.01888700
C	-0.19891100	2.54710900	-1.04707600
C	-1.15179800	1.66186400	-0.51562600
C	-2.33226000	2.18295300	0.03107100
C	-2.56085900	3.56188000	0.05247400
C	-1.61066800	4.44013900	-0.47290500
H	0.32354000	4.59055800	-1.42734400
H	0.74766800	2.20696500	-1.47422200
H	-3.08144100	1.51689600	0.44219300
H	-3.48306000	3.94476900	0.48082200
H	-1.78707400	5.51210600	-0.45585000
C	-0.90386300	0.14070800	-0.59125800
C	0.52960000	-0.23260400	-0.23065600
H	-1.08747700	-0.17841300	-1.61863400
H	3.20713700	3.04022000	-2.31762100
C	0.70435800	-0.12995700	1.20939600
O	1.89795100	0.23720500	1.79393000
C	-0.31185400	-0.26859900	2.07807600
C	1.69402700	0.13638300	3.25246500
C	0.16776200	0.00436600	3.47912600
H	2.13729700	1.02790500	3.69892700
H	2.24378800	-0.74984400	3.58245000
H	-0.07445400	-0.80583800	4.17266800
H	-0.27577400	0.92347700	3.88179500
C	-1.64943800	-0.69621200	1.64279800
O	-2.48760800	-1.11795000	2.43990800
N	-1.85049500	-0.63441800	0.26328900
C	-3.00431600	-1.22848300	-0.34586400
C	-4.29121200	-1.03886200	0.17814500
C	-2.84267000	-2.02184900	-1.49211100
C	-5.39304800	-1.62531400	-0.44740900
H	-4.42430500	-0.45386700	1.07864200

C	-3.95064900	-2.59238000	-2.12029800
H	-1.84788000	-2.21019000	-1.88379800
C	-5.23242700	-2.39695400	-1.60067200
H	-6.38350500	-1.47143100	-0.02896500
H	-3.80636200	-3.20197700	-3.00760900
H	-6.09440200	-2.84551300	-2.08535800
Na	3.07073600	1.57057500	0.16558900
C	3.03225500	-2.15189800	0.02145600
C	2.81608100	-1.11474700	-0.90667800
C	3.90347900	-0.63910800	-1.66712100
C	5.17756700	-1.18263600	-1.48062300
C	5.38180300	-2.21351500	-0.55829900
C	4.30451400	-2.69770300	0.19188100
H	2.19311200	-2.54767700	0.58607900
H	3.74225600	0.20856800	-2.33233100
H	6.01156300	-0.79739200	-2.06036700
H	6.37172200	-2.64147000	-0.42745400
H	4.45325100	-3.50792700	0.90009200
C	1.45695500	-0.58117900	-1.14902600
O	2.97687400	2.29942400	-1.74965600
H	1.17851200	-0.47914700	-2.19633400

Int3a

C	2.53140000	3.96701300	-0.36240700
C	2.26065400	2.82760800	0.40475700
C	2.39357600	1.54490500	-0.13706700
C	2.82412700	1.42327900	-1.46821100
C	3.10302000	2.55511600	-2.23631600
C	2.95192200	3.83557700	-1.68671000
H	2.42385300	4.95381900	0.07980000
H	1.94495300	2.93827000	1.43986300
H	2.94477400	0.43374600	-1.90168400
H	3.44950600	2.44050300	-3.26032200
H	3.17338500	4.71632600	-2.28268100
C	2.01410800	0.30785300	0.69546800
C	0.66778500	-0.24882300	0.29458000
H	1.95124000	0.65161000	1.73674100
H	-0.19631400	0.28476500	0.68552800
C	0.47744400	-1.48794400	-0.27965700
O	-0.66999300	-1.98640800	-0.59309400
C	1.70222100	-2.30943200	-0.59175900
C	1.50950000	-3.81888000	-0.72205300
C	1.76292100	-3.01918700	-1.95143000

H	0.49647600	-4.16003400	-0.54088900
H	2.32164600	-4.42865800	-0.34241400
H	2.74500600	-3.08827500	-2.40844100
H	0.92757500	-2.82241100	-2.61618900
C	3.03119900	-1.90169100	-0.02136500
O	4.02189700	-2.62752400	-0.13083400
N	3.09519700	-0.70025300	0.65511000
C	4.32543800	-0.34319700	1.31061600
C	5.49276700	-0.09832900	0.58059200
C	4.34375700	-0.22702700	2.70470400
C	6.66693600	0.26379800	1.24303300
H	5.47898800	-0.20543700	-0.49771000
C	5.51758100	0.14393000	3.36507900
H	3.44104400	-0.44179900	3.26952900
C	6.68311800	0.39055300	2.63515200
H	7.57092100	0.44709400	0.66920000
H	5.52256700	0.22749300	4.44824200
H	7.59838700	0.67364700	3.14711500
Na	-2.63959100	-1.83513200	-1.32353800
C	-6.60129600	1.47524100	1.09041400
C	-6.22024200	0.15427800	0.80229200
C	-6.99994400	-0.91971300	1.26845100
C	-8.14677900	-0.66820800	2.01453100
C	-8.52218800	0.65242000	2.29960400
C	-7.75137300	1.72414100	1.83930300
H	-5.99219200	2.29937200	0.72755800
H	-6.68899900	-1.93348500	1.03748900
H	-8.75164700	-1.49349100	2.37760400
H	-9.41803000	0.84370900	2.88327900
H	-8.04622200	2.74439800	2.06413200
C	-5.00075200	-0.07616600	0.01575400
O	-4.57406700	-1.19268900	-0.28083500
H	-4.45637700	0.82530200	-0.32017500
O	-2.56295800	-0.46849700	-3.16725800
H	-1.64928000	-0.12746100	-3.11630500
H	-3.09295100	0.33482700	-3.02682600
O	-0.40898300	1.10425700	-2.14988400
H	0.32848400	1.63700800	-2.48004000
H	-0.01602900	0.59928200	-1.38221200
O	-3.00331600	2.04515800	-1.82388300
H	-2.03066200	1.89256700	-1.82333800
H	-3.13300800	2.96845700	-2.07156000

TS3a

C	2.33632700	-2.52518800	-2.62300400
C	1.74363600	-1.36367900	-2.11490300
C	1.26147700	-1.31509500	-0.80172200
C	1.38684800	-2.45883800	0.00099400
C	1.98808100	-3.61645600	-0.49363900
C	2.46583600	-3.65545300	-1.81129000
H	2.71236400	-2.53899900	-3.64221100
H	1.67103600	-0.48008900	-2.74425500
H	1.01162200	-2.44576400	1.02008800
H	2.08283000	-4.48993500	0.14527800
H	2.94614700	-4.55249000	-2.19221100
C	0.63942300	-0.02464500	-0.25208600
C	-0.87539800	-0.14066800	0.03277700
H	0.75958100	0.73200500	-1.03475200
H	-1.31148800	-1.41286000	-0.08263900
C	-1.32395600	0.07240500	1.39052100
O	-2.52916800	0.23485400	1.71219300
C	-0.31311500	-0.05284600	2.48973800
C	-0.78402000	0.26606400	3.90636800
C	-0.55762000	-1.15395400	3.54368800
H	-1.80727500	0.61719800	3.97244700
H	-0.04347300	0.74994700	4.53258800
H	0.33494000	-1.64386800	3.92069300
H	-1.41715300	-1.79100400	3.35973900
C	1.12074200	0.29015600	2.20614800
O	1.93232000	0.44945400	3.11729500
N	1.44864000	0.47952200	0.88373200
C	2.76309100	0.96862500	0.55308000
C	3.91424800	0.24041400	0.86811500
C	2.87283900	2.19288800	-0.11513600
C	5.16917600	0.73676000	0.51021700
H	3.82369400	-0.69875700	1.40086500
C	4.12959700	2.68201200	-0.47923300
H	1.97477900	2.76256300	-0.33641500
C	5.28098300	1.95421000	-0.16755200
H	6.06076300	0.16976200	0.76192700
H	4.20746600	3.63486800	-0.99485600
H	6.25923900	2.33590500	-0.44527500
Na	-4.29692200	-0.41388600	0.58959800
C	-1.34325000	2.58547000	-2.43544100
C	-1.80129500	1.95100600	-1.27161500
C	-2.36853300	2.74694900	-0.26210800
C	-2.47006400	4.13064600	-0.41808200
C	-2.00505800	4.75001400	-1.58265000

C	-1.43840900	3.97162200	-2.59309500
H	-0.91348700	1.98560300	-3.23431500
H	-2.71931400	2.28303800	0.65231100
H	-2.90897900	4.72834900	0.37622300
H	-2.08326000	5.82722000	-1.69882600
H	-1.07423400	4.43817500	-3.50421000
C	-1.68507400	0.43655900	-1.16873800
O	-2.99881600	-0.14793500	-1.27687500
H	-1.12600900	0.11521500	-2.05942500
O	-2.10624100	-2.41764800	-0.38973000
H	-1.66831300	-3.12376800	-0.89694900
H	-2.81449000	-1.12966100	-1.23705500
O	-0.86844600	-4.49146200	-2.09600900
H	0.08207100	-4.30091900	-2.07362100
H	-1.13706700	-4.39366500	-3.01789900
O	-4.45643900	-2.63134900	0.62248000
H	-3.50935000	-2.75042000	0.26644000
H	-4.69172700	-3.41273800	1.13167500

Int4a

C	2.03880700	-1.79410200	-3.46042700
C	1.60350200	-0.73037500	-2.66007600
C	1.45518200	-0.87880300	-1.27665500
C	1.77768400	-2.11985200	-0.70153200
C	2.23368100	-3.17731500	-1.49176200
C	2.35718100	-3.02137300	-2.88001400
H	2.14428300	-1.65381200	-4.53256100
H	1.38823100	0.23098900	-3.12071900
H	1.69031400	-2.25372900	0.37302500
H	2.51851900	-4.11624500	-1.02255800
H	2.71618600	-3.84278700	-3.49336000
C	0.93283800	0.28757100	-0.41837500
C	-0.52479700	0.10502400	-0.03512800
H	1.01435200	1.18615100	-1.04218400
H	-2.41445400	-2.20062400	0.90342300
C	-0.88283200	-0.35394300	1.20617800
O	-2.10840500	-0.63897500	1.57649000
C	0.19418300	-0.55684000	2.23964700
C	-0.24346400	-0.55293900	3.70335600
C	0.16666700	-1.84167100	3.08301700
H	-1.30346000	-0.38593100	3.85610800
H	0.44852800	-0.08510100	4.39454000
H	1.13375000	-2.25265100	3.35590000
H	-0.60819100	-2.55830800	2.82919800

C	1.56030800	0.02320700	2.00335200
O	2.40352900	0.07067700	2.90019700
N	1.81321600	0.52564900	0.74327800
C	3.08732700	1.13534700	0.46937400
C	4.28145300	0.42093600	0.61132800
C	3.12298500	2.46453500	0.03338300
C	5.49992600	1.03498600	0.31624600
H	4.25252700	-0.60281200	0.96490300
C	4.34285100	3.07307100	-0.27089100
H	2.19547900	3.02329900	-0.05406400
C	5.53566800	2.35930700	-0.12950300
H	6.42336400	0.47526600	0.43422400
H	4.35977400	4.10616800	-0.60621600
H	6.48575200	2.83259100	-0.35993000
Na	-3.96643500	-0.08139400	0.51699900
C	-3.06875500	2.30823900	-1.94324900
C	-2.19828800	1.85450100	-0.93521800
C	-1.99493200	2.66685900	0.18749300
C	-2.64628900	3.90125400	0.30461100
C	-3.50901400	4.34069300	-0.70111900
C	-3.71842100	3.53843900	-1.82900200
H	-3.23487700	1.68660700	-2.81884400
H	-1.31827400	2.32854900	0.96588600
H	-2.47307200	4.51757000	1.18246800
H	-4.00973200	5.30065500	-0.61266800
H	-4.38291200	3.87403600	-2.62051800
C	-1.51160700	0.48992100	-1.11248200
O	-2.61112200	-0.44680700	-1.31424100
H	-0.96671700	0.53584500	-2.06677400
O	-2.78576700	-2.86398500	0.26068300
H	-2.12899600	-3.57080700	0.11220900
H	-2.32095700	-1.34944900	-1.08891000
O	-0.70168700	-4.62048900	-0.47637100
H	0.00342800	-4.05689200	-0.83435000
H	-0.86306600	-5.30008500	-1.14273000
O	-5.28383000	-1.94498900	0.52736000
H	-4.52420100	-2.56606400	0.41262100
H	-5.94012800	-2.39014900	1.07367400
TS4a			
C	-1.95230400	2.96282600	-2.34316700
C	-1.66796600	1.62238900	-2.06104000
C	-1.39542500	1.20194100	-0.75387900
C	-1.41940400	2.15648000	0.27443700

C	-1.70841100	3.49339700	0.00093300
C	-1.97417000	3.90413300	-1.31135700
H	-2.16247700	3.26688200	-3.36459900
H	-1.66473400	0.89503800	-2.86917000
H	-1.21407400	1.85824800	1.29790300
H	-1.72211500	4.21737700	0.81064700
H	-2.20236900	4.94469500	-1.52332900
C	-1.08101900	-0.27563900	-0.48238600
C	0.36916000	-0.54561000	-0.07223300
H	-1.25929400	-0.80340600	-1.42258000
H	3.36295600	4.50244600	0.89296800
C	0.68962100	-0.44823200	1.31258100
O	1.85647500	-0.21854200	1.74647500
C	-0.42206800	-0.60834000	2.30033200
C	-0.03505000	-1.21749400	3.65492800
C	-0.35661500	0.22711400	3.59269400
H	1.00565300	-1.50773800	3.74556100
H	-0.77834200	-1.88387500	4.07774900
H	-1.31504400	0.55165600	3.98460200
H	0.45933900	0.94144000	3.63778500
C	-1.80946300	-0.95441700	1.82858600
O	-2.67923900	-1.30692900	2.62529000
N	-2.04351700	-0.86221100	0.47882000
C	-3.35276000	-1.17912800	-0.03032700
C	-4.46140300	-0.39249100	0.29508200
C	-3.50180900	-2.27794000	-0.88245000
C	-5.71476100	-0.70710500	-0.23300100
H	-4.34022100	0.45107900	0.96519100
C	-4.75569100	-2.58501000	-1.41595000
H	-2.63836400	-2.89581000	-1.11257400
C	-5.86515600	-1.79972400	-1.09180000
H	-6.57431600	-0.09583400	0.02615600
H	-4.86562100	-3.44211300	-2.07400200
H	-6.84165500	-2.04027000	-1.50192100
Na	3.10785200	1.44605300	0.62998000
C	2.93062500	-1.89639700	-2.51952000
C	2.48985200	-1.58154800	-1.21635700
C	3.17330000	-2.16907600	-0.13545200
C	4.25509800	-3.02237800	-0.35618800
C	4.68707400	-3.31090100	-1.65383100
C	4.01542400	-2.74334700	-2.73975200
H	2.40630600	-1.47076500	-3.37197700
H	2.86424400	-1.95072000	0.87717400
H	4.76589500	-3.46256100	0.49558500

H	5.53233300	-3.97330300	-1.81637200
H	4.33014900	-2.96448700	-3.75560400
C	1.28501600	-0.72197600	-1.12004900
O	2.31105200	1.09730600	-1.44509700
H	0.81990400	-0.61691400	-2.09612300
O	2.82921200	3.71957600	0.72232700
H	2.34968400	3.86728600	-0.14207500
H	2.91263200	0.88823400	-2.17271400
O	1.62360400	3.60985000	-1.62654600
H	1.80118700	2.61367200	-1.67295700
H	0.66461600	3.72034400	-1.67754200
O	4.28181700	0.66880300	2.52200000
H	3.47736500	0.15834600	2.72768500
H	4.63106300	1.01025600	3.35242300

Int5a

C	-1.19987300	3.18991400	-2.27772700
C	-1.24720600	1.87633900	-1.80052300
C	-2.33659500	1.44184700	-1.03077200
C	-3.37466300	2.34342800	-0.75483800
C	-3.32533200	3.65403900	-1.23546600
C	-2.23637900	4.08290500	-1.99936400
H	-0.34006300	3.50697400	-2.86038000
H	-0.41560300	1.21492200	-2.02850500
H	-4.22604800	2.02607700	-0.16348300
H	-4.13859000	4.33847200	-1.01051300
H	-2.19577700	5.10355900	-2.36913500
C	-2.41677100	-0.02463900	-0.56561100
C	-1.05204700	-0.64399700	-0.29519800
H	-2.89548100	-0.59453000	-1.36374600
H	5.76638500	3.17289000	-1.85732700
C	-0.39392500	-0.03101000	0.88178100
O	0.82958500	0.08357800	1.00368100
C	-2.79002300	0.16575700	1.87111500
O	-3.48664500	0.21091600	2.88196200
N	-3.27782000	-0.19611000	0.63191600
C	-4.61241500	-0.70299700	0.47659400
C	-5.71158000	-0.05016000	1.05065700
C	-4.81860600	-1.87490800	-0.26498000
C	-6.99790500	-0.56162000	0.86897200
H	-5.55680500	0.83821300	1.64934300
C	-6.10908600	-2.37317300	-0.45265200
H	-3.97004900	-2.41057700	-0.67910100

C	-7.20526700	-1.71827500	0.11337700
H	-7.84140500	-0.04772900	1.32072400
H	-6.25226800	-3.28202700	-1.02981100
H	-8.20876800	-2.10843700	-0.02737600
Na	2.73146100	0.64325900	-0.20025600
C	0.82494300	-3.22966100	-2.29632600
C	0.59840500	-2.48778100	-1.11733400
C	1.47725000	-2.68806400	-0.03382000
C	2.53769700	-3.58549200	-0.13705400
C	2.75690700	-4.29904900	-1.32013700
C	1.89427900	-4.11655300	-2.40354700
H	0.15118000	-3.10067200	-3.13944600
H	1.33833700	-2.14107200	0.88849200
H	3.20159100	-3.71992300	0.71136900
H	3.58995700	-4.99200300	-1.39479400
H	2.04931900	-4.66709700	-3.32672600
C	-0.58160400	-1.61489500	-1.11632000
O	1.89647600	0.86791400	-2.47343800
H	-1.23540300	-1.82788000	-1.96292400
O	5.44513100	2.76730100	-1.04465400
H	4.42503700	2.82284400	-1.08148600
H	2.36023100	0.70841300	-3.30289400
O	2.86897700	2.70176300	-1.07260700
H	2.25031800	1.76163100	-2.08643700
H	2.42405000	3.53843700	-0.90271600
C	6.64232000	-1.27278800	2.07770900
H	7.72918000	-1.17922100	2.15403300
H	6.37667800	-2.28855900	1.77928000
H	6.15798500	-1.02134400	3.02463100
S	6.02635400	-0.14936200	0.77119800
O	4.49599500	-0.26621100	0.86144000
C	6.47877200	1.42751800	1.56335400
H	5.96315500	1.50027500	2.52469700
H	7.56491900	1.45234300	1.69425600
H	6.16352100	2.21041700	0.86673500
C	-1.31676500	0.49391400	1.92763100
C	-0.72338100	0.63699600	3.33634300
C	-0.94964700	1.86543100	2.55152700
H	0.29496100	0.27647100	3.43341500
H	-1.41873800	0.40262400	4.13419000
H	-1.79975400	2.49265100	2.79852300
H	-0.10021300	2.36030300	2.09194200

Int5a'

C	-0.14371000	3.37181300	-1.88542400
C	-0.25105900	2.01853000	-1.55196800
C	-1.42037100	1.52680000	-0.95199900
C	-2.47678600	2.41304900	-0.69972500
C	-2.36726600	3.76451900	-1.03635600
C	-1.19930500	4.24969100	-1.63027300
H	0.77542600	3.73100600	-2.33853200
H	0.59583800	1.36890200	-1.75548200
H	-3.38963600	2.05259900	-0.23958400
H	-3.19628800	4.43634100	-0.83228300
H	-1.11287300	5.30134600	-1.88803000
C	-1.55059800	0.02312800	-0.64481800
C	-0.23763500	-0.61331400	-0.21543000
H	-1.88538400	-0.47364600	-1.55735200
H	6.98921900	2.39984700	-0.16024300
C	0.22481600	-0.09791000	1.09730000
O	1.41531800	0.05243700	1.38949200
C	-0.85710700	0.27801600	2.04485100
C	-0.48878700	0.23125700	3.53762300
C	-0.62843300	1.55200600	2.89821500
H	0.51283800	-0.13133900	3.74230700
H	-1.29092600	-0.11686100	4.17834500
H	-1.52473300	2.13129800	3.09310500
H	0.26661000	2.11193500	2.64734000
C	-2.29581400	-0.04909600	1.71695200
O	-3.14080700	-0.12172900	2.60527500
N	-2.58136800	-0.26687200	0.38368900
C	-3.87449600	-0.73961700	-0.02910000
C	-5.05106600	-0.13298300	0.42978800
C	-3.95824700	-1.82810000	-0.90823100
C	-6.29176700	-0.60511800	-0.00224800
H	-4.99443400	0.68787400	1.13316300
C	-5.20217500	-2.28708000	-1.34532000
H	-3.05385700	-2.33043300	-1.23738800
C	-6.37485900	-1.67689800	-0.89453300
H	-7.19691600	-0.12785600	0.36163800
H	-5.25111800	-3.13135200	-2.02672500
H	-7.34282800	-2.03683600	-1.22986900
Na	3.39261800	0.55431000	0.33135000
C	2.32583400	-2.75205100	-1.89725300
C	1.57337600	-2.35729300	-0.77393200
C	1.95229000	-2.84948900	0.48933600
C	3.06101300	-3.68283400	0.62274200

C	3.81744100	-4.04054000	-0.49851500
C	3.44459200	-3.57323500	-1.76099000
H	2.03513700	-2.39556600	-2.88182200
H	1.36861500	-2.59620500	1.36665200
H	3.33301500	-4.05923600	1.60444800
H	4.68420900	-4.68523200	-0.38858900
H	4.01992200	-3.85187500	-2.63878200
C	0.38841300	-1.51622200	-1.00296800
O	2.99858500	1.08593700	-1.98007800
H	-0.06595200	-1.67345000	-1.98205000
O	6.33910100	2.24359000	0.53391500
H	5.40887200	2.53373000	0.16473200
H	3.53816700	0.92581400	-2.76207000
O	3.98913300	2.65888500	-0.28896500
H	3.41206400	1.88740900	-1.47869600
H	3.62755400	3.53525500	-0.11971500
O	5.41345100	-0.13233900	1.15132400
H	5.72879300	-0.48645700	1.98925600
H	5.93143900	0.70723900	0.97152200

TS5a

C	-1.52177400	-0.67976200	3.90041800
C	-1.55919500	0.21720500	2.82979300
C	-1.42425600	-0.23093500	1.50964300
C	-1.26235300	-1.60377000	1.27952100
C	-1.22725200	-2.50397400	2.34675500
C	-1.35319400	-2.04515500	3.66149100
H	-1.63223700	-0.31221200	4.91656900
H	-1.70315600	1.27727400	3.02536300
H	-1.16506500	-1.97826300	0.26587800
H	-1.10388100	-3.56499200	2.14862000
H	-1.32620700	-2.74677900	4.48996900
C	-1.44142400	0.79658200	0.36805800
C	-0.02910200	1.15495700	-0.10146100
H	-1.88223800	1.70882600	0.77525300
H	2.42600700	-5.17731300	-0.58812300
C	0.54868800	0.19916400	-1.08517500
O	1.78154300	-0.09228500	-1.10829000
C	-0.36745400	-0.34182200	-2.00293200
C	1.07731900	-1.87859100	-2.71385300
C	0.16306200	-0.94388100	-3.30897900
H	0.70497700	-2.70907200	-2.11896800
H	2.15610900	-1.79814800	-2.79564600

H	0.61428600	-0.21886900	-3.98996000
H	-0.73513600	-1.40338600	-3.74737800
C	-1.83076500	-0.28373500	-1.86476500
O	-2.58315800	-0.77038000	-2.71703900
N	-2.31365700	0.37710900	-0.74815400
C	-3.73081200	0.52670800	-0.56318500
C	-4.56698100	-0.59015700	-0.46110600
C	-4.27381600	1.81308300	-0.46444100
C	-5.93687000	-0.41637200	-0.25789500
H	-4.14508700	-1.58401300	-0.55257600
C	-5.64325000	1.98248400	-0.24899000
H	-3.62568800	2.67823700	-0.57242800
C	-6.47864900	0.86739000	-0.14590700
H	-6.58105200	-1.28759000	-0.18330800
H	-6.05637500	2.98432200	-0.17555300
H	-7.54470400	0.99765200	0.01547300
Na	3.36640900	-1.18434200	0.04716800
C	2.42504300	3.62356700	1.29526000
C	1.90354800	2.84204800	0.24369700
C	2.64665600	2.76146000	-0.95005900
C	3.87272200	3.41433600	-1.07003700
C	4.38991300	4.15977700	-0.00533900
C	3.65857400	4.26313100	1.18074500
H	1.85669400	3.71697500	2.21732100
H	2.26296400	2.19291600	-1.78678800
H	4.42544700	3.34473100	-2.00270500
H	5.34705300	4.66351000	-0.10405000
H	4.04378000	4.84594300	2.01230700
C	0.58443000	2.22695200	0.45166000
O	4.48677300	-1.58743500	2.03690700
H	-0.00371300	2.75154200	1.20533300
O	2.30358200	-4.23571700	-0.75433900
H	2.29264600	-3.72250900	0.20249300
H	5.23525800	-2.01518700	2.46399100
O	2.41073500	-2.86433900	1.28554200
H	3.71725800	-2.24717400	1.98886700
H	1.59751900	-2.79247700	1.79837100
O	4.07375700	-2.56798200	-1.71485300
H	3.51057700	-3.35507000	-1.43898900
H	4.95637100	-2.89989300	-1.91202900
TS5a'			
C	2.75327600	-0.09131500	-3.88490300
C	2.85562700	0.49453100	-2.62044600

C	2.28611000	-0.11538200	-1.49538600
C	1.61704500	-1.33610000	-1.65912700
C	1.51501300	-1.92558400	-2.92096500
C	2.07958700	-1.30452800	-4.03912200
H	3.20594900	0.39590200	-4.74381900
H	3.39262000	1.43355900	-2.50778800
H	1.17048200	-1.83368200	-0.80472500
H	0.99381000	-2.87268500	-3.02796500
H	1.99888900	-1.76531100	-5.01927000
C	2.40333900	0.58159300	-0.13174900
C	1.12169100	1.32731600	0.24672600
H	3.18964500	1.33252300	-0.23261000
H	-2.07129800	-4.35638800	-0.97162000
C	0.07636600	0.46191100	0.85846500
O	-1.16030500	0.63302900	0.64309100
C	0.56036600	-0.54226400	1.71361700
C	-1.41413700	-1.57059300	1.81722700
C	-0.39368700	-1.15997500	2.74229100
H	-1.22265600	-2.35415100	1.08374700
H	-2.40237400	-1.12003500	1.78766300
H	-0.71871300	-0.46943400	3.52393600
H	0.19941600	-1.98810600	3.15702400
C	1.96008200	-0.98771100	1.77830400
O	2.32738800	-1.86789900	2.56594000
N	2.84728900	-0.34321000	0.93209500
C	4.24145100	-0.68686700	0.96056800
C	4.66909200	-1.99062100	0.68682000
C	5.18440400	0.30672300	1.24901300
C	6.03167200	-2.29241800	0.69876700
H	3.93564300	-2.76068700	0.47883700
C	6.54767900	0.00355000	1.24788800
H	4.84776900	1.31121900	1.48958400
C	6.97505600	-1.29797200	0.97336100
H	6.35618600	-3.30747600	0.48892700
H	7.27170900	0.78088400	1.47456300
H	8.03453900	-1.53680100	0.97786400
Na	-2.82337500	0.17389100	-0.79986900
C	0.09128100	4.84161300	-0.61465500
C	-0.00699900	3.66395300	0.15623400
C	-1.04771800	3.58294300	1.10277400
C	-1.95910200	4.62785400	1.24872700
C	-1.86169200	5.77676600	0.45700300
C	-0.82878800	5.87990000	-0.47823300
H	0.89907800	4.93477200	-1.33643000

H	-1.14737200	2.70153000	1.72111600
H	-2.75091100	4.54415700	1.98788300
H	-2.57775400	6.58503700	0.57407000
H	-0.73512200	6.76890100	-1.09520500
C	1.03198600	2.64509500	-0.05105100
O	-3.88011800	0.18955200	-2.87780100
H	1.91344800	3.05601400	-0.54427200
O	-2.26771100	-3.53802600	-0.50140900
H	-2.24909800	-2.78138600	-1.21495200
H	-4.63459700	-0.00551600	-3.44161700
O	-2.23627700	-1.58032700	-2.12808000
H	-3.28567200	-0.64299200	-2.81469500
H	-1.40311900	-1.55815900	-2.61438900
C	-6.93588400	-1.10534700	1.33646300
H	-7.74197500	-1.82298600	1.16018000
H	-7.26153800	-0.10196500	1.05611400
H	-6.61765000	-1.11837600	2.38191500
S	-5.50993400	-1.52487100	0.27308000
O	-4.38202200	-0.58097700	0.73122300
C	-5.11947200	-3.15665300	0.98136700
H	-5.00775700	-3.06380700	2.06526200
H	-5.92739300	-3.85015700	0.72939300
H	-4.17864900	-3.47210100	0.51230900

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C	-5.97747200	0.53322200	-0.08823700
C	-4.78910400	-0.02209800	-0.56333800
C	-3.68837300	0.79219300	-0.89301200
C	-3.82288900	2.18840300	-0.74720500
C	-5.01129800	2.74230900	-0.27798900
C	-6.09263100	1.91774100	0.05726300
H	-6.81218800	-0.11378300	0.16469000
H	-4.70195500	-1.09943300	-0.67603200
H	-3.00221300	2.84355000	-1.02249400
H	-5.10108700	3.82063600	-0.18170400
H	-7.01856000	2.35405800	0.42035800
C	-2.46291200	0.14852400	-1.37540100
C	-1.26624800	0.74322900	-1.57262200
H	-2.56227500	-0.91401900	-1.58687400
H	-1.11759800	1.80267400	-1.38135700
C	-0.07606500	0.08779900	-2.14339900
O	0.84080100	0.80151700	-2.57493700
C	-0.02398300	-1.40965200	-2.30546800
C	-0.26816700	-1.88642600	-3.73718000

C	1.10551000	-1.97249200	-3.15457100
H	-0.45937200	-1.11823800	-4.48027300
H	-0.86162800	-2.79083400	-3.82130700
H	1.47562000	-2.95247900	-2.86903700
H	1.85308100	-1.25843000	-3.48330300
C	-0.53305000	-2.33330800	-1.19935500
O	-1.30970000	-3.25829700	-1.46150900
N	-0.02021500	-2.07099200	0.03318300
H	0.65936400	-1.26696700	0.12806600
C	-0.28819000	-2.76025100	1.23545600
C	0.40521800	-2.31983200	2.38102100
C	-1.18641100	-3.83723000	1.35192100
C	0.20012700	-2.93736700	3.61262400
H	1.10258000	-1.49368300	2.27889200
C	-1.37903100	-4.44412500	2.59654400
H	-1.71214300	-4.19048900	0.47667000
C	-0.69574700	-4.00539300	3.73235400
H	0.74654100	-2.58362700	4.48324400
H	-2.07443900	-5.27611900	2.67024400
H	-0.85397800	-4.48801800	4.69241000
Na	2.14847100	1.64312700	-0.84050200
H	1.66000200	-0.05775100	0.43254900
C	4.62342300	-1.14018600	-0.93244800
H	5.20104700	-1.95343900	-0.48339500
H	4.70769300	-1.18153800	-2.02012600
H	3.57523000	-1.16823600	-0.61598000
S	5.34210100	0.45801400	-0.40512200
O	4.42427100	1.55305300	-0.97002200
C	4.92488900	0.30880100	1.37038100
H	3.84331100	0.15397300	1.45416900
H	5.48697900	-0.52584600	1.79944600
H	5.22724200	1.24386700	1.84625100
C	-0.40016400	1.93175600	2.17226400
H	-0.54300900	1.85127100	3.25374800
H	-0.02450700	0.99022300	1.76061700
H	-1.32445300	2.23268900	1.67278300
S	0.90855600	3.15470000	1.83208700
O	0.99804300	3.28596200	0.30252300
C	0.02138000	4.65253500	2.38664700
H	-0.90403800	4.75301700	1.81422700
H	-0.18396500	4.57566800	3.45800600
H	0.67633500	5.50360500	2.19135600

TS1e

C	6.85764300	-0.20077200	-0.16854800
C	5.54478600	-0.31009700	-0.62721600
C	4.59072600	-1.06915300	0.07887000
C	4.99885700	-1.72820300	1.25674300
C	6.31043100	-1.62255200	1.71140900
C	7.24479000	-0.85658100	1.00257900
H	7.57650300	0.39361100	-0.72473700
H	5.24130200	0.20154500	-1.53651900
H	4.29079400	-2.33529900	1.81205200
H	6.60967500	-2.14082100	2.61790300
H	8.26708800	-0.77719200	1.36076800
C	3.22874200	-1.13450000	-0.45460200
C	2.14741400	-1.68201400	0.14809400
H	3.09344700	-0.66762500	-1.42822100
H	2.21006500	-2.14885100	1.12790000
C	0.80377700	-1.74124300	-0.44274300
O	-0.08262700	-2.36549400	0.15952300
C	0.53031100	-1.07849600	-1.77547500
C	0.88896800	-1.88384400	-3.01018100
C	-0.55588600	-1.65973100	-2.64800900
H	1.30150800	-2.87808300	-2.86182000
H	1.32448900	-1.32254700	-3.83108200
H	-1.12927900	-0.95883700	-3.24653000
H	-1.12450300	-2.49583100	-2.25207000
C	0.77553100	0.44337200	-1.83682800
O	1.75091700	0.87846100	-2.47183900
N	-0.14446200	1.16017600	-1.15565700
H	-1.19019900	0.59215300	-0.73770700
C	-0.13030000	2.56149300	-1.02375900
C	-1.29583900	3.16205500	-0.49584800
C	0.96348600	3.39610400	-1.34004300
C	-1.36240800	4.53807300	-0.28461700
H	-2.14592800	2.53094600	-0.26060000
C	0.88159100	4.77365000	-1.12082500
H	1.85480600	2.95868800	-1.76674900
C	-0.27249600	5.35879700	-0.59369200
H	-2.27473200	4.97200400	0.11769800
H	1.73607000	5.39626800	-1.37447500
H	-0.32549700	6.43203400	-0.43452200
Na	-2.21676900	-1.74168900	0.69103800
H	-2.11682800	0.16813000	-0.36084500
C	-4.50127500	-1.08199000	-2.38881900
H	-5.23167200	-0.45154600	-2.90399100
H	-4.20949400	-1.91328500	-3.03343500

H	-3.62513500	-0.50820600	-2.07029500
S	-5.28448400	-1.81043700	-0.90496900
O	-4.17129900	-2.55026300	-0.15005200
C	-5.55851400	-0.24030900	-0.00422800
H	-4.60254100	0.28396300	0.08566600
H	-6.29301700	0.35949900	-0.54924600
H	-5.95046700	-0.50438200	0.97984900
C	-0.26081600	1.04337900	2.60444100
H	-0.03805900	2.06843300	2.91273200
H	-0.21044400	0.97194000	1.51677900
H	0.42179800	0.32870800	3.07124200
S	-1.97174800	0.63315900	3.08831800
O	-2.16646700	-0.86298300	2.79706000
C	-1.74201400	0.72853700	4.89910600
H	-0.95623300	0.02976000	5.19667500
H	-1.48703700	1.75430100	5.17917700
H	-2.69027600	0.44068500	5.35660200

Int1e

C	6.93038300	0.95470000	-0.06090000
C	5.61471300	0.85548200	-0.51362500
C	4.86345000	-0.31819700	-0.30643500
C	5.47884600	-1.39722000	0.36086200
C	6.79368200	-1.29962000	0.80759200
C	7.52446900	-0.12252500	0.60101700
H	7.49042300	1.87047300	-0.22549500
H	5.15009400	1.69391100	-1.02521400
H	4.92998500	-2.32025900	0.51989600
H	7.25441200	-2.14217100	1.31532900
H	8.54996900	-0.05014100	0.95147800
C	3.48730100	-0.35392700	-0.80321200
C	2.55866300	-1.31095500	-0.56751400
H	3.18758000	0.51046300	-1.39367100
H	2.76896900	-2.17870200	0.05344700
C	1.18101300	-1.24273500	-1.06851100
O	0.34529300	-2.08459600	-0.68469400
C	0.78557000	-0.12614000	-1.99639600
C	1.31102300	-0.10558800	-3.40469100
C	-0.14527500	-0.42758100	-3.15340800
H	1.95819700	-0.91749100	-3.72643000
H	1.56739300	0.87417900	-3.79685100
H	-0.88720800	0.32532600	-3.40405200
H	-0.47503500	-1.45420500	-3.29623400

C	0.61442400	1.23223000	-1.24841400
O	1.38079700	2.16720800	-1.56178800
N	-0.36624300	1.16035500	-0.33827200
C	-0.71529300	2.25226500	0.46515800
C	-1.76741800	2.04104100	1.39172900
C	-0.12772700	3.54275100	0.44490400
C	-2.20954000	3.04812100	2.24785600
H	-2.23021400	1.05829500	1.43355500
C	-0.57925900	4.54443300	1.30777300
H	0.67393500	3.73786300	-0.25368100
C	-1.61794700	4.31612400	2.21517100
H	-3.01960200	2.84217800	2.94459300
H	-0.10743600	5.52363900	1.26521700
H	-1.95916100	5.10511100	2.87945400
Na	-1.68989100	-0.81544100	-0.56614000
C	-6.01901400	0.27173800	-2.18537000
H	-7.05314200	0.34739900	-1.83789400
H	-5.99701700	-0.06903800	-3.22205600
H	-5.49914000	1.22853700	-2.09339600
S	-5.13703100	-0.98356200	-1.19164800
O	-3.67402500	-0.90075700	-1.64189300
C	-5.23397600	-0.13465600	0.42307300
H	-4.84541800	0.88251400	0.32437200
H	-6.27515100	-0.12916200	0.75858300
H	-4.60841700	-0.70872100	1.11166800
C	-0.20345900	-1.08192100	2.89829600
H	0.42514200	-1.49712800	3.69109700
H	-0.56649900	-0.09343200	3.18485700
H	0.33727700	-1.01667400	1.95213500
S	-1.66628100	-2.15826700	2.69497300
O	-2.45120400	-1.61083000	1.48835100
C	-0.79659100	-3.64909000	2.09247400
H	-0.23058100	-3.39354900	1.19206400
H	-0.14411300	-4.02160300	2.88745900
H	-1.56486100	-4.39156100	1.86763000

TS2e

C	-5.01931000	1.47889700	1.10669900
C	-3.73632700	1.38207800	0.56864800
C	-3.54034600	0.89643200	-0.73502000
C	-4.66383800	0.49518900	-1.47642900
C	-5.94986900	0.60077100	-0.94484900
C	-6.13078300	1.09319000	0.35054200
H	-5.15288000	1.84835500	2.11945700

H	-2.87644100	1.66779000	1.16593500
H	-4.52482200	0.10606500	-2.48202000
H	-6.80768700	0.29592300	-1.53758600
H	-7.12960200	1.16965800	0.77079500
C	-2.19238300	0.80101400	-1.34212200
C	-1.21492900	1.81485400	-1.10571600
H	-2.21381300	0.35680000	-2.33164900
H	-1.43599100	2.65067700	-0.45016400
C	0.10583600	1.56397400	-1.49899300
O	1.14046000	2.26011900	-1.24656400
C	0.30161000	0.16501500	-2.08095600
C	0.03802300	-0.12417500	-3.54395700
C	1.45139400	-0.11528100	-3.00967800
H	-0.27869400	0.70515600	-4.17102000
H	-0.40529800	-1.08329200	-3.79902800
H	1.96282000	-1.06760100	-2.91087900
H	2.08571200	0.72543600	-3.27853500
C	-0.07263800	-0.85627100	-1.00155900
O	0.86378400	-1.51189800	-0.46397900
N	-1.36244700	-0.87365500	-0.67743200
C	-1.86065700	-1.56163400	0.44271900
C	-1.29926400	-1.40717500	1.72500300
C	-2.99973900	-2.37221400	0.29941800
C	-1.86318600	-2.05314500	2.82581500
H	-0.41755400	-0.78747100	1.84656700
C	-3.56157900	-3.01297200	1.40438400
H	-3.43576900	-2.49068400	-0.68755400
C	-2.99659000	-2.85876900	2.67411200
H	-1.41592900	-1.92434800	3.80826200
H	-4.44316100	-3.63454600	1.27276400
H	-3.43379200	-3.35834000	3.53384000
Na	2.53148700	0.38199100	-0.39826600
C	3.39745700	-3.58675200	-0.99550400
H	3.38483000	-4.57687100	-0.53071800
H	3.87824800	-3.64428000	-1.97413700
H	2.39147700	-3.16505900	-1.07157700
S	4.41613500	-2.46574800	0.02935300
O	4.26825400	-1.06684600	-0.58757600
C	3.35791900	-2.49327500	1.52281100
H	2.32548700	-2.27153100	1.23953800
H	3.43673300	-3.48000600	1.98841000
H	3.75166700	-1.73053600	2.19788500
C	1.18174500	3.51596700	1.81685900
H	1.11212000	4.59147300	2.00470700

H	0.67133700	2.96803000	2.61132800
H	0.78725500	3.25112600	0.83128400
S	2.94014000	3.02209500	1.87932200
O	2.98548200	1.53222800	1.50666300
C	3.48614500	3.94170300	0.39436000
H	2.85800100	3.64946000	-0.45128600
H	3.40913000	5.01399100	0.59644200
H	4.53101200	3.67339700	0.22520700

Int2e

C	2.60867100	2.62472800	-2.64788700
C	1.88696000	1.94827000	-1.66428900
C	2.17336600	2.13833400	-0.30458100
C	3.18964300	3.03259000	0.04578700
C	3.91251800	3.72009700	-0.93552200
C	3.62655900	3.51517400	-2.28611900
H	2.37389900	2.46586300	-3.69724800
H	1.08178400	1.27346600	-1.94115300
H	3.42053000	3.19193900	1.09626100
H	4.69782100	4.41153600	-0.64275300
H	4.18608400	4.04622900	-3.05115200
C	1.36671400	1.41492800	0.77341800
C	-0.11049900	1.62184700	0.56178900
H	1.70482700	1.82307900	1.74320100
H	-0.41349200	2.54636200	0.08133200
C	-1.05475900	0.73495400	0.98514200
O	-2.34671100	0.84642300	0.83658200
C	-0.53189600	-0.51539700	1.67103600
C	-0.81861200	-0.68505100	3.17193100
C	-1.50262700	-1.55876200	2.16569400
H	-1.38637200	0.11493100	3.63818500
H	-0.03659400	-1.12572900	3.78375600
H	-1.18512600	-2.59325300	2.10598900
H	-2.55034600	-1.35623900	1.97016700
C	0.82261700	-0.99986100	1.23649000
O	1.13591000	-2.19881000	1.29152100
N	1.71059400	-0.04881700	0.79435500
C	3.10522200	-0.41498400	0.76830500
C	3.72759400	-0.78790000	-0.42521200
C	3.84711900	-0.38082300	1.95385600
C	5.08307900	-1.12430600	-0.43390700
H	3.14993600	-0.80295300	-1.34283700
C	5.20312300	-0.71422400	1.94488400
H	3.35507400	-0.10218600	2.88113600

C	5.82459400	-1.08714400	0.74994400
H	5.56037800	-1.41103200	-1.36671700
H	5.77114200	-0.68699900	2.87046800
H	6.87912300	-1.34745900	0.74147800
Na	-3.13194900	-0.51594900	-0.72010900
C	-0.73670000	-4.33638700	-0.58018200
H	-0.07414800	-5.15329100	-0.88139600
H	-1.67077500	-4.74682700	-0.19131700
H	-0.24755000	-3.68894400	0.15421100
S	-1.16973900	-3.38025200	-2.07493500
O	-2.09247000	-2.24055100	-1.62194000
C	0.47165100	-2.63020600	-2.35915200
H	0.80339500	-2.12100700	-1.45223900
H	1.17237200	-3.42301100	-2.63589100
H	0.35997300	-1.92781100	-3.18721700
C	-4.51998400	2.91614800	-0.33766500
H	-4.83042700	3.78505600	0.25020000
H	-4.53646900	3.16657400	-1.40054600
H	-3.53822500	2.54282400	-0.02199000
S	-5.74124900	1.57848400	-0.09395000
O	-5.19975400	0.35507600	-0.85956200
C	-5.39682300	1.27270100	1.67587000
H	-4.32598300	1.07094600	1.79129300
H	-5.70434300	2.15370600	2.24705300
H	-6.00438300	0.41422100	1.97001500

Int3e

C	-3.63473300	2.52130200	1.48626600
C	-3.04358100	1.34114300	1.03600900
C	-3.30809800	0.85097500	-0.25230200
C	-4.16842700	1.57960400	-1.08015700
C	-4.75416000	2.77300600	-0.63950900
C	-4.49226800	3.24578000	0.64713100
H	-3.42687700	2.87981600	2.49105900
H	-2.36870600	0.79089800	1.68628900
H	-4.39236200	1.20587200	-2.07693300
H	-5.42265300	3.32192800	-1.29749700
H	-4.95511500	4.16370500	0.99901100
C	-2.65015600	-0.44495400	-0.75711600
C	-1.16128800	-0.30707800	-0.91273700
H	-3.09384100	-0.64306800	-1.74246200
H	-0.83273100	0.35636900	-1.70877100
C	-0.23649100	-0.88973800	-0.09469800
O	1.05554400	-0.73521500	-0.19938400

C	-2.19137500	-2.20383800	1.00646700
O	-2.60580300	-3.07493500	1.77579800
N	-3.03025200	-1.59138200	0.10050500
C	-4.40611700	-2.00530400	0.04488700
C	-5.26632700	-1.80333200	1.12899600
C	-4.89357600	-2.60072900	-1.12340200
C	-6.60392600	-2.19178000	1.04033600
H	-4.88069400	-1.35456400	2.03715000
C	-6.23500800	-2.98072800	-1.21357800
H	-4.21627500	-2.77570400	-1.95451100
C	-7.09429600	-2.77696200	-0.13094700
H	-7.26466900	-2.03487300	1.88823200
H	-6.60352300	-3.44477400	-2.12423600
H	-8.13654700	-3.07592200	-0.19724600
Na	3.11478300	-0.13691000	0.16988800
C	7.14967100	-1.41089100	2.66373900
H	8.04661300	-2.01246600	2.49219900
H	6.64998100	-1.73688000	3.57771100
H	7.39176500	-0.34723800	2.72895000
S	5.97161100	-1.67031100	1.29090700
O	4.83695100	-0.67144900	1.54986800
C	6.98587900	-0.96172000	-0.05183600
H	7.27205300	0.05914800	0.21487200
H	7.86684400	-1.59189300	-0.20529700
H	6.34831500	-0.96668700	-0.93960600
C	2.12076800	-0.63870300	-3.32330500
H	1.51258300	-1.09021800	-4.11229900
H	2.62405500	0.25175100	-3.70564900
H	1.52302400	-0.41652500	-2.43203200
S	3.42766700	-1.81886200	-2.84059700
O	4.16868900	-1.16589200	-1.65285000
C	2.33425200	-3.08676000	-2.11174600
H	1.73075300	-2.60313500	-1.33566500
H	1.70894900	-3.51057100	-2.90267300
H	2.97977900	-3.86226500	-1.69458800
C	-0.34842700	4.15955900	-0.09522400
C	1.03063900	3.90288100	-0.02768500
C	1.94539100	4.97127000	-0.00693700
C	1.48022100	6.28150800	-0.05585300
C	0.10199000	6.53350900	-0.12385600
C	-0.81113100	5.47572700	-0.14217100
H	-1.05198600	3.33113200	-0.10398000
H	3.00684400	4.75073500	0.04777700
H	2.18240200	7.10990600	-0.04047400

H	-0.25721700	7.55822500	-0.16102500
H	-1.87758200	5.67183200	-0.19159400
C	1.49253400	2.50522300	0.02086300
O	2.67666600	2.17591600	0.08946800
H	0.71104900	1.72529200	-0.01375500
C	-0.74600400	-1.78424000	1.01146800
C	-0.13713400	-1.61519200	2.41003800
C	0.20587400	-2.81853500	1.59859500
H	-0.81434000	-1.74540100	3.24835900
H	0.60830200	-0.83168900	2.50681900
H	1.18972700	-2.85061500	1.14400100
H	-0.24177600	-3.76308800	1.88697700

TS3e

C	-3.00480100	3.56078900	0.53015900
C	-2.62266100	2.22270100	0.61782600
C	-2.75619400	1.36471500	-0.48372300
C	-3.27859800	1.87948800	-1.67357700
C	-3.65287000	3.22472700	-1.77183200
C	-3.51927000	4.06894000	-0.66927500
H	-2.90489300	4.20892500	1.39690400
H	-2.22042800	1.83618400	1.55094500
H	-3.40129200	1.22326900	-2.53193200
H	-4.05582500	3.60580500	-2.70609200
H	-3.81738500	5.11132300	-0.73817000
C	-2.33013600	-0.10664300	-0.38818100
C	-0.81943600	-0.24868900	-0.20381400
H	-2.59254500	-0.56747700	-1.34965100
H	-0.05754800	0.85683100	-0.01483100
C	-0.26821600	-1.04351500	0.86568500
O	0.95024700	-1.32531900	0.96031700
C	-2.67192600	-1.34210300	1.81352700
O	-3.43535700	-1.77183100	2.68012800
N	-3.14386900	-0.80950200	0.63405000
C	-4.56146300	-0.86675800	0.38061300
C	-5.46528200	-0.13906600	1.16009900
C	-5.03220700	-1.65582600	-0.67364200
C	-6.83170000	-0.20140000	0.88281500
H	-5.09617700	0.45957500	1.98464800
C	-6.39954500	-1.70939800	-0.95536100
H	-4.32910500	-2.23660300	-1.26396000
C	-7.30304200	-0.98185600	-0.17701700
H	-7.52896600	0.36225200	1.49597300
H	-6.75645400	-2.32696300	-1.77466300

H	-8.36693500	-1.02597100	-0.39151400
Na	2.67411400	-0.10583200	0.09234300
C	1.73853500	3.60026600	1.00399500
H	1.38355200	4.61579500	0.80669000
H	1.87167500	3.45664500	2.07803300
H	1.06041300	2.85557800	0.58149500
S	3.38384200	3.39799100	0.23604200
O	3.81664000	1.94276300	0.50525400
C	2.83803300	3.46133700	-1.50640900
H	2.08909500	2.67340900	-1.65785200
H	2.42921400	4.45638200	-1.70606900
H	3.72687200	3.29956900	-2.12011100
C	6.74649200	0.48068900	0.67288200
H	7.59277500	0.72783300	1.32038600
H	6.06157700	1.32758600	0.58336700
H	7.08476900	0.15344500	-0.31389400
S	5.76419700	-0.85011700	1.44646200
O	4.65219900	-1.19666800	0.45259300
C	6.98819400	-2.19819100	1.28285100
H	7.24007900	-2.32208100	0.22664300
H	7.87441400	-1.95939800	1.87742100
H	6.51527500	-3.10555000	1.66273000
C	0.21185900	-2.45193900	-2.15166900
C	0.75598800	-1.15962700	-2.12852200
C	1.95568100	-0.93143600	-2.81918300
C	2.60028100	-1.96703700	-3.50327700
C	2.04998800	-3.25061000	-3.51427200
C	0.85063200	-3.48791200	-2.83588200
H	-0.70977000	-2.65439000	-1.61301000
H	2.37807000	0.06963000	-2.82287900
H	3.53163400	-1.76908200	-4.02732200
H	2.54982300	-4.05792500	-4.04195100
H	0.41656000	-4.48413300	-2.83049300
C	0.03448100	0.00145500	-1.45977700
O	0.90569000	1.02237700	-0.93290000
H	-0.62467500	0.44223800	-2.22853900
C	-1.18463900	-1.42970800	1.98693300
C	-0.66455800	-1.20903000	3.41841600
C	-0.71129800	-2.58717400	2.87481700
H	-1.41624000	-0.92133700	4.14626900
H	0.30152900	-0.71853500	3.48511200
H	0.22269600	-3.03826300	2.55846300
H	-1.49786100	-3.24361000	3.22930500

Int4e

C	3.21987300	2.00786000	3.09290000
C	2.76729000	1.47827100	1.88476300
C	2.88312000	0.10586200	1.61342700
C	3.45863800	-0.72016900	2.58464900
C	3.90358600	-0.19637900	3.80487200
C	3.78705300	1.16970400	4.06200000
H	3.13202200	3.07464200	3.28197200
H	2.32034800	2.13231400	1.14045000
H	3.56839500	-1.78348800	2.38341300
H	4.34586300	-0.85595700	4.54650300
H	4.13578700	1.58179800	5.00471000
C	2.37169200	-0.48218700	0.28457400
C	0.87853200	-0.29250600	0.10942800
H	2.58353200	-1.55964700	0.33017800
H	-0.49985400	0.33869500	2.13712000
C	0.34106400	0.62946900	-0.76142700
O	-0.92434800	0.90003600	-0.88450800
C	2.73767100	0.98888200	-1.73495500
O	3.49873000	1.48556500	-2.56909400
N	3.16957500	0.02951000	-0.84929900
C	4.53433200	-0.41995000	-0.92608500
C	5.59553800	0.43685800	-0.61906000
C	4.79434700	-1.74456700	-1.29191500
C	6.90894800	-0.03221200	-0.67749300
H	5.38672100	1.46519600	-0.34692800
C	6.10914300	-2.21436100	-1.34192500
H	3.96592200	-2.39946600	-1.54666500
C	7.16997400	-1.35839200	-1.03500000
H	7.72930100	0.63958900	-0.44141000
H	6.30269900	-3.24380200	-1.62998000
H	8.19317200	-1.72071100	-1.07762600
Na	-2.65935800	-0.02510300	0.19527900
C	-3.03511400	3.23655300	-1.64278900
H	-2.66177200	4.21630700	-1.95490500
H	-3.92008600	2.97727800	-2.22771000
H	-2.25977800	2.46545000	-1.72020800
S	-3.57529100	3.34045500	0.09916800
O	-3.97484600	1.90714400	0.50584900
C	-1.93407300	3.62211100	0.84935800
H	-1.27626400	2.80648300	0.53349800
H	-1.55271500	4.59448300	0.52493000
H	-2.07980200	3.62455700	1.93143900
C	-6.57854400	0.13862000	1.26980700

H	-7.61730900	0.46639300	1.16922200
H	-5.92300400	0.99039200	1.46284700
H	-6.47678100	-0.61821900	2.05201900
S	-6.01284400	-0.56263700	-0.31836800
O	-4.62165500	-1.15082600	-0.06125200
C	-7.13142600	-2.00833100	-0.36677900
H	-6.97295500	-2.61248200	0.52993500
H	-8.16750900	-1.66528300	-0.43642700
H	-6.86729900	-2.58444500	-1.25536800
C	-0.65096800	-2.57898900	-1.03661800
C	-0.71755200	-2.32527100	0.33864400
C	-1.46688900	-3.19757500	1.14724000
C	-2.13113400	-4.29318300	0.59477600
C	-2.05617200	-4.53797200	-0.78028200
C	-1.31647800	-3.67681900	-1.59271400
H	-0.07127400	-1.91209300	-1.66636800
H	-1.52724100	-3.00973800	2.21571000
H	-2.70412600	-4.95705600	1.23651100
H	-2.56879200	-5.39307200	-1.21233400
H	-1.25342600	-3.85628400	-2.66255900
C	0.04490300	-1.17350700	1.00112100
O	-0.95872000	-0.43941000	1.78982100
H	0.71781100	-1.63906000	1.73571200
C	1.28942300	1.38422600	-1.66666200
C	1.02552200	2.87161200	-1.92515000
C	0.72369700	1.88012000	-2.99596900
H	1.90345100	3.49769900	-2.04817000
H	0.19522000	3.30302700	-1.37668900
H	-0.31404400	1.61873900	-3.16969700
H	1.40061000	1.83551000	-3.84185000

TS4e

C	1.31356200	-2.59223600	-2.34384400
C	1.54411900	-1.74275400	-1.26179100
C	2.00292300	-0.43236800	-1.46510800
C	2.22424800	0.00174900	-2.77775200
C	1.98969500	-0.84509600	-3.86635500
C	1.53398900	-2.14657900	-3.65189500
H	0.95478000	-3.60202500	-2.16563700
H	1.35822800	-2.10517700	-0.25525600
H	2.59037900	1.01071300	-2.95278500
H	2.16969100	-0.48800900	-4.87654300
H	1.35243100	-2.80929900	-4.49320300
C	2.24384400	0.53380100	-0.29722900

C	0.96478100	0.91856200	0.44918300
H	2.65471600	1.44753900	-0.73394000
H	-0.72546800	0.74441300	-2.18596900
C	0.54725500	0.05365700	1.52238200
O	-0.64306300	-0.05960200	1.90010100
C	3.03807500	-0.66035100	1.77730300
O	3.93601200	-1.16996100	2.44873100
N	3.29548500	0.03376400	0.61903400
C	4.65604200	0.15492900	0.16513600
C	5.37268400	-0.96658700	-0.26224900
C	5.25356600	1.41891700	0.13240500
C	6.68319800	-0.82084600	-0.72054000
H	4.90539500	-1.94414600	-0.22330400
C	6.56184900	1.56298100	-0.33563600
H	4.69656300	2.28188600	0.48627400
C	7.27973300	0.44275300	-0.76254400
H	7.23753800	-1.69603900	-1.04688900
H	7.02151600	2.54697000	-0.35511800
H	8.29906200	0.55280900	-1.12120200
Na	-2.08350900	-0.35907900	0.05903000
C	-4.20226200	0.36601800	-2.88866000
H	-4.57360900	1.02373400	-3.68031200
H	-4.47384700	-0.66877400	-3.10745400
H	-3.12088300	0.48527000	-2.73266700
S	-5.02640900	0.81636700	-1.32196400
O	-4.39632600	-0.08717600	-0.23847900
C	-4.25219000	2.45795700	-1.13337300
H	-3.16849400	2.34282500	-1.24650600
H	-4.66837900	3.12184600	-1.89729000
H	-4.51637900	2.82553600	-0.14020500
C	-4.80376500	-2.72437500	1.52251400
H	-5.71332400	-3.32978500	1.57772600
H	-5.03795900	-1.70476600	1.20701800
H	-4.26976100	-2.72603000	2.47650700
S	-3.71184700	-3.40657700	0.22674700
O	-2.38769400	-2.64003300	0.31895500
C	-3.37991800	-5.02472500	1.01258800
H	-2.94626200	-4.85938600	2.00199200
H	-4.31108700	-5.59435600	1.07908500
H	-2.66614100	-5.54926100	0.37481600
C	-1.35268400	2.81742200	1.74711800
C	-0.73777000	2.91521300	0.48414500
C	-0.97631000	4.08465200	-0.26946400
C	-1.78626100	5.11183500	0.20896500

C	-2.38600200	4.99920500	1.46756500
C	-2.16204600	3.84883200	2.22844700
H	-1.20610300	1.92938000	2.34615500
H	-0.51852600	4.17699500	-1.25034100
H	-1.94523200	6.00024900	-0.39611300
H	-3.01500900	5.79814100	1.85038000
H	-2.62014800	3.74897400	3.20880700
C	0.22232400	1.95486200	-0.09888200
O	-1.35274900	1.04977900	-1.51673000
H	0.67172500	2.37536000	-0.99421700
C	1.59795600	-0.77407800	2.19249600
C	1.16806500	-2.16163000	2.70879500
C	1.36770400	-1.06456300	3.68263000
H	1.93004400	-2.93198500	2.64836300
H	0.15183600	-2.44393100	2.45169800
H	0.48677600	-0.59385700	4.10523300
H	2.27038600	-1.07594700	4.28308200

Int5e

C	-2.89335600	1.95264200	-3.13962500
C	-2.68123800	1.37888400	-1.88421200
C	-3.14451500	0.08645900	-1.60289900
C	-3.82920500	-0.61390700	-2.60411400
C	-4.04389900	-0.04293400	-3.86084700
C	-3.57426900	1.24381800	-4.13316700
H	-2.52513300	2.95464700	-3.34053700
H	-2.15390500	1.94790400	-1.12508100
H	-4.20211800	-1.61476500	-2.39967800
H	-4.58129700	-0.60102200	-4.62214000
H	-3.74004200	1.69194600	-5.10841400
C	-2.89482900	-0.59852000	-0.25215100
C	-1.49164100	-1.19601100	-0.16663100
H	-3.60261700	-1.42830200	-0.18693100
C	-0.42025600	-0.23472900	0.17492700
O	0.74678700	-0.33402900	-0.21001700
C	-2.24961900	1.04129200	1.53906800
O	-2.54224900	1.83544000	2.43211100
N	-3.19568800	0.27759900	0.89933900
C	-4.58210100	0.42176100	1.26349100
C	-5.28845400	1.58389000	0.94153000
C	-5.22615400	-0.62818300	1.92517700
C	-6.63814800	1.69193500	1.28131300
H	-4.77817900	2.39672900	0.43696200
C	-6.57890200	-0.52041100	2.25625300

H	-4.66255400	-1.51809100	2.19088800
C	-7.28717000	0.64038600	1.93469500
H	-7.18291200	2.59804200	1.03297000
H	-7.07371100	-1.33726100	2.77346500
H	-8.33776200	0.72711000	2.19594600
C	6.54450600	-0.50996900	-0.02090100
H	7.35681600	-1.22264100	0.15457900
H	6.95921100	0.48410600	-0.20396500
H	5.85924400	-0.84835900	-0.82283900
S	5.54502600	-0.39296200	1.50233500
O	4.36971900	0.55968000	1.16346600
C	4.85349600	-2.08137300	1.44608100
H	4.43839000	-2.23288100	0.43542700
H	5.66098100	-2.78782000	1.66342900
H	4.09415000	-2.13779800	2.22908100
C	3.83464700	3.69137100	1.17123600
H	4.59214000	4.42339700	1.46669000
H	4.02219300	2.72613700	1.64886700
H	2.82808100	4.05376400	1.39502300
S	3.98247400	3.37918800	-0.62129400
O	2.80661900	2.46919600	-1.00674900
C	3.50557400	5.04362900	-1.20976200
H	2.51327500	5.29089900	-0.82432400
H	4.25006500	5.77273300	-0.87804300
H	3.48354200	5.00241600	-2.30028600
C	-0.58291100	-4.82894400	0.02795100
C	-0.25511400	-3.49857000	-0.32875200
C	1.07617600	-3.22277700	-0.69927800
C	2.04407400	-4.22776700	-0.67845700
C	1.70782300	-5.52738200	-0.29274700
C	0.38585500	-5.82725700	0.05971900
H	-1.60953700	-5.07115500	0.29284300
H	1.36685500	-2.23502300	-1.02169000
H	3.05429300	-3.95479000	-0.97095400
H	2.46409000	-6.30760300	-0.27858200
H	0.11112600	-6.83764600	0.34921900
C	-1.36612300	-2.54234600	-0.32833500
H	-2.32535700	-3.05411400	-0.42385300
O	4.07159600	-1.55525500	-1.46334900
H	4.11764100	-1.93052500	-2.34995300
Na	2.98971900	0.15816700	-0.71406200
C	-0.82229100	0.87788500	1.08727400
C	-0.01610300	2.19260100	0.98897600
C	0.23784000	1.29018300	2.12969200

H	-0.60269600	3.08678700	1.17558800
H	0.71589900	2.23378800	0.18736300
H	1.14589800	0.69633900	2.11842500
H	-0.17508900	1.55620800	3.09642500

TS5e

C	-3.25442200	2.37148400	-3.23733800
C	-3.45358800	1.51848700	-2.15025400
C	-2.43802600	0.64724100	-1.72547000
C	-1.21902500	0.64466300	-2.41823900
C	-1.01858800	1.50785800	-3.50077800
C	-2.03264500	2.37150900	-3.91682500
H	-4.05450900	3.03687100	-3.55015700
H	-4.40515600	1.53589100	-1.63069500
H	-0.40027600	-0.00731300	-2.12572600
H	-0.05673900	1.50269700	-4.00447400
H	-1.87376300	3.03953600	-4.75876600
C	-2.70038000	-0.32925500	-0.55979700
C	-1.42446000	-0.84404700	0.09526600
H	-3.24127900	-1.18689600	-0.96362800
C	-0.72881100	0.26807800	0.80137000
O	0.52603400	0.42511700	0.78113600
C	-1.58009900	1.15999000	1.48025500
C	0.04960600	2.66095800	1.67281600
C	-0.94833300	2.07712800	2.53028800
H	-0.28714500	3.27338000	0.84029900
H	1.12073200	2.51436500	1.77259400
H	-0.56071600	1.56162900	3.41186100
H	-1.77162400	2.75468600	2.79844700
C	-3.04521700	1.17303600	1.38316400
O	-3.73869900	1.89177700	2.11224900
N	-3.58891400	0.27658800	0.46659600
C	-4.97463600	-0.07663100	0.50889600
C	-5.97486100	0.90344600	0.60232700
C	-5.34582500	-1.42945500	0.45500900
C	-7.31936700	0.52839100	0.62761800
H	-5.69485700	1.94623500	0.67139100
C	-6.69296300	-1.79454000	0.46653000
H	-4.58170500	-2.19976600	0.42604700
C	-7.68744800	-0.81740600	0.55329300
H	-8.08235700	1.29806000	0.70156000
H	-6.96132700	-2.84627600	0.42409900
H	-8.73537700	-1.10174900	0.56861800
C	5.35638100	-0.49308100	-2.54063700

H	5.77888000	-1.15103400	-3.30680000
H	6.06323400	0.30753000	-2.31027100
H	4.35305400	-0.11817700	-2.82085100
S	5.13664500	-1.46033100	-1.00867700
O	4.45670700	-0.49633500	-0.00094400
C	3.81765900	-2.56413800	-1.61894600
H	3.03594300	-1.92174300	-2.06548700
H	4.25945200	-3.24244200	-2.35615700
H	3.45884000	-3.13366200	-0.75911600
C	5.23039600	1.54283300	2.24881700
H	6.28011600	1.76398500	2.46373500
H	5.12500600	0.53224700	1.84569500
H	4.60724300	1.68862600	3.13518700
S	4.65255700	2.64991100	0.91933800
O	3.13947200	2.41224600	0.78349200
C	4.80417100	4.23343100	1.82259200
H	4.21325200	4.18459800	2.74076900
H	5.85791500	4.42417500	2.04435700
H	4.41501600	5.01422600	1.16650000
C	0.08253200	-4.30169800	0.08996700
C	0.00693800	-2.96450100	0.53433300
C	0.93268600	-2.54198300	1.50953900
C	1.88730800	-3.42503500	2.01208000
C	1.95006500	-4.74619000	1.55640500
C	1.04218300	-5.18174900	0.58741100
H	-0.62520200	-4.65016400	-0.65812100
H	0.91661900	-1.51922100	1.86103800
H	2.59183800	-3.07588700	2.76147700
H	2.69677400	-5.42775700	1.95380700
H	1.07752900	-6.20453200	0.22340800
C	-1.07246400	-2.14289100	-0.02949700
H	-1.74962900	-2.72961400	-0.65114200
O	2.33733000	-0.08701000	-2.58596400
H	1.89135800	0.05888200	-3.42626000
Na	2.41588000	0.56429800	-0.54735300

Pr+NaOH

C	2.23990900	-2.39772700	2.50374200
C	2.28884700	-1.29445600	1.65039700
C	2.85725400	-1.40630800	0.37356000
C	3.38023900	-2.64243700	-0.02383300
C	3.33394600	-3.74930200	0.82881300
C	2.76132400	-3.62973600	2.09597300

H	1.78752300	-2.29539000	3.48585300
H	1.87479300	-0.34719300	1.98033200
H	3.83466200	-2.74237800	-1.00675200
H	3.74965800	-4.69874300	0.50341800
H	2.72156500	-4.48678700	2.76200400
C	2.91551200	-0.21994200	-0.59874900
C	1.52948000	0.10611600	-1.17162600
H	3.53506800	-0.53820100	-1.44079400
C	0.83795000	1.15816100	-0.44912200
O	-0.48074000	1.47520300	-0.63217500
C	1.48320400	2.00938400	0.38383300
C	-0.64881100	2.83975600	-0.09564000
C	0.51620200	3.04967600	0.88659300
H	-1.64568500	2.89282800	0.34046300
H	-0.58000100	3.51810500	-0.95388300
H	0.92770800	4.06133000	0.83944400
H	0.22517800	2.86032100	1.92889100
C	2.92458200	1.98496800	0.62532400
O	3.49423700	2.85728700	1.28591300
N	3.60636000	0.94701700	0.00271600
C	5.03303100	0.85381900	0.12902200
C	5.64353100	0.73901000	1.38274600
C	5.82155100	0.86178000	-1.02770800
C	7.03220800	0.63117400	1.47315800
H	5.03097900	0.74506900	2.27657200
C	7.20975200	0.74009000	-0.93429100
H	5.34585700	0.97869900	-1.99752200
C	7.81916600	0.62598100	0.31783100
H	7.49931700	0.54641900	2.45011300
H	7.81291000	0.74892500	-1.83769900
H	8.89914500	0.53836600	0.39323000
C	-3.94666000	-2.40417800	2.60768000
H	-4.02900700	-3.40258400	3.04866400
H	-4.45150300	-1.67649600	3.24733400
H	-2.89721200	-2.13284000	2.38738600
S	-4.83116100	-2.40851800	1.01042400
O	-4.60628900	-0.99928500	0.40028500
C	-3.69047800	-3.52463700	0.12687600
H	-2.67760900	-3.09706400	0.24412900
H	-3.77216600	-4.51991700	0.57516100
H	-4.02175600	-3.56206000	-0.91322900
C	-6.12610200	1.70318300	-0.08620900
H	-7.17752400	1.85960900	0.17215700
H	-5.93959300	0.65246400	-0.31992600

H	-5.81940400	2.35616800	-0.90752200
S	-5.09862300	2.06193800	1.37703000
O	-3.63632900	2.02541300	0.90070400
C	-5.48995200	3.84091800	1.53216700
H	-5.23300400	4.34865000	0.59919900
H	-6.55186800	3.95835300	1.76543000
H	-4.88377500	4.23220400	2.35124400
C	-0.31564000	-0.20113200	-4.29976300
C	-0.20489100	-0.54667400	-2.94129100
C	-1.35025500	-0.98446000	-2.25347500
C	-2.58569600	-1.02304700	-2.90569900
C	-2.69444600	-0.64180100	-4.24675700
C	-1.55310400	-0.23597700	-4.94489000
H	0.57007300	0.11307200	-4.84659000
H	-1.25725600	-1.32651400	-1.21937200
H	-3.46503400	-1.35708800	-2.36140000
H	-3.65786400	-0.67361700	-4.74829900
H	-1.62484700	0.04995700	-5.99067400
C	1.12169500	-0.53775300	-2.28942800
H	1.87390700	-1.15419300	-2.78440200
O	-1.44028200	-1.68920700	1.02707800
H	-0.53407600	-1.93009400	1.24746500
Na	-2.48563800	0.07407200	0.43285800

TS3e'

C	-2.96519000	-3.04195900	0.20659700
C	-2.43907600	-1.76989900	-0.02776100
C	-1.87788000	-1.02410500	1.01761000
C	-1.85047200	-1.58501700	2.30021500
C	-2.36203800	-2.86531500	2.53745600
C	-2.92421600	-3.59875800	1.48992900
H	-3.42122200	-3.59482900	-0.61085700
H	-2.48325100	-1.33368900	-1.02083900
H	-1.43455400	-1.01042000	3.12536600
H	-2.33600900	-3.28035700	3.54144700
H	-3.33995700	-4.58560000	1.67339200
C	-1.23012900	0.34482000	0.77898400
C	0.21686800	0.12642000	0.40227900
H	-1.28294700	0.88500300	1.74452600
H	0.75384600	-0.63247900	0.96361700
C	0.87336400	0.96504700	-0.47125500
O	2.17284300	0.90967800	-0.72019600
C	0.12580700	1.98549500	-1.14097900
C	1.83263100	2.09581500	-2.68917100

C	0.89476500	2.96763700	-1.98484000
H	1.43227000	1.34328900	-3.35982300
H	2.90991400	2.19533100	-2.64166600
H	1.38109000	3.78028900	-1.43211500
H	0.14985000	3.40479300	-2.66618400
C	-1.31108300	2.00653100	-1.14574800
O	-1.97536900	2.75800800	-1.87996600
N	-1.96900300	1.12670600	-0.23927600
C	-3.37011400	1.32573500	-0.02177100
C	-4.26160500	1.30480200	-1.10700500
C	-3.88626600	1.51932800	1.26784800
C	-5.62952700	1.47886400	-0.90184800
H	-3.87209100	1.16941800	-2.10777600
C	-5.25961200	1.68277300	1.46935600
H	-3.22125200	1.54856400	2.12380600
C	-6.13997900	1.66571400	0.38694500
H	-6.30081200	1.46411700	-1.75623300
H	-5.63604900	1.82933400	2.47819000
H	-7.20709700	1.79479600	0.54337000
Na	3.59123400	-0.71762100	-0.26955400
C	0.78583100	-2.36805100	-2.40088000
H	-0.09522900	-2.90736800	-2.75976500
H	1.31622300	-1.92468600	-3.24577400
H	0.50832200	-1.59990600	-1.67039000
S	1.92950400	-3.56434900	-1.63069900
O	3.05843000	-2.73653300	-0.99260900
C	0.85589100	-4.09168700	-0.25176000
H	0.51163500	-3.21789100	0.30535400
H	0.00445400	-4.64589500	-0.65478600
H	1.45940900	-4.74442100	0.38171000
C	3.21074100	1.68757300	2.63305800
H	3.05859500	2.68555600	3.05389400
H	3.18651600	0.94379800	3.43199300
H	2.46277700	1.46278500	1.86718000
S	4.87884500	1.61028900	1.88919800
O	4.98384600	0.23384900	1.20665300
C	4.59072300	2.82003900	0.54989800
H	3.73113600	2.48135100	-0.03837800
H	4.41439600	3.80433900	0.99316300
H	5.50129100	2.84578600	-0.05236800

Int3e'

C	3.75653300	3.05553300	-1.53533900
C	2.54892500	2.45674600	-1.17446100

C	2.33782000	2.00074000	0.13656400
C	3.36254500	2.17607100	1.07518600
C	4.57086800	2.78656800	0.72188500
C	4.77292900	3.22475100	-0.58769000
H	3.90417100	3.39710100	-2.55650300
H	1.76030700	2.34085400	-1.91060700
H	3.21638200	1.82765100	2.09522800
H	5.35054700	2.91501300	1.46792400
H	5.71007300	3.69707200	-0.86911900
C	1.01925700	1.33195300	0.56050100
C	-0.21649300	2.09767800	0.13448900
H	1.05426300	1.27405200	1.65434300
H	-0.40475700	3.06856900	0.57770900
C	-0.79326200	1.70440700	-1.03421300
O	-1.81931300	2.39305500	-1.65713400
C	-0.46499900	0.52571200	-1.75801300
C	-1.94789700	1.85974100	-3.00675500
C	-1.31673700	0.44956400	-3.00112000
H	-1.41015700	2.53709400	-3.68138400
H	-3.01084900	1.87717800	-3.26162000
H	-2.08954700	-0.33403500	-2.95473900
H	-0.74308900	0.27156800	-3.91856400
C	0.43656900	-0.41514200	-1.23746800
O	0.72854500	-1.52673500	-1.74825000
N	0.92088900	-0.10275600	0.09874800
C	1.89189800	-0.97742600	0.69150500
C	3.02190700	-1.43165900	-0.00424100
C	1.72180000	-1.36227600	2.02965500
C	3.95022700	-2.26098600	0.62872600
H	3.15997000	-1.14331600	-1.03857900
C	2.66024600	-2.17743700	2.66667700
H	0.84605800	-1.01886700	2.57535000
C	3.77855000	-2.63601000	1.96486000
H	4.81931700	-2.60638000	0.07539000
H	2.51076100	-2.46019000	3.70518500
H	4.50839600	-3.27512400	2.45360500
Na	-1.62060900	-0.56378700	0.55937800
C	-4.64632800	2.20435100	0.27360100
H	-5.22259400	3.12398100	0.41136700
H	-5.25325000	1.46996100	-0.26032700
H	-3.71277200	2.39449300	-0.26546000
S	-4.28987800	1.48424200	1.91602800
O	-3.36040500	0.28998200	1.67654900
C	-3.23102300	2.83219900	2.55138400

H	-2.36504000	2.93676400	1.89332500
H	-3.81432100	3.75573800	2.60194300
H	-2.91285700	2.53926000	3.55379900
C	0.16726200	-4.31105800	-0.16418500
H	0.45954400	-5.23291300	-0.67630800
H	0.32927300	-4.41827300	0.90998900
H	0.69927900	-3.44148200	-0.56194700
S	-1.62507300	-4.06687300	-0.40958900
O	-1.98707200	-2.73289200	0.26458400
C	-1.57174000	-3.73461900	-2.20538000
H	-0.87793900	-2.90559200	-2.38398400
H	-1.24828200	-4.64625600	-2.71683000
H	-2.59039000	-3.48454700	-2.50959400

Int4e'

C	-2.53948000	3.38758000	1.92160600
C	-2.27860100	2.07738600	1.51868400
C	-2.27750200	1.73208100	0.15628000
C	-2.54762700	2.73477500	-0.78291200
C	-2.80807300	4.05103300	-0.38393100
C	-2.80575100	4.38251500	0.97167200
H	-2.54780600	3.63243800	2.98083300
H	-2.08147600	1.31029200	2.26122600
H	-2.56460800	2.48294600	-1.84137700
H	-3.02395200	4.80971800	-1.13178700
H	-3.02169400	5.39923000	1.28891300
C	-1.96496900	0.30048000	-0.31634100
C	-0.51096700	-0.07690800	-0.10104100
H	-2.16761500	0.29830900	-1.39337000
H	0.23910200	0.30728600	-0.77803100
C	-0.24991100	-0.77855400	1.04433200
O	1.04247900	-1.09794000	1.48195100
C	-1.21166500	-1.33664300	1.89609700
C	0.91400200	-1.64156600	2.83542500
C	-0.53427600	-2.14534000	2.97032000
H	1.12005400	-0.82213300	3.53482600
H	1.68118800	-2.41215100	2.94750600
H	-0.60402700	-3.23224300	2.79958600
H	-0.92115200	-1.96330300	3.97971300
C	-2.57407200	-1.41534000	1.48922400
O	-3.44262800	-2.10328700	2.05742500
N	-2.88929000	-0.70143700	0.29074900
C	-4.22747100	-0.71187400	-0.20202500
C	-5.32686000	-0.46668100	0.63576100

C	-4.46375500	-0.95629400	-1.56463500
C	-6.62273100	-0.46909100	0.11734800
H	-5.15866300	-0.29336600	1.69081600
C	-5.75999400	-0.94228100	-2.08322000
H	-3.62425400	-1.16628200	-2.22169100
C	-6.84981600	-0.70119500	-1.24251300
H	-7.46090500	-0.28087000	0.78300300
H	-5.91735300	-1.13280400	-3.14178100
H	-7.86055900	-0.69575700	-1.64054800
Na	2.58261900	-1.61303300	-0.15995800
C	6.06228500	-0.07196100	1.58132000
H	7.02095000	0.45053700	1.51936500
H	5.91556000	-0.45718000	2.59210100
H	5.23407300	0.58168300	1.29892300
S	6.09173700	-1.52016600	0.46348100
O	4.68434400	-2.12060200	0.50542100
C	6.20751900	-0.59840000	-1.11348900
H	5.35093200	0.07584200	-1.19510400
H	7.15366000	-0.05056800	-1.14089500
H	6.18754400	-1.34088500	-1.91372000
C	-0.65278700	-2.71673600	-2.72474400
H	-1.61368200	-3.18872900	-2.94756900
H	-0.16351700	-2.40807700	-3.65083100
H	-0.77037900	-1.86958200	-2.04111600
S	0.44271100	-3.94121700	-1.92995200
O	1.69649700	-3.16395700	-1.49668000
C	-0.55621000	-4.22016500	-0.42648900
H	-0.75564700	-3.27116900	0.07851800
H	-1.49264200	-4.70599100	-0.71493300
H	0.02152700	-4.88933000	0.21422400
C	1.41870500	3.89987200	0.27929600
C	2.25414200	2.98970400	-0.39260500
C	3.00957500	3.42204500	-1.49987500
C	2.93367500	4.74662900	-1.91844600
C	2.10170700	5.64967300	-1.24121400
C	1.34301500	5.22527400	-0.14548500
H	0.81304800	3.55717800	1.11403000
H	3.64205400	2.70635400	-2.01548300
H	3.51560500	5.08183400	-2.77206700
H	2.04157300	6.68210500	-1.57353700
H	0.68672300	5.92098400	0.36749400
C	2.32500600	1.60435500	0.08272800
O	2.99541000	0.71343200	-0.46096100
H	1.73990900	1.37181900	0.98656700

TS4e'

C	-2.82843600	3.69437700	1.20800700
C	-2.67350300	2.31244000	1.06125200
C	-2.48652500	1.74204600	-0.20541600
C	-2.48396700	2.59218000	-1.32173100
C	-2.64568400	3.97270500	-1.18136000
C	-2.81405000	4.53189500	0.08909100
H	-2.97478700	4.11451800	2.19964500
H	-2.70535600	1.67721900	1.93984800
H	-2.35914800	2.16610600	-2.31481100
H	-2.65740200	4.60755200	-2.06368000
H	-2.95199200	5.60352800	0.20397000
C	-2.25253900	0.23965000	-0.41853400
C	-0.75610900	-0.10871900	-0.37441300
H	-2.60349000	0.01770300	-1.42941800
H	0.25339500	0.74406100	-0.88724400
C	-0.37647700	-0.55999100	0.93385200
O	0.95639300	-0.72394500	1.27567500
C	-1.21415300	-0.82635000	1.96781100
C	0.97944700	-1.37683600	2.59078400
C	-0.41987100	-1.16229100	3.20472700
H	1.79961000	-0.92852900	3.15492500
H	1.19096100	-2.43691900	2.41587900
H	-0.78736800	-2.06102300	3.70839800
H	-0.42496700	-0.34792700	3.94312800
C	-2.64587200	-0.96086600	1.77031900
O	-3.40457800	-1.42597500	2.63014100
N	-3.09836700	-0.58305300	0.49628500
C	-4.47326700	-0.75598900	0.14020200
C	-5.50988100	-0.28854500	0.95997400
C	-4.79436700	-1.39131500	-1.06843200
C	-6.84023100	-0.45394900	0.57082700
H	-5.26969100	0.18504100	1.90333200
C	-6.12588600	-1.54117300	-1.46104200
H	-3.99830200	-1.78134000	-1.69638500
C	-7.15642900	-1.07418700	-0.64122000
H	-7.63317900	-0.09046900	1.21866500
H	-6.35545100	-2.03644000	-2.40050900
H	-8.19330800	-1.19612100	-0.94104900
Na	2.69718900	-0.09844200	-0.21940000
C	1.28555900	3.57455300	0.20199300
H	0.76471400	4.46415300	-0.16158600
H	1.51922100	3.68963300	1.26205600

H	0.67785700	2.68169200	0.03921000
S	2.88057600	3.42137100	-0.67029100
O	3.50769500	2.09158400	-0.19775400
C	2.24410900	3.12247700	-2.35629400
H	1.66880200	2.18945800	-2.37205700
H	1.63659000	3.98200700	-2.65385000
H	3.11665400	3.04699500	-3.00889200
C	6.54802100	0.90638600	0.05277700
H	7.43350600	1.36628900	0.50097500
H	5.75911300	1.64713600	-0.10366700
H	6.79584500	0.40646600	-0.88740100
S	5.85327700	-0.31272900	1.22025700
O	4.65880500	-0.96100400	0.50844500
C	7.19312500	-1.55113700	1.12665600
H	7.30676200	-1.87409100	0.08885700
H	8.11872400	-1.11208700	1.50904200
H	6.89330500	-2.39498200	1.75052700
C	-0.40401900	-3.18636400	-1.01780600
C	0.41901000	-2.18131500	-1.55105400
C	1.65921500	-2.55076300	-2.09109800
C	2.07513600	-3.88645800	-2.08585300
C	1.25109100	-4.87693600	-1.54661300
C	0.00726900	-4.52102800	-1.01483400
H	-1.36839000	-2.92051900	-0.59328000
H	2.28751500	-1.78291900	-2.53320200
H	3.04065400	-4.15180400	-2.50860200
H	1.57138800	-5.91507500	-1.54220800
H	-0.64270800	-5.28232200	-0.59191000
C	-0.05746400	-0.73946700	-1.60631200
O	1.01825100	0.22338600	-1.73648400
H	-0.74327100	-0.65357800	-2.46649100

Int5e'

C	-2.73349000	3.70290900	-0.57878100
C	-2.66268300	2.37487100	-0.14175400
C	-2.32314300	1.34384400	-1.03023300
C	-2.08052500	1.68363000	-2.37232000
C	-2.15809000	3.00645800	-2.81534800
C	-2.48193200	4.02708700	-1.91454200
H	-3.01208900	4.48287200	0.12571300
H	-2.90022500	2.13631300	0.88855600
H	-1.85966500	0.89509400	-3.09022300
H	-1.99098600	3.23634100	-3.86461200
H	-2.56292900	5.05542200	-2.25621600

C	-2.21806800	-0.13600500	-0.60297200
C	-0.78034800	-0.60493600	-0.39841000
H	-2.63180900	-0.70847100	-1.43839300
H	0.67141500	0.45112900	-2.22758900
C	-0.36201100	-0.48601800	0.90989500
O	0.95666600	-0.71495900	1.31196000
C	-1.16547400	-0.15753300	2.00008200
C	0.93569600	-0.87815300	2.76791600
C	-0.34042900	-0.16968000	3.26239000
H	1.87287300	-0.46218100	3.14749900
H	0.90750100	-1.95449800	2.97235000
H	-0.82572800	-0.72874300	4.06900500
H	-0.11446200	0.83266900	3.66131300
C	-2.58724100	-0.25243900	1.90350300
O	-3.36532800	-0.24222100	2.87418900
N	-3.07589500	-0.42493300	0.57444200
C	-4.45603900	-0.69171100	0.33661600
C	-5.47425600	0.04669900	0.96189700
C	-4.82037400	-1.71487800	-0.55549500
C	-6.81517400	-0.23223500	0.69128100
H	-5.20891700	0.81705500	1.67348500
C	-6.16218000	-1.97795500	-0.83575400
H	-4.04710000	-2.32092300	-1.01900800
C	-7.17022000	-1.23809700	-0.21178700
H	-7.58777700	0.34774000	1.18924700
H	-6.41753400	-2.77519700	-1.52888300
H	-8.21551800	-1.44637200	-0.42157100
Na	2.59096600	-0.17870800	-0.22784500
C	0.99171300	3.03108300	1.68677000
H	0.40145300	3.93548100	1.85881700
H	1.53118100	2.76526000	2.59751400
H	0.34948100	2.20724600	1.36356100
S	2.24763200	3.40241100	0.41716800
O	2.97859600	2.08085100	0.10556700
C	1.11289600	3.70141400	-0.97872500
H	0.43130900	2.85616100	-1.09506000
H	0.54665800	4.61573000	-0.78567300
H	1.73319200	3.82907900	-1.86795400
C	6.22832700	1.50520400	-0.46079700
H	7.08757900	2.06775000	-0.08455200
H	5.31879100	2.10910000	-0.41499000
H	6.40364300	1.15016100	-1.47970800
S	5.92015100	0.07542800	0.63130800
O	4.76837100	-0.71004000	-0.00874100

C	7.42443000	-0.88227900	0.23594900
H	7.45069200	-1.07672500	-0.83905500
H	8.30602600	-0.32249900	0.56022200
H	7.35599200	-1.82322600	0.78470600
C	0.00754800	-3.50703400	-0.31100900
C	0.63881100	-2.61041400	-1.18612000
C	1.81269700	-3.02415100	-1.83472900
C	2.35139100	-4.29345600	-1.59741400
C	1.71690500	-5.17591300	-0.72126300
C	0.53891800	-4.77746300	-0.08191800
H	-0.90043800	-3.19666000	0.19679800
H	2.30210500	-2.35316700	-2.53227600
H	3.26532400	-4.59112100	-2.10454600
H	2.13254700	-6.16309900	-0.53941500
H	0.03316600	-5.45463500	0.60098500
C	-0.01150200	-1.25739300	-1.48933200
O	1.09558100	-0.39300800	-2.01726900
H	-0.68766200	-1.41591800	-2.34170100

TS5e'

C	2.36946900	2.89939700	-2.33792000
C	2.46475600	1.65499100	-1.71050300
C	2.51705000	1.55786100	-0.31049100
C	2.49875200	2.74646000	0.43521500
C	2.40621400	3.99466900	-0.18846900
C	2.33515900	4.07559300	-1.58132400
H	2.33380900	2.95057400	-3.42305000
H	2.50591800	0.75466700	-2.31371300
H	2.56913200	2.69620200	1.51983800
H	2.40688300	4.90016400	0.41284900
H	2.27361100	5.04259600	-2.07289300
C	2.54725500	0.20800800	0.42949600
C	1.15493600	-0.39033600	0.63747300
H	2.96804500	0.41525700	1.41751300
H	-0.18744500	1.87061500	0.47902100
C	0.76962600	-1.23970000	-0.41550800
O	-0.55167500	-1.58304400	-0.64737700
C	1.61320800	-1.78194700	-1.35112600
C	-0.54115100	-2.65835800	-1.64622400
C	0.81706000	-2.55858600	-2.36804200
H	-1.42265000	-2.50994900	-2.27040200
H	-0.63555800	-3.60213800	-1.09588900
H	1.23657300	-3.54733300	-2.57962800
H	0.73046100	-2.03102300	-3.33051300

C	3.04103200	-1.63699400	-1.24711900
O	3.85378300	-2.24427500	-1.95960400
N	3.46826200	-0.76302000	-0.22030700
C	4.86200100	-0.61772200	0.06067500
C	5.79111100	-0.31880500	-0.94612400
C	5.31386000	-0.76412000	1.38098000
C	7.14278100	-0.16582800	-0.63076800
H	5.45189900	-0.22576300	-1.97003300
C	6.66352600	-0.59415200	1.69488300
H	4.60387900	-1.02908300	2.15943100
C	7.58610100	-0.29556300	0.68838900
H	7.85179300	0.06063100	-1.42249600
H	6.99471600	-0.71193400	2.72319000
H	8.63825100	-0.17124700	0.92855100
Na	-2.28306000	-0.03277800	-0.11599400
C	-3.01952800	3.74464300	-0.76379300
H	-2.99187100	4.81761100	-0.55430100
H	-3.36763900	3.57510900	-1.78441500
H	-2.04021000	3.28725600	-0.60451600
S	-4.23038000	2.95145000	0.35280400
O	-4.15329100	1.44065300	0.06060900
C	-3.32472800	3.22757600	1.91377700
H	-2.32332200	2.78992500	1.81130000
H	-3.29155300	4.30363900	2.10913900
H	-3.89658600	2.72960500	2.69950300
C	-6.11530800	-1.10955100	-0.56160100
H	-7.15942600	-1.01023800	-0.87209100
H	-5.82689400	-0.27627300	0.08233200
H	-5.94059500	-2.06751800	-0.06494300
S	-5.04062600	-0.98343900	-2.03146100
O	-3.60926600	-1.24997500	-1.54689100
C	-5.55461400	-2.53721800	-2.84763200
H	-5.34808300	-3.37477800	-2.17672400
H	-6.61775800	-2.48291000	-3.09821500
H	-4.96181200	-2.63364400	-3.75905900
C	-0.51781800	-2.19208500	2.39509000
C	-0.69119900	-0.79819500	2.36451700
C	-1.74402200	-0.24824600	3.11811800
C	-2.60742600	-1.06351000	3.85419900
C	-2.43369600	-2.45054900	3.85845400
C	-1.38279600	-3.00935500	3.12625400
H	0.31271500	-2.63059700	1.85301100
H	-1.87756800	0.82718200	3.11563400
H	-3.41117900	-0.61400100	4.43176600

H	-3.10091900	-3.08598000	4.43422700
H	-1.22647300	-4.08464000	3.13126900
C	0.29984700	0.08923900	1.65414100
O	-0.84501100	1.37653400	0.98975800
H	0.79670700	0.75668800	2.35884100

TS3d

C	-2.63102400	3.24502900	-0.77923500
C	-1.70542500	2.29691200	-1.22987700
C	-1.01473100	1.48174200	-0.32724100
C	-1.27402100	1.62666400	1.04316800
C	-2.20562300	2.56138500	1.49712900
C	-2.88491600	3.37998500	0.58686000
H	-3.15939400	3.86700100	-1.49664100
H	-1.52252100	2.18718700	-2.29669400
H	-0.75619600	0.98283400	1.74825500
H	-2.41066400	2.64578800	2.56117700
H	-3.61219500	4.10553300	0.94004200
C	0.07108500	0.53313200	-0.83869100
C	1.40865600	1.21683000	-0.65904400
H	-0.12618400	0.37066600	-1.91593200
H	1.47764700	2.21345600	-1.09897200
C	2.57339600	0.46691700	-0.48225600
O	3.77249700	1.01062400	-0.38240700
C	2.45591000	-0.94441500	-0.33299300
C	3.73086700	-1.75668500	-0.38389600
C	4.57382300	-0.98608600	0.51668000
H	4.15410500	-1.89217700	-1.38407500
H	3.45226200	-2.73280100	0.03913200
H	4.29389500	-0.93664500	1.56441100
H	5.49817600	-0.50725200	0.21989100
C	1.20067300	-1.58121900	-0.02363900
O	1.11920200	-2.76463800	0.34176100
N	0.03413500	-0.77879600	-0.14589200
C	-1.22780200	-1.45487500	-0.07470300
C	-1.57596500	-2.15696800	1.08876800
C	-2.13582800	-1.41925200	-1.14131300
C	-2.80508600	-2.80865900	1.17903300
H	-0.87065000	-2.19990800	1.90972000
C	-3.37215300	-2.06369500	-1.04221700
H	-1.88359500	-0.89348200	-2.05559100
C	-3.71336900	-2.76304700	0.11622700
H	-3.05504100	-3.35221300	2.08602800
H	-4.06389900	-2.02168400	-1.87908000

H	-4.67278700	-3.26673800	0.19119000
Na	2.82488200	2.51563200	0.90336200

Int3d

C	-2.54161800	3.28422400	-0.82460600
C	-1.61890800	2.32108900	-1.24862200
C	-0.98014500	1.48256600	-0.32926700
C	-1.29451300	1.61712800	1.03053300
C	-2.22460800	2.56543600	1.45799900
C	-2.84818300	3.40976200	0.53138500
H	-3.02660200	3.92579000	-1.55536000
H	-1.39615600	2.21884900	-2.30868300
H	-0.82245800	0.95270300	1.74879300
H	-2.47285300	2.64039500	2.51359100
H	-3.57335500	4.14719900	0.86369400
C	0.10702800	0.52113000	-0.81169300
C	1.46853000	1.19090000	-0.63575600
H	-0.06595500	0.35962000	-1.89341200
H	1.61815800	2.05998000	-1.27762200
C	2.52886500	0.29473900	-0.48691600
O	3.84176100	0.76956400	-0.35910400
C	2.44652800	-1.05135000	-0.22911100
C	3.80021000	-1.57296700	0.17720900
C	4.69932000	-0.42189300	-0.31171100
H	4.07462800	-2.52063200	-0.29681800
H	3.88151500	-1.72573800	1.26670500
H	5.54491100	-0.18484900	0.33793400
H	5.06023300	-0.59723800	-1.33074600
C	1.16896600	-1.65655300	0.02274700
O	1.03603500	-2.82013700	0.42109100
N	0.03183800	-0.79907700	-0.12149700
C	-1.25315400	-1.43691600	-0.08331600
C	-1.65888000	-2.11677400	1.07429400
C	-2.12295200	-1.39367000	-1.18125600
C	-2.90595700	-2.73835400	1.12936800
H	-0.98341500	-2.16697100	1.91959300
C	-3.37703000	-2.00737500	-1.11877200
H	-1.82644900	-0.88493900	-2.09201300
C	-3.77541900	-2.68379700	0.03527800
H	-3.20011400	-3.26532900	2.03292800
H	-4.03809600	-1.95916400	-1.97984000
H	-4.74917800	-3.16287500	0.08246700
Na	2.63831700	2.22885100	1.19424100

Int4d

C	3.56694100	-1.84616100	2.74242700
C	2.37755700	-1.24051300	2.30904700
C	2.26422500	-0.71552300	1.01268100
C	3.36465900	-0.83028400	0.14316400
C	4.55212300	-1.44123300	0.56712900
C	4.66094300	-1.94630200	1.87345000
H	3.63100900	-2.24979200	3.75347000
H	1.52527400	-1.17325900	2.98702100
H	3.27480900	-0.46216100	-0.87974000
H	5.39004300	-1.54021500	-0.12600700
H	5.58078700	-2.42851200	2.20224000
C	0.98963700	0.04330600	0.60461800
C	1.19441200	1.54865600	0.80340300
H	0.20763000	-0.28756200	1.30302100
H	0.91775800	1.93234200	1.78781500
C	0.95097900	2.34511700	-0.31444200
O	1.25717300	3.71893600	-0.27384200
C	0.57729700	1.95070700	-1.57367700
C	0.68544800	3.11542800	-2.52799700
C	0.74427600	4.28757500	-1.52782000
H	-0.16986400	3.21324000	-3.20656300
H	1.59092500	3.07212600	-3.16024900
H	1.41827200	5.09923500	-1.80606200
H	-0.25171100	4.68913200	-1.31870000
C	0.32638700	0.57018200	-1.85364600
O	-0.04368800	0.14735200	-2.95749300
N	0.55561900	-0.32910600	-0.77492700
C	0.21519800	-1.70894300	-0.97345400
C	0.83179100	-2.45112700	-1.99283800
C	-0.72793800	-2.33944000	-0.14746800
C	0.51283400	-3.79767400	-2.17781700
H	1.54652700	-1.96167600	-2.64652200
C	-1.03731300	-3.69178300	-0.32651900
H	-1.23544200	-1.77412300	0.63079300
C	-0.41825900	-4.42720000	-1.34206100
H	0.99734800	-4.35725200	-2.97563900
H	-1.77254000	-4.16370200	0.32405000
H	-0.66055900	-5.47794900	-1.48341600
Na	3.22816700	2.86774900	0.81666000
C	-4.59627300	0.26729500	1.92408900
C	-3.55123900	0.72849500	1.09889300
C	-3.55642400	0.43904400	-0.27605200
C	-4.60300600	-0.30660500	-0.82697400

C	-5.64183000	-0.75969400	-0.00336200
C	-5.63807100	-0.47604200	1.37224000
H	-4.56663600	0.49583600	2.98928200
H	-2.73949300	0.78654400	-0.91038900
H	-4.60336700	-0.53305100	-1.89399700
H	-6.45748100	-1.33980800	-0.43171600
H	-6.44497600	-0.83801400	2.00762300
C	-2.42280600	1.50720700	1.66059100
O	-2.29536700	1.79470500	2.84262800
H	-1.65170700	1.82227000	0.91893900

TS4d

C	0.46905500	0.56199900	4.11376100
C	0.27998900	0.01014900	2.84606500
C	0.45531500	0.78036400	1.68629500
C	0.84522300	2.11708800	1.82991600
C	1.02992500	2.67647300	3.09893500
C	0.84072700	1.90377500	4.24624500
H	0.33511300	-0.05706700	4.99685600
H	-0.00810600	-1.03410700	2.75308500
H	1.01801700	2.72956300	0.95176100
H	1.33263600	3.71656300	3.18633400
H	0.99315800	2.33650300	5.23100200
C	0.18579900	0.12632900	0.32205800
C	-1.31893400	0.12415000	0.00248100
H	0.49734900	-0.91543400	0.41022000
H	-2.28810200	-0.09524500	1.03153100
C	-1.65627100	1.27087400	-0.79046400
O	-2.99770200	1.62658100	-1.03691500
C	-0.79505700	2.13971700	-1.36579600
C	-1.53720800	3.27519900	-2.01906900
C	-2.96593100	2.70006200	-2.04492600
H	-1.16694200	3.49549100	-3.02414700
H	-1.47992600	4.20461200	-1.43567300
H	-3.74826700	3.41418900	-1.77775800
H	-3.20053400	2.23877600	-3.01072400
C	0.62582400	1.83537300	-1.48030200
O	1.37996600	2.48252800	-2.21711600
N	1.04415800	0.72379700	-0.74702200
C	2.40200000	0.27257800	-0.83189200
C	3.47881100	1.16343600	-0.71872100
C	2.66261000	-1.09336600	-1.01176400
C	4.78998200	0.68927700	-0.78427700
H	3.28697500	2.22159300	-0.59761500

C	3.97632700	-1.56352500	-1.06261200
H	1.83732900	-1.78967700	-1.12022600
C	5.04768000	-0.67413700	-0.95117600
H	5.61393300	1.39225900	-0.69831100
H	4.15826600	-2.62584900	-1.19994000
H	6.07016100	-1.03804700	-0.99581400
Na	-4.56653200	0.44477100	0.09439500
C	-1.38726000	-3.23964100	0.94539500
C	-1.42892800	-2.48764600	-0.23563700
C	-0.79330900	-2.99344100	-1.38051000
C	-0.12082100	-4.21665100	-1.34399700
C	-0.07495500	-4.95588400	-0.15722400
C	-0.71152700	-4.46315700	0.98499000
H	-1.91104000	-2.86325800	1.81760700
H	-0.82739700	-2.42489800	-2.30765100
H	0.36250100	-4.59438000	-2.24094500
H	0.44563600	-5.90880900	-0.12654600
H	-0.68933500	-5.03602400	1.90823700
C	-2.15016400	-1.15887600	-0.29641100
O	-3.12741500	-0.98807600	0.76835300
H	-2.64087100	-1.09719300	-1.28321000

Int5d

C	-0.00628200	-0.13725300	3.93295300
C	0.10134000	0.35362200	2.62705100
C	-0.48192000	-0.32158600	1.54359100
C	-1.22307800	-1.48945200	1.81422200
C	-1.32360700	-1.98820300	3.11801000
C	-0.70641900	-1.32037100	4.18338100
H	0.44690100	0.41118900	4.75444300
H	0.64004100	1.28187000	2.44590000
H	-1.74299100	-1.99008500	1.00241300
H	-1.91309600	-2.88209400	3.30697600
H	-0.79725600	-1.70145700	5.19620500
C	-0.20732600	0.15708700	0.10349200
C	0.88162500	-0.70978100	-0.52304200
H	0.16459100	1.18145500	0.18847700
H	2.53865400	-0.51267300	1.74216700
C	0.36914800	-1.77678100	-1.24510000
O	1.15139100	-2.89959200	-1.55975400
C	-0.94215400	-1.95196200	-1.64908800
C	-1.09744000	-3.28701200	-2.33036000
C	0.38080100	-3.66357200	-2.55143800
H	-1.63879200	-3.22473900	-3.28008400

H	-1.62117700	-4.03751600	-1.71496800
H	0.62197200	-4.71763500	-2.39666800
H	0.73317800	-3.35020800	-3.54006400
C	-1.90522100	-0.90760300	-1.48033900
O	-3.05176400	-0.92413300	-1.95318000
N	-1.44068900	0.20964100	-0.72455700
C	-2.30001200	1.33245200	-0.50921600
C	-3.62560700	1.17531600	-0.07667400
C	-1.80318500	2.62983000	-0.70914500
C	-4.42836100	2.29479900	0.15057000
H	-4.02597000	0.17867500	0.05693500
C	-2.60426200	3.74669400	-0.46458600
H	-0.78757900	2.76394400	-1.06988700
C	-3.92389000	3.58497200	-0.03441200
H	-5.45449600	2.15454700	0.47950400
H	-2.19923700	4.74209200	-0.62575700
H	-4.55185100	4.45214500	0.14879000
Na	1.29719400	-2.83303200	0.90703900
C	3.94891200	1.35668200	0.37462200
C	2.87260700	0.90177700	-0.40172100
C	2.34219100	1.76213000	-1.37669700
C	2.86123100	3.04525700	-1.55864800
C	3.92219700	3.49523500	-0.76723400
C	4.46456600	2.64493400	0.19794900
H	4.40027300	0.69570100	1.10688100
H	1.52087500	1.41315900	-1.99584100
H	2.43501700	3.69347200	-2.31923600
H	4.32400900	4.49474300	-0.90601800
H	5.29738000	2.97769100	0.81131700
C	2.33172300	-0.52097500	-0.28508000
O	2.79523200	-1.12779400	1.03730900
H	2.88089900	-1.15367500	-0.99039100

TS5d

C	0.18086000	0.02480200	3.84210700
C	0.21593900	0.46160900	2.51493200
C	-0.40839700	-0.26746500	1.49264300
C	-1.10228600	-1.44063400	1.84375200
C	-1.13201600	-1.88527100	3.17093100
C	-0.48332600	-1.15849800	4.17536600
H	0.66838600	0.61171600	4.61555400
H	0.73968600	1.38145700	2.26637300
H	-1.64760900	-1.99262900	1.08438000
H	-1.68809600	-2.78468100	3.42343100

H	-0.51593600	-1.49864500	5.20619300
C	-0.23826900	0.18943200	0.03172300
C	0.85168900	-0.63921500	-0.65195300
H	0.08233400	1.23041200	0.07495600
H	2.93680800	-0.53232300	1.73165300
C	0.32047600	-1.80775700	-1.24694700
O	1.11048000	-2.92548100	-1.50513300
C	-0.98934800	-2.01585900	-1.57286000
C	-1.16500300	-3.39651200	-2.15166300
C	0.30820300	-3.79666100	-2.37751800
H	-1.73088100	-3.39932700	-3.08826500
H	-1.68127400	-4.08398600	-1.46409200
H	0.55479700	-4.82706300	-2.11428500
H	0.62983500	-3.59650800	-3.40480000
C	-1.98231300	-0.97864200	-1.39953600
O	-3.14135100	-1.06653800	-1.82147200
N	-1.52081300	0.16916300	-0.72352700
C	-2.41851500	1.26105000	-0.48501500
C	-3.66717000	1.06330800	0.11951400
C	-2.02979800	2.55986000	-0.84029500
C	-4.50735600	2.15099400	0.36424800
H	-3.98158100	0.05949000	0.37716200
C	-2.86642100	3.64721900	-0.58088900
H	-1.07464600	2.71618700	-1.33262000
C	-4.11093600	3.44679600	0.02169400
H	-5.47526900	1.98300400	0.82814400
H	-2.54979800	4.64738700	-0.86318000
H	-4.76668100	4.29027600	0.21721300
Na	1.51762400	-2.74174500	0.94009400
C	4.07072200	1.26125000	0.03102200
C	2.82524500	0.98111000	-0.55850800
C	2.18962100	2.00847100	-1.27941600
C	2.75562900	3.28221600	-1.37174400
C	3.97906200	3.55414500	-0.75557900
C	4.63657600	2.53442900	-0.06182600
H	4.58729100	0.46682600	0.55717000
H	1.26108200	1.79541300	-1.79931300
H	2.24357500	4.05714500	-1.93541100
H	4.42095900	4.54392900	-0.82632800
H	5.59829400	2.72740400	0.40567100
C	2.23709300	-0.40116300	-0.56842700
O	2.99148500	-1.20148300	1.03523500
H	2.83586800	-1.10650900	-1.13951700

Int3b

C	-5.23669300	-0.85344700	-1.46146200
C	-3.85722100	-0.65830300	-1.59620300
C	-3.12403700	0.00166900	-0.60418400
C	-3.80032400	0.46997900	0.53221500
C	-5.17277700	0.26894800	0.67637900
C	-5.89773100	-0.39306600	-0.32222100
H	-5.78888600	-1.36722000	-2.24359600
H	-3.34587400	-1.02810400	-2.48220000
H	-3.24864700	1.00380400	1.30052400
H	-5.68112300	0.63590600	1.56396500
H	-6.96786200	-0.54369600	-0.21145600
C	-1.61177100	0.21475100	-0.77311400
C	-1.20163400	1.66166600	-0.71675800
H	-1.35970500	-0.18402900	-1.76340500
H	-1.55732700	2.28586100	-1.53353800
C	-0.64268800	2.24561700	0.38563400
O	-0.32825900	3.51389700	0.49502800
C	-0.29632000	1.35746200	1.55583300
C	0.66247000	1.89828700	2.60902400
C	-0.78564900	1.79055500	2.94621300
H	1.04902600	2.89111600	2.40711500
H	1.33494500	1.17502300	3.05716800
H	-1.09711400	0.99604600	3.61746300
H	-1.37381300	2.70279300	2.97041000
C	-0.23351900	-0.12848300	1.32261000
O	0.37190300	-0.87531000	2.10227900
N	-0.84594400	-0.61708200	0.19419200
C	-0.82915100	-2.03577000	-0.04310800
C	-1.50828800	-2.91159700	0.80952900
C	-0.14512900	-2.54067800	-1.15389400
C	-1.49999200	-4.28302200	0.55113200
H	-2.03192500	-2.51511700	1.67218900
C	-0.14508600	-3.91322500	-1.41560700
H	0.39124000	-1.85920900	-1.80822600
C	-0.82183300	-4.78828700	-0.56231600
H	-2.02856200	-4.95721900	1.21883100
H	0.38939300	-4.29623000	-2.28035300
H	-0.82075100	-5.85577800	-0.76283000
Na	1.15997900	3.43416400	-1.22692100
C	3.72261400	-1.07197400	0.62674300
C	3.94710300	0.00728200	-0.24792200
C	5.14770500	0.09466900	-0.97784900
C	6.11481700	-0.89314200	-0.83030300

C	5.88874900	-1.96943200	0.04158200
C	4.69749300	-2.06039700	0.76686600
H	2.78932600	-1.13333800	1.18380600
H	5.29916300	0.93641900	-1.64621700
H	7.04453600	-0.83355400	-1.38801800
H	6.64763200	-2.73886400	0.15259900
H	4.52761300	-2.89671600	1.43748200
C	2.89857200	1.01974100	-0.37233800
O	2.94349300	2.00614700	-1.11499300
H	2.01389800	0.85662100	0.26356200
O	-0.39385200	5.04591500	-1.57700200
H	-0.65756800	4.61827100	-0.70409400
H	-0.73013100	5.94697000	-1.60576400

TS3b

C	2.73111800	-2.00732500	-2.88791100
C	1.88348500	-1.05134600	-2.31633700
C	1.47379400	-1.15819900	-0.98324500
C	1.94235000	-2.24033200	-0.22252400
C	2.79275800	-3.19223900	-0.78459400
C	3.18826300	-3.08092400	-2.12333500
H	3.03830700	-1.90524700	-3.92490200
H	1.54687900	-0.20746600	-2.91409300
H	1.64073300	-2.33820300	0.81718900
H	3.15076800	-4.02036900	-0.17885100
H	3.85112200	-3.82204200	-2.56049400
C	0.51942900	-0.11998000	-0.37958800
C	-0.88962800	-0.70366000	-0.12861100
H	0.41751300	0.67442700	-1.12662900
H	-0.89927500	-2.05884300	-0.30614200
C	-1.39863700	-0.72173500	1.22445700
O	-2.56817900	-1.10160300	1.50697600
C	-0.46954400	-0.42171000	2.35433800
C	-1.12382100	-0.11411700	3.70758100
C	-0.44864600	-1.41915500	3.53150300
H	-2.20729700	-0.09396800	3.68790100
H	-0.61396200	0.64288700	4.29220400
H	0.52118600	-1.56121900	3.99727100
H	-1.06133400	-2.30492500	3.39719500
C	0.81311600	0.31383800	2.10093000
O	1.50123800	0.72720700	3.03490300
N	1.14629900	0.54133400	0.78873600
C	2.29001000	1.37109000	0.50215000
C	3.58504300	0.95969000	0.82922500

C	2.08737900	2.60210100	-0.12985100
C	4.67266800	1.77810600	0.51932200
H	3.73359800	0.01151900	1.33266400
C	3.17860800	3.41493000	-0.44639100
H	1.07553100	2.92473900	-0.35832100
C	4.47418100	3.00404300	-0.12241700
H	5.67672800	1.45605400	0.77980100
H	3.01380200	4.37160300	-0.93374200
H	5.32328700	3.63713700	-0.36319100
Na	-3.29051900	-2.74823000	0.25249000
C	-2.09730200	2.08367300	-1.98115400
C	-2.54739800	1.01230600	-1.19587300
C	-3.63678700	1.22779100	-0.33608100
C	-4.24322400	2.48240900	-0.25909400
C	-3.77477700	3.54729300	-1.03551800
C	-2.69754100	3.34386500	-1.89916600
H	-1.27539100	1.92945600	-2.67651200
H	-3.99701500	0.41504600	0.28214300
H	-5.08496700	2.63005200	0.41202400
H	-4.24926700	4.52230500	-0.97123400
H	-2.33062800	4.15804500	-2.51794500
C	-1.84712700	-0.33044800	-1.30901100
O	-2.83132800	-1.35352000	-1.58904300
H	-1.19893100	-0.27140700	-2.19256900
O	-1.32354000	-3.25167400	-0.59197500
H	-0.57430400	-3.83195100	-0.76821000
H	-2.29762400	-2.15949100	-1.76383200

Int4b

C	2.38648400	-3.59764500	1.20534700
C	1.90590800	-2.66167100	0.28151100
C	1.41178900	-1.42252300	0.70367800
C	1.41196400	-1.13319200	2.07813300
C	1.89903300	-2.05833600	3.00205000
C	2.38534500	-3.29830600	2.56810900
H	2.76493500	-4.55467900	0.85708300
H	1.92381400	-2.89596100	-0.78050500
H	1.03006700	-0.17513400	2.42147900
H	1.89992500	-1.81417700	4.06100000
H	2.76063100	-4.02004800	3.28789700
C	0.85738800	-0.40775200	-0.31478000
C	-0.59525800	-0.07009800	-0.04986200
H	0.93389700	-0.89393300	-1.29715900
H	-3.23656800	1.98846700	2.13547500

C	-0.98377100	1.12379000	0.51343400
O	-2.20684600	1.39753200	0.86251000
C	0.05084700	2.19294900	0.72876300
C	-0.43543400	3.64025600	0.75118000
C	-0.01523200	3.00368100	2.03039200
H	-1.49669400	3.76636300	0.56777800
H	0.23760500	4.36579000	0.30823100
H	0.93979300	3.30000400	2.45215300
H	-0.78221100	2.69948800	2.73600600
C	1.43218800	2.00834200	0.16821200
O	2.25860300	2.92215500	0.18970200
N	1.72686300	0.78480900	-0.39202400
C	3.02565100	0.59189000	-0.98176400
C	4.18086100	0.58491800	-0.19435300
C	3.12399700	0.38939300	-2.36209900
C	5.42670400	0.37488400	-0.78768100
H	4.09886500	0.75676700	0.87297700
C	4.37105300	0.17060700	-2.95273400
H	2.22446800	0.41810100	-2.97057200
C	5.52575600	0.16302400	-2.16611400
H	6.32120000	0.37594000	-0.17146300
H	4.43953800	0.01827400	-4.02613400
H	6.49669300	-0.00160800	-2.62439900
Na	-3.75538800	-0.10509800	1.33100300
C	-3.87146400	-1.81955800	-1.12531900
C	-2.76630000	-0.94943600	-1.16796200
C	-2.77569900	0.09614600	-2.10134400
C	-3.85930700	0.27294500	-2.96428500
C	-4.95882100	-0.58867700	-2.90764400
C	-4.96210700	-1.63630900	-1.98347700
H	-3.86551400	-2.65355200	-0.42943200
H	-1.93230000	0.77780300	-2.13213900
H	-3.84789900	1.09307700	-3.67659400
H	-5.80146800	-0.44695300	-3.57818200
H	-5.80397800	-2.32193700	-1.93789200
C	-1.56050000	-1.20034500	-0.25913300
O	-2.13106300	-1.71670900	1.01274600
H	-1.01266800	-2.04668600	-0.69672900
O	-4.02817800	1.72494700	2.67210000
H	-4.49767100	2.52096300	2.94106800
H	-1.37981100	-1.83122800	1.61317400
TS4b			
C	-1.65216000	3.19887900	-2.15680800

C	-1.25715900	1.87344300	-1.95298300
C	-1.20856600	1.32237600	-0.66673000
C	-1.58129000	2.12986300	0.41850200
C	-1.98133100	3.45366800	0.22145200
C	-2.01491000	3.99611900	-1.06906200
H	-1.68199600	3.60424400	-3.16413000
H	-0.98261400	1.26038100	-2.80777300
H	-1.56490300	1.72663000	1.42624400
H	-2.27657800	4.05883800	1.07455000
H	-2.33046600	5.02392300	-1.22308000
C	-0.72743300	-0.12469800	-0.47722100
C	0.70464000	-0.22349900	0.05609100
H	-0.74468200	-0.58769200	-1.46729100
H	0.70239300	4.04340000	0.09967700
C	0.87079300	-0.13806900	1.46831400
O	1.92700000	0.26424100	2.04326500
C	-0.28468700	-0.54936900	2.32710800
C	0.08346600	-1.19707700	3.67061500
C	-0.47262800	0.17545000	3.67240800
H	1.14716200	-1.31358500	3.84510700
H	-0.56865400	-2.00894600	3.97242300
H	-1.50186500	0.30731900	3.99022500
H	0.20863000	1.00204500	3.84711800
C	-1.54767700	-1.07611600	1.69915200
O	-2.41681900	-1.62247600	2.37875900
N	-1.67471700	-0.91252300	0.34128000
C	-2.86094100	-1.39430900	-0.31723000
C	-4.10062700	-0.78600200	-0.10159600
C	-2.75635100	-2.47277300	-1.20151300
C	-5.23135900	-1.25688000	-0.77167700
H	-4.17502200	0.04186600	0.59459500
C	-3.88794800	-2.93696200	-1.87611600
H	-1.79207200	-2.95191400	-1.34563300
C	-5.12804900	-2.32935300	-1.66225700
H	-6.19369000	-0.78441300	-0.59747600
H	-3.80147700	-3.77805800	-2.55793800
H	-6.00970000	-2.69264900	-2.18223900
Na	2.79753300	2.01748400	0.97888200
C	3.60942400	-1.24853600	-2.14223600
C	3.04682900	-0.93476500	-0.88766900
C	3.74222800	-1.35091100	0.26336800
C	4.95065600	-2.04161800	0.15371300
C	5.49969300	-2.33251100	-1.09833600
C	4.81895300	-1.93334100	-2.25124700

H	3.08226400	-0.95448300	-3.04706200
H	3.33821400	-1.13002100	1.24255200
H	5.46547400	-2.35604500	1.05744900
H	6.44127400	-2.86852100	-1.17440900
H	5.22421000	-2.16007300	-3.23328400
C	1.73120100	-0.23866300	-0.91152400
O	2.43595800	1.63851600	-1.17373700
H	1.33275600	-0.23979900	-1.92190600
O	1.63814000	3.80488600	0.07546600
H	1.74468900	3.15851500	-0.67381400
H	3.02394300	1.60697400	-1.93969100

Int5b

C	-0.09659200	3.89104700	-0.90995100
C	-0.01396900	2.49589400	-0.93283700
C	-1.11179400	1.71635500	-0.53359300
C	-2.28660200	2.35832400	-0.12082900
C	-2.36600100	3.75367400	-0.10318500
C	-1.27065800	4.52569700	-0.49677800
H	0.76685000	4.47635100	-1.21282900
H	0.92043400	2.03649400	-1.25664500
H	-3.14538900	1.77357900	0.18813100
H	-3.28531600	4.23393500	0.21998500
H	-1.33086700	5.61010000	-0.47901400
C	-1.01497900	0.18176300	-0.61073200
C	0.34187500	-0.34179200	-0.17281700
H	-1.17516300	-0.11302000	-1.64970900
C	0.59166400	-0.09219500	1.26849500
O	1.70233500	0.22848700	1.71133200
C	-0.60317800	-0.18825900	2.14125400
C	-0.33929200	-0.63018400	3.59415000
C	-0.67598900	0.78255400	3.34490100
H	0.69456300	-0.87946600	3.80858300
H	-1.10778000	-1.27710800	4.00190600
H	-1.67573400	1.12734800	3.58645600
H	0.11671300	1.52277300	3.37688700
C	-1.92824600	-0.62212600	1.55518500
O	-2.81948800	-1.05502500	2.28108100
N	-2.06142600	-0.50776900	0.18526100
C	-3.22131800	-1.02888700	-0.48702500
C	-4.51534600	-0.71093600	-0.05621800
C	-3.04951700	-1.87018000	-1.59451000
C	-5.62092000	-1.22107700	-0.73904100
H	-4.65414100	-0.08671600	0.81743200

C	-4.15958000	-2.36697800	-2.28005300
H	-2.05000800	-2.15207200	-1.91124600
C	-5.45030100	-2.04373000	-1.85532700
H	-6.61991800	-0.97011700	-0.39487900
H	-4.01179600	-3.01710900	-3.13731100
H	-6.31406900	-2.43407100	-2.38494900
Na	3.31050400	1.13575000	0.31503100
C	3.62770800	-1.37277600	-1.45530600
C	2.46790000	-1.63228100	-0.69999100
C	2.51217900	-2.61559000	0.30526200
C	3.69117300	-3.31542900	0.56064800
C	4.84437500	-3.04149000	-0.18176200
C	4.80910000	-2.06738200	-1.18405300
H	3.60689700	-0.57564300	-2.19532000
H	1.61343400	-2.84600200	0.86985300
H	3.70785100	-4.07811800	1.33373000
H	5.76238900	-3.58657900	0.01786400
H	5.70323500	-1.84456400	-1.75893000
C	1.20921500	-0.92542600	-1.02422500
O	3.22817000	1.77084300	-1.76875800
H	0.94748800	-0.91088200	-2.08222000
H	2.97510000	2.32786400	-2.51109500
O	5.11871700	2.36346900	-0.26695400
H	6.03172300	2.29926400	-0.56336400
H	4.47464300	2.25114500	-1.08906800

TS5b

C	-0.05913400	3.84189200	-0.90260400
C	-0.02506800	2.44637600	-0.96907200
C	-1.10541900	1.68708900	-0.49173700
C	-2.21639800	2.35241500	0.04225700
C	-2.24888800	3.74887100	0.10356000
C	-1.16991500	4.49959400	-0.36779400
H	0.79363700	4.40814000	-1.26566700
H	0.86425000	1.97179400	-1.38176100
H	-3.06219800	1.78496000	0.41244800
H	-3.12028100	4.24604200	0.52064200
H	-1.19357700	5.58445100	-0.31742900
C	-1.06274500	0.14947700	-0.61163100
C	0.29423700	-0.41914900	-0.22609300
H	-1.25071200	-0.10870900	-1.65539300
C	0.54051300	-0.25135300	1.23493400
O	1.65560600	0.14027600	1.69759400
C	-0.57040700	-0.51685400	2.04887000

C	0.43616000	0.39270200	3.82037300
C	-0.32733500	-0.79094000	3.53354800
H	-0.04403400	1.36308400	3.73726200
H	1.48407300	0.37433800	4.09482200
H	0.17740600	-1.73498800	3.74980600
H	-1.34561000	-0.78595500	3.95181500
C	-1.94587600	-0.69519800	1.55379600
O	-2.86129800	-1.03593800	2.31055000
N	-2.12377700	-0.51084700	0.18637100
C	-3.32843700	-0.93740700	-0.46547700
C	-4.59180300	-0.60009200	0.04007000
C	-3.24025600	-1.70818000	-1.63437300
C	-5.74407100	-1.01904900	-0.62752400
H	-4.66921800	-0.03182800	0.95781000
C	-4.39665300	-2.11256400	-2.30293700
H	-2.26823800	-2.00956900	-2.01233700
C	-5.65489800	-1.76935400	-1.80261400
H	-6.71670100	-0.75212200	-0.22453000
H	-4.31039500	-2.70868100	-3.20669100
H	-6.55519700	-2.08824500	-2.31914100
Na	3.17022000	1.12740700	0.26370200
C	3.57774000	-1.30583700	-1.60667700
C	2.43606100	-1.62488500	-0.84629000
C	2.52506800	-2.63821300	0.12562600
C	3.72723000	-3.31206600	0.34083000
C	4.86040400	-2.98167500	-0.40940300
C	4.78227500	-1.97506500	-1.37651700
H	3.52912300	-0.48164200	-2.31510300
H	1.64117100	-2.91158300	0.69453600
H	3.77785200	-4.09936400	1.08756400
H	5.79645100	-3.50675800	-0.24195400
H	5.66121000	-1.70523700	-1.95474200
C	1.15315700	-0.94059100	-1.12107300
O	3.27251700	1.86722800	-1.78640700
H	0.87581000	-0.87292100	-2.17278200
H	3.05868300	2.46728500	-2.50715600
O	5.01057400	2.40297600	-0.09993900
H	5.94375700	2.33535400	-0.32441100
H	4.43432700	2.32061400	-0.97960700

Int3c

C	-5.30575200	-0.65563900	-1.53854600
C	-3.91213600	-0.57992200	-1.64553900
C	-3.14010400	-0.03604900	-0.61339900

C	-3.79134400	0.43552500	0.53629900
C	-5.17860600	0.35301500	0.65247900
C	-5.94271000	-0.19176300	-0.38708200
H	-5.88797100	-1.08046600	-2.35165700
H	-3.42050300	-0.95269200	-2.54139400
H	-3.20711700	0.87766400	1.33817200
H	-5.66719000	0.72045100	1.55093000
H	-7.02378700	-0.25012700	-0.29771500
C	-1.61299300	0.05143300	-0.75358900
C	-1.07912000	1.45309800	-0.64015900
H	-1.37883800	-0.32810100	-1.75607200
H	-1.29866200	2.11476500	-1.47435800
C	-0.45577000	1.93854500	0.46655800
O	-0.01258900	3.17180600	0.61481200
C	-0.21883600	0.99160100	1.61671000
C	0.74728000	1.40877200	2.71622900
C	-0.71510600	1.40998100	3.00948800
H	1.21966300	2.37398800	2.57143100
H	1.34413100	0.61491900	3.15169400
H	-1.11105100	0.62001400	3.64054900
H	-1.22601100	2.36687800	3.05796000
C	-0.27534800	-0.48516500	1.32773600
O	0.27011000	-1.30769100	2.07442800
N	-0.93556800	-0.87788100	0.18967100
C	-1.03025500	-2.28285800	-0.10419600
C	-1.79824000	-3.13014900	0.70008500
C	-0.36457400	-2.80020000	-1.22038700
C	-1.89668800	-4.48716400	0.38868100
H	-2.30749100	-2.72332300	1.56668000
C	-0.47135600	-4.15727600	-1.53534700
H	0.24141600	-2.14092100	-1.83558600
C	-1.23710400	-5.00450600	-0.73035500
H	-2.49381000	-5.13979800	1.01897300
H	0.04950600	-4.55099300	-2.40359800
H	-1.31918600	-6.06014400	-0.97258200
Na	1.75340400	3.51829000	-0.66330400
C	3.58274700	-1.60415900	0.53577900
C	3.96653900	-0.43839200	-0.15252400
C	5.18568100	-0.39573500	-0.85495300
C	6.01174400	-1.51397300	-0.86687800
C	5.62683100	-2.67614100	-0.18073100
C	4.41715300	-2.72258700	0.51775600
H	2.63784700	-1.63026100	1.07588700
H	5.46152700	0.51439800	-1.37817900

H	6.95406100	-1.49002600	-1.40588500
H	6.27582200	-3.54730700	-0.19384300
H	4.12352100	-3.62473800	1.04498500
C	3.06437000	0.71408200	-0.11438500
O	3.26810200	1.79493400	-0.67565300
H	2.14422400	0.56995400	0.47382300
O	1.20011800	5.43713700	-1.69649400
H	0.28104800	5.56130000	-1.32497000
H	1.53727900	6.30338000	-1.94656100
O	-1.09364100	5.29998600	-0.40179500
H	-0.81552400	4.43344900	0.04552500
H	-1.96599400	5.15609200	-0.78633800

TS3c

C	3.67811100	-1.52076800	-1.92016100
C	2.47611600	-0.82070100	-1.76374600
C	1.85529500	-0.72025600	-0.51309300
C	2.46750100	-1.33997900	0.58759400
C	3.66893300	-2.03325600	0.44148200
C	4.28222100	-2.12736500	-0.81522300
H	4.14637600	-1.57767000	-2.89872700
H	2.02352000	-0.33787300	-2.62632600
H	2.00552500	-1.27885400	1.56820600
H	4.13175000	-2.49704900	1.30833800
H	5.22685600	-2.65262700	-0.92623300
C	0.54029800	0.05950400	-0.37108200
C	-0.68506500	-0.84982200	-0.13069800
H	0.38886300	0.56674500	-1.32769100
H	-0.36040700	-2.15697900	-0.29250600
C	-1.20257400	-0.89591400	1.22715000
O	-2.18073500	-1.61708300	1.55586100
C	-0.51137900	-0.12378000	2.30576300
C	-1.28867400	0.05944600	3.61370900
C	-0.14713900	-0.88176500	3.60191700
H	-2.29018300	-0.35430700	3.60166200
H	-1.14350600	1.02208400	4.09021200
H	0.77876800	-0.56998700	4.07521100
H	-0.35255300	-1.94772900	3.58739600
C	0.38482300	1.02773700	1.94430100
O	0.77296600	1.82510100	2.79826300
N	0.69832500	1.15896100	0.61411800
C	1.48310500	2.29207000	0.19329200
C	2.81432500	2.44425400	0.59246200
C	0.89361200	3.24039200	-0.64877000

C	3.55256000	3.54131000	0.14443300
H	3.26010300	1.71443800	1.25853100
C	1.63749100	4.33301300	-1.10096900
H	-0.14858200	3.12383700	-0.93092200
C	2.96910300	4.48518200	-0.70578600
H	4.58488700	3.65825300	0.46130500
H	1.17266600	5.06918500	-1.75056800
H	3.54679200	5.33715400	-1.05252600
Na	-2.48141000	-3.42906800	0.35304800
C	-2.56422000	1.51689700	-2.00760500
C	-2.73576200	0.37259800	-1.21562400
C	-3.85248200	0.31211500	-0.36661800
C	-4.75575600	1.37419600	-0.30258400
C	-4.56402000	2.51758900	-1.08484100
C	-3.46395000	2.58493300	-1.94126300
H	-1.72486400	1.56892700	-2.69728200
H	-4.00593700	-0.56485000	0.25010200
H	-5.61355900	1.30897400	0.36127300
H	-5.26920000	3.34209900	-1.03230500
H	-3.31090700	3.45997200	-2.56697800
C	-1.72270500	-0.75488600	-1.31050400
O	-2.41968200	-1.99358800	-1.53927800
H	-1.11540600	-0.55767400	-2.20395100
O	-0.50548700	-3.42989300	-0.56195800
H	0.31497700	-3.85380200	-0.86250600
H	-1.69392500	-2.66204500	-1.62825100
O	2.02608500	-4.64305900	-1.53011100
H	2.39736300	-5.33594300	-0.97011600
H	2.65403900	-3.90555000	-1.48114300

Int4c

C	-2.08612400	2.57172300	-2.84083600
C	-1.59797200	1.34835200	-2.36365400
C	-1.40014800	1.13261900	-0.99552700
C	-1.72064400	2.17249700	-0.10399400
C	-2.22276800	3.38897400	-0.57279400
C	-2.40099300	3.59678400	-1.94874400
H	-2.23239500	2.71389500	-3.90800100
H	-1.37821200	0.54881500	-3.06736000
H	-1.59100200	2.02178900	0.96416400
H	-2.48956900	4.17008200	0.13467600
H	-2.79639400	4.54059300	-2.31280800
C	-0.81765400	-0.20009300	-0.48778800
C	0.62530800	-0.06352100	-0.03979800

H	-0.85381900	-0.89036000	-1.33937500
H	2.59475200	2.09959600	1.98687800
C	0.94905500	0.07890200	1.29144300
O	2.14343800	0.32501300	1.74409400
C	-0.14196400	-0.09226800	2.31812200
C	0.29680500	-0.50758500	3.72200400
C	-0.18736900	0.88218100	3.50622300
H	1.36478900	-0.65572900	3.83345100
H	-0.36649200	-1.19694800	4.23223500
H	-1.17635000	1.13825600	3.87348900
H	0.54574900	1.68278400	3.49147400
C	-1.47423900	-0.64765400	1.90004400
O	-2.32111900	-0.98304600	2.72954400
N	-1.69378200	-0.78987300	0.54534900
C	-2.93668200	-1.35237000	0.08848900
C	-4.16061800	-0.73653600	0.36933200
C	-2.91035600	-2.52719800	-0.67104600
C	-5.34705000	-1.29181000	-0.11327700
H	-4.17937500	0.16216000	0.97466300
C	-4.09815100	-3.07608800	-1.15993700
H	-1.95963800	-3.01538000	-0.86588000
C	-5.32049700	-2.45879800	-0.88241200
H	-6.29416800	-0.81044600	0.11292200
H	-4.06739600	-3.98992300	-1.74642600
H	-6.24571100	-2.88694500	-1.25713100
Na	3.87647700	0.92331200	0.52296200
C	3.88463000	-1.05907300	-1.85956700
C	2.70562300	-1.17501000	-1.09965200
C	2.49920400	-2.35252900	-0.36860900
C	3.44382800	-3.38199500	-0.38710400
C	4.61672000	-3.25353600	-1.13589900
C	4.83423000	-2.08658800	-1.87339500
H	4.04793500	-0.16429600	-2.45286400
H	1.59947800	-2.44692900	0.23032900
H	3.26518100	-4.28257600	0.19366800
H	5.35087700	-4.05400200	-1.14700500
H	5.73590900	-1.97821800	-2.47035100
C	1.65867000	-0.05068000	-1.13730300
O	2.43847200	1.18917500	-1.23587700
H	1.13156600	-0.15502900	-2.09754700
O	3.17525100	2.83693100	1.68338000
H	2.60249300	3.37947700	1.11750700
H	1.84992700	1.95162000	-1.08556400
O	1.20311600	3.68443100	-0.47610000

H	1.24301400	4.42038600	-1.10065800
H	0.25575000	3.49780900	-0.35076200

TS4c

C	-1.63370600	3.03601100	-2.29387300
C	-1.35324100	1.69143100	-2.02842600
C	-1.19993400	1.23075200	-0.71520400
C	-1.34569000	2.14895700	0.33620100
C	-1.63213300	3.49003800	0.07892000
C	-1.77350300	3.94197400	-1.23967700
H	-1.74945900	3.37122800	-3.32063900
H	-1.25739000	0.99183000	-2.85531500
H	-1.23787400	1.81794100	1.36456500
H	-1.74538800	4.18452200	0.90672900
H	-2.00219800	4.98491200	-1.43949000
C	-0.86721000	-0.24712300	-0.45929200
C	0.55346100	-0.47965000	0.05922200
H	-0.95322000	-0.75067400	-1.42589800
H	3.59057500	4.46312100	1.50681800
C	0.76183900	-0.41875800	1.46347100
O	1.88024900	-0.17736400	2.01184600
C	-0.42084600	-0.64479500	2.35501500
C	-0.11884400	-1.28815200	3.71533300
C	-0.48135800	0.14761200	3.67465200
H	0.92263700	-1.54253200	3.87632000
H	-0.86944700	-1.99072800	4.05933500
H	-1.47632400	0.43131700	4.00221200
H	0.31000900	0.87817200	3.80863100
C	-1.75541800	-1.01252200	1.76666400
O	-2.67728000	-1.41160100	2.47857000
N	-1.88579700	-0.88512900	0.40423100
C	-3.14069700	-1.22092200	-0.21608300
C	-4.29651600	-0.48048800	0.04897700
C	-3.18890700	-2.29096300	-1.11551400
C	-5.49446200	-0.81089700	-0.58710800
H	-4.25482100	0.33942900	0.75698200
C	-4.38701400	-2.61353800	-1.75714700
H	-2.29144900	-2.87542400	-1.29777200
C	-5.54280100	-1.87363300	-1.49391700
H	-6.39080000	-0.23563000	-0.37415200
H	-4.41839100	-3.44847200	-2.45122000
H	-6.47644400	-2.12686700	-1.98774200
Na	3.04304900	1.44466800	1.02776500
C	3.29156400	-1.76199400	-2.22402200

C	2.77463500	-1.44098600	-0.95175200
C	3.40470200	-2.00568300	0.17318200
C	4.50908900	-2.84622700	0.02169700
C	5.01657400	-3.14280500	-1.24665400
C	4.39868300	-2.59663300	-2.37421400
H	2.80866300	-1.35555500	-3.10995200
H	3.03172100	-1.78169700	1.16394800
H	4.97486300	-3.27421200	0.90515300
H	5.87732700	-3.79633700	-1.35469500
H	4.77137700	-2.82530600	-3.36858700
C	1.56116700	-0.57571100	-0.92842600
O	2.48483000	1.17435800	-1.11686700
H	1.14813800	-0.49606800	-1.93042800
O	3.09507600	3.68885100	1.22181200
H	2.61584000	3.92097900	0.37750200
H	3.13717300	1.02731800	-1.81601700
O	1.83766700	3.74192300	-1.10632000
H	1.97651200	2.75790800	-1.24737900
H	0.88447000	3.89427700	-1.16843600

Int5c

C	-1.05282000	3.49342800	-1.87198400
C	-1.06861100	2.09676500	-1.84935700
C	-1.13287200	1.39894800	-0.63680900
C	-1.18789700	2.12836400	0.55878000
C	-1.17123600	3.52434400	0.54020300
C	-1.10287400	4.21212500	-0.67511900
H	-1.00371700	4.01688500	-2.82222500
H	-1.03149500	1.54569900	-2.78589100
H	-1.24786100	1.61439200	1.51284700
H	-1.20557000	4.07382800	1.47616600
H	-1.09219100	5.29803400	-0.68795200
C	-1.09921000	-0.13325300	-0.66192900
C	0.28046500	-0.69792500	-0.34294300
H	-1.34747100	-0.44116000	-1.68073500
H	3.43914100	3.26449700	2.78611600
C	0.63063000	-0.74345600	1.09925400
O	1.77804400	-0.54642800	1.51235000
C	-0.48906200	-1.02360400	2.02980000
C	-0.13830800	-1.90493000	3.24809200
C	-0.36386400	-0.46415000	3.46491600
H	0.88249700	-2.27224900	3.26321700
H	-0.92512700	-2.59460400	3.53299600
H	-1.30380400	-0.15867000	3.91253200

H	0.49534100	0.17964000	3.62362200
C	-1.89565900	-1.16193700	1.50250000
O	-2.79222900	-1.60217700	2.21867600
N	-2.12144900	-0.75908900	0.20740600
C	-3.45870100	-0.85225600	-0.32647500
C	-4.40272100	0.14097600	-0.05410100
C	-3.79292100	-1.93580600	-1.14394300
C	-5.68305700	0.04839100	-0.60409000
H	-4.13401800	0.97313300	0.58747000
C	-5.07338300	-2.02328000	-1.69481900
H	-3.05447900	-2.70933500	-1.33405000
C	-6.01970600	-1.03070400	-1.42593700
H	-6.41687100	0.81940000	-0.38884000
H	-5.33213900	-2.86862300	-2.32556400
H	-7.01649800	-1.10006700	-1.85140600
Na	3.31831500	0.98630600	0.73836800
C	3.51788100	-1.32032300	-1.94958300
C	2.41427000	-1.78705500	-1.21411500
C	2.55386300	-2.95447900	-0.44306500
C	3.77248500	-3.63076400	-0.39405100
C	4.87122100	-3.14946900	-1.11324600
C	4.74024300	-1.99242000	-1.88648500
H	3.42843500	-0.39875800	-2.51633800
H	1.69871200	-3.34107100	0.10365200
H	3.86253400	-4.53592700	0.19954800
H	5.82034700	-3.67625800	-1.07532300
H	5.59078000	-1.60915900	-2.44255500
C	1.11407100	-1.09252900	-1.32859800
O	3.67993300	1.91945500	-1.16791800
H	0.78271900	-0.91200300	-2.35191300
O	2.94412100	2.76103400	2.13156800
H	2.80912500	3.36748600	1.32540800
H	4.41784500	2.09513800	-1.76026100
O	2.72212800	3.93763300	-0.14753300
H	3.16118100	3.09876300	-0.70923300
H	1.84192500	4.10911300	-0.50371100

TS5c

C	-1.95765600	0.59271800	4.02579900
C	-1.86407200	1.05235200	2.71006700
C	-1.70997000	0.15669000	1.64420400
C	-1.66431300	-1.21588900	1.92121200
C	-1.75741900	-1.67927800	3.23530900
C	-1.90136100	-0.77699800	4.29282200

H	-2.08219100	1.30305600	4.83806500
H	-1.91887100	2.12016500	2.51135000
H	-1.56233200	-1.92918600	1.10970400
H	-1.71927100	-2.74685200	3.43234100
H	-1.97555700	-1.13902700	5.31396200
C	-1.56985100	0.71293400	0.21943500
C	-0.10369700	0.84044500	-0.19463600
H	-1.98766100	1.72189400	0.23299600
H	4.90670200	-3.17439000	-1.81137600
C	0.49882600	-0.42917900	-0.68919500
O	1.69343600	-0.76100800	-0.44189000
C	-0.35472000	-1.22258400	-1.47286600
C	0.26818600	-2.24576300	-2.42852500
C	1.04968600	-2.95845500	-1.45443400
H	0.84179000	-1.80723200	-3.24800000
H	-0.60762100	-2.79771000	-2.80104600
H	0.52043000	-3.51544400	-0.68528300
H	2.14061500	-2.96509600	-1.43143800
C	-1.81607200	-1.07041800	-1.53477200
O	-2.51388200	-1.79603600	-2.25290000
N	-2.35950200	-0.05288200	-0.76709900
C	-3.77337600	0.20030200	-0.81381700
C	-4.69494900	-0.78084800	-0.43342100
C	-4.22829300	1.45609800	-1.23251200
C	-6.06196600	-0.50178000	-0.46923900
H	-4.34014500	-1.75725300	-0.12533900
C	-5.59636000	1.73550200	-1.25559400
H	-3.51124900	2.20584100	-1.55495900
C	-6.51711900	0.75632100	-0.87429300
H	-6.77230600	-1.26945100	-0.17663000
H	-5.94045700	2.71188300	-1.58413700
H	-7.58164500	0.96993800	-0.89763100
Na	3.79220900	-0.99785500	0.22362900
C	2.51264800	3.42211200	0.44448100
C	1.91041500	2.42887200	-0.35189100
C	2.63304500	1.93346300	-1.45419000
C	3.92248700	2.39124000	-1.72430000
C	4.51965300	3.35315400	-0.90226900
C	3.80762700	3.86953000	0.18309800
H	1.96136500	3.83352100	1.28622600
H	2.17632700	1.20378800	-2.11238400
H	4.45953400	2.00356900	-2.58545200
H	5.52531400	3.70403700	-1.11378300
H	4.25748900	4.62288300	0.82293000

C	0.53362300	2.02015800	-0.02986900
O	5.63259300	-0.50479200	1.51673800
H	-0.06072200	2.81873700	0.41520900
O	4.20016900	-2.90385600	-1.21512500
H	4.51845100	-3.09514200	-0.22471200
H	6.57239400	-0.30354300	1.47326100
O	4.77542700	-2.85141200	1.17871600
H	5.51671700	-1.51835400	1.56227800
H	4.65314100	-3.56141200	1.81569600

TS3'

C	-3.77148100	2.20302200	-2.02377800
C	-2.64446300	1.38357200	-1.89466000
C	-1.90744800	1.35904100	-0.70613300
C	-2.32277100	2.17049100	0.35992600
C	-3.44844000	2.98502000	0.23843400
C	-4.17720600	3.00569500	-0.95674100
H	-4.33348200	2.20586300	-2.95356700
H	-2.34044600	0.75128800	-2.72578000
H	-1.76160500	2.16437500	1.29070700
H	-3.75813300	3.60528700	1.07513400
H	-5.05406700	3.63983200	-1.05090000
C	-0.64969100	0.48750000	-0.59507100
C	0.60370200	1.34663600	-0.51683500
H	-0.60356000	-0.10900900	-1.51752700
H	0.51708500	2.23492900	-1.13861000
C	1.20744600	1.60838500	0.74694000
O	2.00966300	2.57213400	0.93553700
C	0.93982100	0.66567200	1.86992900
C	2.08866100	0.37198900	2.84322700
C	0.98903900	1.25658600	3.29244100
H	3.03655300	0.83148000	2.58553000
H	2.11476700	-0.64329800	3.22275200
H	0.26074000	0.84893400	3.98527400
H	1.17596100	2.32445900	3.33530900
C	-0.05273500	-0.44895600	1.68932700
O	-0.22865500	-1.28209000	2.57920000
N	-0.76487900	-0.48644100	0.51353600
C	-1.77223000	-1.50876100	0.36711100
C	-2.97690500	-1.41995200	1.07091700
C	-1.54941900	-2.58191000	-0.49900000
C	-3.95531600	-2.40119600	0.90467700
H	-3.13798000	-0.58951400	1.74942200
C	-2.53376300	-3.55894100	-0.67031900

H	-0.59977600	-2.65626300	-1.01742900
C	-3.73887500	-3.47048300	0.03045400
H	-4.88755100	-2.32893800	1.45738500
H	-2.35286100	-4.39335000	-1.34207600
H	-4.50264300	-4.23189400	-0.09928700
Na	3.34705200	3.28269600	-0.60169600
C	1.92312100	-1.83741900	-1.89276400
C	2.50767700	-0.71040300	-1.29895500
C	3.51964300	-0.89951000	-0.34616900
C	3.91403000	-2.18354400	0.02606400
C	3.31494200	-3.30339100	-0.56298000
C	2.32264600	-3.12687500	-1.52945700
H	1.16787700	-1.70224800	-2.66392700
H	3.99713500	-0.02872600	0.09121100
H	4.69269200	-2.31586100	0.77229600
H	3.62572800	-4.30358500	-0.27545600
H	1.86678400	-3.99071400	-2.00559300
C	2.11877200	0.66717100	-1.75753500
O	3.01217800	1.58429800	-1.80364300
H	1.37531800	0.63101100	-2.57401300

Int3'

C	3.76788500	-2.08747100	-2.10735100
C	2.62058100	-1.30022800	-1.96941000
C	1.95603100	-1.20483700	-0.74035500
C	2.47094700	-1.91256200	0.35572600
C	3.61684900	-2.69898200	0.22297300
C	4.26995600	-2.79047700	-1.01047600
H	4.27148300	-2.14282500	-3.06832000
H	2.24144900	-0.74852000	-2.82641500
H	1.98256200	-1.84458900	1.32361500
H	4.00218000	-3.23769000	1.08426700
H	5.16374400	-3.39912100	-1.11205500
C	0.66992600	-0.38001300	-0.64015600
C	-0.58867200	-1.29024000	-0.67971600
H	0.62441300	0.24834200	-1.53619200
H	-0.30147700	-2.19995100	-1.21663200
C	-1.03390400	-1.75125100	0.67636000
O	-1.68745800	-2.80197600	0.81436400
C	-0.70472900	-0.92811400	1.86370400
C	-1.73226400	-0.91855000	3.00916100
C	-0.49035100	-1.69234700	3.19340700
H	-2.64753000	-1.46291800	2.80307500
H	-1.81958800	0.03659700	3.51458600

H	0.27961000	-1.27498700	3.83368200
H	-0.53655800	-2.77316700	3.10860000
C	0.11125000	0.32949700	1.71840700
O	0.25177900	1.09328600	2.67317200
N	0.69254000	0.56007300	0.50005500
C	1.50517600	1.74640800	0.35140900
C	2.85266600	1.73323200	0.72254000
C	0.93451400	2.90511200	-0.18119700
C	3.63109300	2.88024800	0.55277400
H	3.28358000	0.83325300	1.14708300
C	1.71719900	4.04986300	-0.35006400
H	-0.11639800	2.90563900	-0.44961200
C	3.06616300	4.03959900	0.01440200
H	4.67716800	2.86751200	0.84492200
H	1.26909100	4.95076200	-0.75934000
H	3.67275900	4.93136000	-0.11509700
Na	-3.08012900	-3.46033800	-0.80340300
C	-2.17883200	1.74133200	-1.92843300
C	-2.36204500	0.58895200	-1.15431700
C	-3.20410200	0.67489600	-0.03558800
C	-3.81569200	1.87800400	0.31704800
C	-3.61371200	3.02500100	-0.45980200
C	-2.79869400	2.95037100	-1.59047500
H	-1.55698800	1.68787200	-2.81963400
H	-3.40270600	-0.21775200	0.54981200
H	-4.45686100	1.92321000	1.19358200
H	-4.09530800	3.96069000	-0.19017800
H	-2.64975300	3.82805800	-2.21431300
C	-1.75653700	-0.75336900	-1.60049400
O	-2.70520300	-1.69306800	-1.80345800
H	-1.18840000	-0.51895300	-2.53149700

TS4''

C	2.15433500	3.77589100	-0.08851200
C	1.55097400	2.62340100	0.42647800
C	1.25710100	1.53672600	-0.40237400
C	1.58369800	1.61926900	-1.76271500
C	2.19160100	2.76224200	-2.28059400
C	2.47744300	3.84735600	-1.44398200
H	2.37323900	4.61129200	0.57051400
H	1.31269700	2.56849800	1.48617600
H	1.35794000	0.78325800	-2.41944900
H	2.43820300	2.81055500	-3.33761700

H	2.94729300	4.73941100	-1.84820500
C	0.58741100	0.28099500	0.16924000
C	-0.78078100	0.03125200	-0.46876300
H	0.42724700	0.47690400	1.24047900
H	-1.09356600	0.64281200	-1.62170900
C	-1.20098900	-1.30258800	-0.82264500
O	-2.38626300	-1.60009100	-1.13707600
C	-0.15039700	-2.35332200	-0.95815600
C	-0.62481300	-3.81001500	-0.82706200
C	-0.26007000	-3.29774300	-2.16782100
H	-1.67792600	-3.92299900	-0.59439700
H	0.07489200	-4.47370400	-0.33172900
H	0.68806100	-3.61012900	-2.59225200
H	-1.06118700	-3.06397000	-2.86127600
C	1.24205700	-2.10388900	-0.45887100
O	2.09558500	-2.99041200	-0.51558800
N	1.51651600	-0.87280400	0.08877700
C	2.79604400	-0.70628500	0.73598200
C	3.95971100	-0.53346300	-0.01700400
C	2.86250600	-0.71126500	2.13194800
C	5.18603800	-0.36332000	0.62693100
H	3.89828100	-0.54097900	-1.09936200
C	4.08994800	-0.53292300	2.77518700
H	1.95698900	-0.86667800	2.71166200
C	5.25425700	-0.35824200	2.02326900
H	6.08866400	-0.23323900	0.03704600
H	4.13578700	-0.53989600	3.86044000
H	6.20964500	-0.22278900	2.52189400
Na	-3.79894600	-0.07345100	-1.82328300
C	-4.24184500	1.46699800	0.55130800
C	-3.02865100	0.78016300	0.73556900
C	-2.93816700	-0.13350600	1.79585500
C	-4.02772400	-0.36606600	2.63784300
C	-5.23440900	0.31197000	2.43699500
C	-5.33736900	1.23276800	1.39152700
H	-4.30511400	2.21023900	-0.24055300
H	-2.01288700	-0.68005800	1.95424800
H	-3.93724500	-1.08456700	3.44784700
H	-6.08124000	0.12793000	3.09163900
H	-6.26297100	1.78129000	1.23732200
C	-1.84826500	1.10323500	-0.17426000
O	-2.21985700	1.42015400	-1.52865500
H	-1.33757500	1.96936500	0.28029300

TS3a'

C	-0.80018800	4.40085500	-0.97125300
C	-0.70347600	3.02904500	-1.22602600
C	-0.93886100	2.08786800	-0.21162900
C	-1.29142100	2.55260800	1.06017000
C	-1.39648800	3.92147300	1.31637200
C	-1.14585700	4.85161900	0.30600100
H	-0.63555900	5.11305900	-1.77652500
H	-0.45781400	2.68312400	-2.22883800
H	-1.48747600	1.84107800	1.85703700
H	-1.67572900	4.26127700	2.31014600
H	-1.23351100	5.91582900	0.50632200
C	-0.71292600	0.59936700	-0.51229700
C	0.75954000	0.26145000	-0.28521900
H	-0.91693800	0.46447800	-1.58204600
H	1.36174000	1.07898600	-0.67068100
C	1.14521200	-0.18311400	1.03296700
O	2.31610900	-0.07043000	1.47388400
C	0.12185900	-0.91502500	1.82449700
C	0.61151200	-2.14690600	2.60748800
C	0.29174900	-0.91676400	3.35676700
H	1.65295800	-2.39910400	2.44336600
H	-0.09558000	-2.96803000	2.63686000
H	-0.63628400	-0.88875700	3.91815000
H	1.11182100	-0.31025600	3.72774000
C	-1.30283900	-0.99628700	1.34849400
O	-2.12648600	-1.66659900	1.96184100
N	-1.64439400	-0.27508200	0.21571700
C	-3.01187900	-0.28325800	-0.23480700
C	-4.05508200	0.05766500	0.63395500
C	-3.30473600	-0.60927300	-1.56338200
C	-5.37058300	0.07041400	0.17441700
H	-3.83414600	0.29351300	1.66783300
C	-4.62260800	-0.58466300	-2.02168600
H	-2.50546700	-0.88973100	-2.24318400
C	-5.66072600	-0.24545900	-1.15449600
H	-6.17218600	0.33287500	0.85951300
H	-4.83435400	-0.84120000	-3.05614600
H	-6.68753700	-0.23040300	-1.50923200
Na	4.06430700	0.37745200	-0.04178000
C	-0.01082500	-2.95219500	-1.27627300
C	1.26037900	-2.38410700	-1.12130700
C	2.29358800	-3.18328400	-0.61768300

C	2.05494600	-4.50717600	-0.24648500
C	0.77808700	-5.05569300	-0.38217500
C	-0.25537200	-4.27366000	-0.90439600
H	-0.82062700	-2.35642100	-1.68942300
H	3.28898400	-2.75691300	-0.54869200
H	2.86942800	-5.11559100	0.13968000
H	0.59112100	-6.08723800	-0.09521900
H	-1.25031000	-4.69370900	-1.02626100
C	1.54701000	-0.95286300	-1.53158700
O	2.79198000	-0.59767400	-1.62739000
H	0.87342600	-0.64501700	-2.35964500
O	4.39046200	1.56538100	-2.02654900
H	3.78774200	0.83623200	-2.30328600
H	3.80884400	2.30134100	-1.75921600
O	2.65672500	3.60458500	-0.69841900
H	2.92635400	4.53337700	-0.77163900
H	1.68254700	3.61817000	-0.71630200
O	3.93882800	2.21480600	1.42541300
H	3.37515200	2.78166500	0.85770700
H	3.29574000	1.64460400	1.88872800

Int3a'

C	0.15390900	4.41143500	-0.90892400
C	-0.04016000	3.05683300	-1.19858400
C	-0.41981500	2.15177800	-0.19585600
C	-0.61351400	2.63858400	1.10180200
C	-0.41915100	3.99001900	1.39616700
C	-0.03177700	4.88185300	0.39504900
H	0.42127600	5.10095200	-1.70631800
H	0.09379200	2.70005900	-2.21795500
H	-0.92416700	1.96036500	1.89075600
H	-0.57569700	4.34638300	2.41066700
H	0.10866400	5.93482700	0.62275100
C	-0.53639300	0.66283000	-0.54067500
C	0.85081500	-0.02541000	-0.39981400
H	-0.78981700	0.60089000	-1.60373400
H	1.57262800	0.75374800	-0.65906800
C	1.13206100	-0.43134000	1.01961700
O	2.28183700	-0.42268900	1.48038200
C	-0.01008100	-0.91893700	1.82288200
C	0.24623700	-2.19493400	2.65453900
C	0.15337200	-0.90567000	3.35883700
H	1.22287000	-2.64135200	2.50468000

H	-0.60152100	-2.86974500	2.69257100
H	-0.75755100	-0.68804600	3.90640400
H	1.06810800	-0.44231300	3.71469800
C	-1.42632200	-0.75323800	1.33838500
O	-2.35362400	-1.24651200	1.97038500
N	-1.62610800	0.00386900	0.19836400
C	-2.97082800	0.30176100	-0.22385500
C	-3.90852400	0.81166700	0.68261300
C	-3.34260700	0.11381900	-1.55964500
C	-5.19718800	1.12331800	0.25421100
H	-3.63226600	0.94445000	1.72126800
C	-4.63166700	0.43727600	-1.98528100
H	-2.63236800	-0.29266300	-2.27291800
C	-5.56484400	0.94185400	-1.08054200
H	-5.91580800	1.51452000	0.96926900
H	-4.90457600	0.28358900	-3.02573700
H	-6.56987000	1.18914300	-1.41079300
Na	4.12541600	-0.41910800	-0.17474000
C	-0.73817600	-2.83062500	-1.31344800
C	0.60277100	-2.52315600	-1.05283800
C	1.41616300	-3.52634900	-0.51294900
C	0.89652100	-4.78389300	-0.20160000
C	-0.44999200	-5.06734700	-0.43914600
C	-1.26572500	-4.08584200	-1.00452000
H	-1.38426100	-2.08773200	-1.77342300
H	2.46941000	-3.30790000	-0.37299500
H	1.54757900	-5.54953100	0.21472200
H	-0.85610400	-6.04743900	-0.20203100
H	-2.31135800	-4.29772300	-1.21327900
C	1.21809400	-1.14547000	-1.39086100
O	2.56940100	-1.20418700	-1.51602300
H	0.71649700	-0.82272300	-2.33588200
O	4.24390300	0.68436800	-2.24055800
H	3.48164300	0.02656200	-2.24653200
H	3.83988200	1.52918000	-1.97350000
O	3.32526100	3.10230600	-0.70441700
H	3.82035900	3.88675200	-0.98705600
H	2.39618000	3.39099700	-0.63824500
O	4.50759300	1.37685300	1.25976200
H	4.16002500	2.08798500	0.68100200
H	3.72560400	1.07386500	1.75465400

TS4a'

C	2.33632700	-2.52518800	-2.62300400
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C	1.74363600	-1.36367900	-2.11490300
C	1.26147700	-1.31509500	-0.80172200
C	1.38684800	-2.45883800	0.00099400
C	1.98808100	-3.61645600	-0.49363900
C	2.46583600	-3.65545300	-1.81129000
H	2.71236400	-2.53899900	-3.64221100
H	1.67103600	-0.48008900	-2.74425500
H	1.01162200	-2.44576400	1.02008800
H	2.08283000	-4.48993500	0.14527800
H	2.94614700	-4.55249000	-2.19221100
C	0.63942300	-0.02464500	-0.25208600
C	-0.87539800	-0.14066800	0.03277700
H	0.75958100	0.73200500	-1.03475200
H	-1.31148800	-1.41286000	-0.08263900
C	-1.32395600	0.07240500	1.39052100
O	-2.52916800	0.23485400	1.71219300
C	-0.31311500	-0.05284600	2.48973800
C	-0.78402000	0.26606400	3.90636800
C	-0.55762000	-1.15395400	3.54368800
H	-1.80727500	0.61719800	3.97244700
H	-0.04347300	0.74994700	4.53258800
H	0.33494000	-1.64386800	3.92069300
H	-1.41715300	-1.79100400	3.35973900
C	1.12074200	0.29015600	2.20614800
O	1.93232000	0.44945400	3.11729500
N	1.44864000	0.47952200	0.88373200
C	2.76309100	0.96862500	0.55308000
C	3.91424800	0.24041400	0.86811500
C	2.87283900	2.19288800	-0.11513600
C	5.16917600	0.73676000	0.51021700
H	3.82369400	-0.69875700	1.40086500
C	4.12959700	2.68201200	-0.47923300
H	1.97477900	2.76256300	-0.33641500
C	5.28098300	1.95421000	-0.16755200
H	6.06076300	0.16976200	0.76192700
H	4.20746600	3.63486800	-0.99485600
H	6.25923900	2.33590500	-0.44527500
Na	-4.29692200	-0.41388600	0.58959800
C	-1.34325000	2.58547000	-2.43544100
C	-1.80129500	1.95100600	-1.27161500
C	-2.36853300	2.74694900	-0.26210800
C	-2.47006400	4.13064600	-0.41808200
C	-2.00505800	4.75001400	-1.58265000
C	-1.43840900	3.97162200	-2.59309500

H	-0.91348700	1.98560300	-3.23431500
H	-2.71931400	2.28303800	0.65231100
H	-2.90897900	4.72834900	0.37622300
H	-2.08326000	5.82722000	-1.69882600
H	-1.07423400	4.43817500	-3.50421000
C	-1.68507400	0.43655900	-1.16873800
O	-2.99881600	-0.14793500	-1.27687500
H	-1.12600900	0.11521500	-2.05942500
O	-2.10624100	-2.41764800	-0.38973000
H	-1.66831300	-3.12376800	-0.89694900
H	-2.81449000	-1.12966100	-1.23705500
O	-0.86844600	-4.49146200	-2.09600900
H	0.08207100	-4.30091900	-2.07362100
H	-1.13706700	-4.39366500	-3.01789900
O	-4.45643900	-2.63134900	0.62248000
H	-3.50935000	-2.75042000	0.26644000
H	-4.69172700	-3.41273800	1.13167500

TS4'

C	-2.37146000	3.73986200	-0.64204900
C	-1.81017300	2.50282700	-0.98183100
C	-1.37822800	1.60943700	0.00632900
C	-1.52720600	1.97991100	1.35403000
C	-2.09378600	3.20774900	1.69720500
C	-2.51528600	4.09601400	0.69922500
H	-2.70210800	4.41642600	-1.42542300
H	-1.71721700	2.22533800	-2.02955800
H	-1.20096200	1.29594600	2.13258500
H	-2.20993100	3.47322000	2.74472600
H	-2.95562300	5.05188700	0.96845400
C	-0.72650900	0.27010700	-0.38945300
C	0.71639900	0.14983700	0.06153200
H	-0.73193800	0.25228100	-1.48591800
H	1.41149800	2.58748500	0.38905100
C	1.00154100	-0.54632600	1.23435000
O	2.19230700	-0.58320000	1.80390800
C	-0.05050300	-1.25673700	1.89510000
C	1.51672100	-2.44875100	3.02685700
C	0.22370500	-1.82055500	3.26633900
H	2.42774600	-2.18009900	3.54621600
H	1.56832500	-3.26730200	2.31698900
H	-0.57319500	-2.56012100	3.43273500
H	0.22855000	-1.09221700	4.08499700
C	-1.29076200	-1.58774300	1.22805600

O	-2.09346400	-2.43318900	1.65920100
N	-1.54408600	-0.88907000	0.03799500
C	-2.75749100	-1.12589500	-0.68250100
C	-4.00971600	-1.03254000	-0.06084500
C	-2.69411700	-1.44091300	-2.04711600
C	-5.17545300	-1.25029900	-0.79729600
H	-4.06152500	-0.80640800	0.99710100
C	-3.86262200	-1.64496200	-2.78406200
H	-1.72451500	-1.54304800	-2.52660800
C	-5.10979200	-1.55141000	-2.16087800
H	-6.13996500	-1.17979900	-0.30209400
H	-3.79584000	-1.89167200	-3.84018800
H	-6.02012100	-1.71642100	-2.73011600
Na	3.61801700	0.96553100	1.40022600
C	3.02476000	-1.16884600	-1.31251300
C	3.00084700	0.22378400	-1.14862600
C	4.15338900	0.95829400	-1.48528400
C	5.30318100	0.31203600	-1.95657200
C	5.31391000	-1.07604800	-2.11064700
C	4.16819700	-1.81150800	-1.79057600
H	2.14021800	-1.73968500	-1.04972500
H	4.13804400	2.04098100	-1.40040400
H	6.18042300	0.89758200	-2.21834100
H	6.20203800	-1.57915900	-2.48191400
H	4.16587000	-2.89155100	-1.90695200
C	1.72554300	0.94154000	-0.69365300
O	2.21123800	2.15278200	0.05721900
H	1.24945800	1.34463200	-1.59742000

Int5'

C	-1.71451800	3.76063300	-1.48231200
C	-1.33689700	2.41523700	-1.54247000
C	-1.40028000	1.58745800	-0.40947100
C	-1.88758100	2.13858800	0.78641400
C	-2.26235200	3.48308200	0.85114500
C	-2.17222900	4.30285700	-0.27856200
H	-1.66852600	4.37595900	-2.37706800
H	-1.00757000	1.99633800	-2.49214300
H	-1.97861300	1.51287800	1.66735300
H	-2.63821200	3.88916800	1.78668000
H	-2.47485600	5.34481200	-0.22597700
C	-0.87245600	0.14341800	-0.50630400
C	0.61174900	0.05451300	-0.15239400
H	-0.97736100	-0.14476800	-1.55734400

H	1.28412300	2.39520300	-1.04988800
C	0.82461900	-0.23242300	1.18771300
O	2.07355500	-0.08156800	1.82920300
C	-0.12630900	-0.68157700	2.08513800
C	1.96825500	-0.78425000	3.11683900
C	0.47120500	-0.81273600	3.45992100
H	2.59715900	-0.24138300	3.82739600
H	2.36923100	-1.79270400	2.96530100
H	0.19114800	-1.74629700	3.95818400
H	0.19822200	0.01259900	4.13717700
C	-1.42377200	-1.09385300	1.64368500
O	-2.25373400	-1.68231000	2.35544700
N	-1.69306200	-0.81474700	0.27693300
C	-2.90959100	-1.26465100	-0.32147300
C	-4.15684800	-1.03710800	0.27908900
C	-2.86405900	-1.94070800	-1.55104400
C	-5.32717700	-1.47453700	-0.34415400
H	-4.20032300	-0.53769300	1.23829400
C	-4.03768500	-2.36147500	-2.17894700
H	-1.90112800	-2.15263200	-2.00749500
C	-5.27772500	-2.13161200	-1.57676900
H	-6.28465000	-1.29422400	0.13710200
H	-3.97970700	-2.88385700	-3.13017000
H	-6.19225400	-2.46477400	-2.05909900
Na	3.27361500	1.47075400	0.79278700
C	2.90946100	-1.76421300	-0.83326000
C	2.91269200	-0.41177100	-1.21005600
C	4.10968500	0.14095100	-1.70256200
C	5.27415800	-0.63279500	-1.79100900
C	5.25772000	-1.97390500	-1.40378900
C	4.06782600	-2.53676500	-0.93088300
H	1.98820700	-2.20061200	-0.46126000
H	4.11718200	1.17071700	-2.04603300
H	6.18619900	-0.18824800	-2.18027400
H	6.15787500	-2.57713300	-1.47806300
H	4.04070500	-3.58154200	-0.63450500
C	1.61717400	0.40324000	-1.16401600
O	2.09891800	1.86886200	-1.06106000
H	1.15984400	0.35567500	-2.16028500
TS5'			
C	-1.75497400	3.86901400	-0.91685500
C	-1.35476200	2.55557100	-1.18034800

C	-1.34774800	1.58077200	-0.17135100
C	-1.78153100	1.95039100	1.11105300
C	-2.18139500	3.26177600	1.37909100
C	-2.16520900	4.22881800	0.36898300
H	-1.75836900	4.60350700	-1.71763600
H	-1.05380700	2.28229300	-2.18976700
H	-1.81672300	1.20927400	1.90228700
H	-2.51704200	3.52606900	2.37839500
H	-2.48423600	5.24580500	0.57835000
C	-0.82477900	0.17190200	-0.49710200
C	0.65970400	-0.00434100	-0.16280600
H	-0.92734600	0.05095000	-1.57910300
H	1.33815100	2.68012400	-0.68211900
C	0.85629600	-0.48366600	1.14890600
O	2.07047000	-0.35502700	1.83968600
C	-0.09620500	-1.07913800	1.92760900
C	1.96145300	-1.20386600	3.03518100
C	0.45545300	-1.38384500	3.29478600
H	2.50992900	-0.70227200	3.83574900
H	2.44954200	-2.15490400	2.79546800
H	0.22277900	-2.39809400	3.63314100
H	0.08680900	-0.69114600	4.06628500
C	-1.40445800	-1.40248900	1.40525700
O	-2.22890900	-2.09742700	2.01344700
N	-1.66091200	-0.89470800	0.11880300
C	-2.89438700	-1.20596900	-0.53864900
C	-4.13210000	-0.98782500	0.08098200
C	-2.86355600	-1.72677100	-1.84005100
C	-5.31617900	-1.28241400	-0.59751600
H	-4.15996300	-0.60593700	1.09379700
C	-4.05004200	-2.00573000	-2.52103700
H	-1.90533100	-1.92721900	-2.31113900
C	-5.28289500	-1.78585500	-1.90088000
H	-6.26930300	-1.11308300	-0.10428900
H	-4.00888400	-2.40881800	-3.52918200
H	-6.20722800	-2.00946800	-2.42574500
Na	3.19111000	1.44789900	1.05408300
C	3.17463100	-1.54636900	-0.85127200
C	3.00715500	-0.18597500	-1.16757600
C	4.11423700	0.51630900	-1.68426500
C	5.34970800	-0.11748300	-1.85318900
C	5.50389900	-1.46562800	-1.51904500
C	4.40875600	-2.17734900	-1.02113300
H	2.32383700	-2.11172900	-0.48653000

H	3.98631300	1.55930800	-1.95228000
H	6.18821500	0.44268800	-2.25819200
H	6.46197600	-1.95891800	-1.65590200
H	4.51076900	-3.22992600	-0.77198200
C	1.64492500	0.45905000	-1.06050800
O	2.18173500	2.20647600	-0.67987800
H	1.25173400	0.72203700	-2.04177300

TS4a-1

C	-2.27084300	2.52364700	-3.00692600
C	-1.84157500	1.31089100	-2.45570800
C	-1.63403900	1.17336200	-1.07704900
C	-1.88791200	2.28414800	-0.25169200
C	-2.32283300	3.49564700	-0.79760200
C	-2.51082300	3.62300500	-2.18054300
H	-2.43076600	2.60200800	-4.07881700
H	-1.67780500	0.45598400	-3.10775000
H	-1.75698400	2.19234000	0.82233000
H	-2.52890700	4.33680300	-0.14086200
H	-2.85849200	4.56188000	-2.60172500
C	-1.10402200	-0.15490000	-0.50511200
C	0.38280700	-0.11076000	-0.19757100
H	-1.25528100	-0.89909600	-1.29497900
H	2.43050000	2.02380800	1.56264800
C	0.77794900	0.14123100	1.10340500
O	2.04660400	0.31628200	1.47104100
C	-0.20578000	0.24034800	2.14090800
C	1.43807400	-0.11604600	3.66960700
C	0.23854100	0.69763000	3.50917200
H	2.43123700	0.28824700	3.81970500
H	1.32807000	-1.19482300	3.69831600
H	-0.56594400	0.38325400	4.18958400
H	0.41474200	1.77305600	3.61742100
C	-1.52824100	-0.31938300	1.97665400
O	-2.30068500	-0.54293600	2.92484000
N	-1.90230400	-0.61325000	0.65305600
C	-3.20109600	-1.14639200	0.37594500
C	-4.36369300	-0.54797400	0.88117700
C	-3.31798900	-2.28586200	-0.43310900
C	-5.61671000	-1.08276400	0.57721400
H	-4.27871800	0.31875000	1.52449100
C	-4.57385100	-2.80957000	-0.74649100
H	-2.42089400	-2.77375400	-0.80365400

C	-5.73042000	-2.21037000	-0.24091400
H	-6.50872300	-0.61159800	0.98068600
H	-4.64502000	-3.69447200	-1.37299800
H	-6.70809000	-2.62047700	-0.47711100
Na	3.82352400	0.25806700	0.11664000
C	3.32962100	-1.79629000	-2.03358800
C	2.19789600	-1.63484800	-1.21259400
C	1.84935700	-2.67864700	-0.34446900
C	2.61195900	-3.84888400	-0.29025200
C	3.73982500	-3.99634600	-1.10190400
C	4.09667600	-2.96489900	-1.97523800
H	3.59939900	-1.00568500	-2.72765600
H	0.98106800	-2.56063500	0.29608400
H	2.32513000	-4.64368700	0.39259300
H	4.33200200	-4.90584200	-1.05740000
H	4.96530100	-3.07150200	-2.61947500
C	1.34150200	-0.36205200	-1.32756100
O	2.29795400	0.72337500	-1.56355600
H	0.75441800	-0.46765000	-2.25213300
O	2.83042400	2.92314800	1.43164200
H	2.33072900	3.30646800	0.69021100
H	1.83005600	1.57367800	-1.46211500
O	1.17482700	3.34768900	-0.96954900
H	1.17282700	4.04783800	-1.63535800
H	0.23742900	3.17605200	-0.76586400
O	5.19431800	1.93218700	0.75005600
H	4.44455100	2.50553800	1.06866400
H	6.00172700	2.21602700	1.19038200

Int5a-1

C	-2.74475300	3.22880100	-2.15337400
C	-2.13421500	1.98675700	-1.95698100
C	-1.91698000	1.47596100	-0.66798600
C	-2.36458800	2.23173600	0.42751800
C	-2.97157200	3.47600300	0.23696000
C	-3.15896500	3.98501800	-1.05266600
H	-2.90763900	3.59793600	-3.16245600
H	-1.82072300	1.40403600	-2.82081400
H	-2.23370300	1.84958400	1.43386000
H	-3.30761400	4.04532500	1.09946900
H	-3.64025700	4.94797700	-1.19805200
C	-1.14994100	0.15388200	-0.50954100
C	0.36116000	0.36354300	-0.29324700

H	-1.27015300	-0.37232500	-1.46066900
H	3.57303500	4.42380400	0.70893600
C	0.69725400	0.32168600	1.06690000
O	1.99339400	0.58424200	1.52160300
C	-0.15163600	0.04233500	2.11327700
C	2.02741800	0.23299400	2.94677600
C	0.56413800	0.22913200	3.42488400
H	2.66785700	0.96887400	3.43980500
H	2.48238700	-0.76129500	3.02350900
H	0.36805200	-0.58495400	4.12915000
H	0.30451400	1.17105600	3.93147800
C	-1.40720800	-0.62035700	1.88670600
O	-2.09623500	-1.12996500	2.78361200
N	-1.77435400	-0.72173500	0.52300000
C	-2.95060200	-1.43864900	0.14372800
C	-4.18314900	-1.22662200	0.77918400
C	-2.88054500	-2.36674800	-0.90703600
C	-5.31633200	-1.92909600	0.36514000
H	-4.24123700	-0.52848700	1.60423500
C	-4.01998200	-3.05421900	-1.32921100
H	-1.92486400	-2.56029000	-1.38649300
C	-5.24535300	-2.84018300	-0.69260100
H	-6.26254000	-1.75653500	0.87080700
H	-3.94437700	-3.76774500	-2.14536000
H	-6.13207200	-3.37915700	-1.01381600
Na	3.65491200	1.38465100	0.15442200
C	3.29650700	-1.64697700	-1.82923300
C	2.09432100	-1.39362200	-1.14355100
C	1.58031800	-2.39578500	-0.30886800
C	2.25692200	-3.60866300	-0.14387200
C	3.46138000	-3.84408900	-0.81074900
C	3.97790800	-2.85869900	-1.65988200
H	3.68899700	-0.89381900	-2.50470400
H	0.64776300	-2.22433300	0.21901200
H	1.83832600	-4.36825800	0.51021200
H	3.98433600	-4.78769500	-0.68385300
H	4.89707500	-3.04115000	-2.21154500
C	1.31745600	-0.09059400	-1.37336700
O	2.34523200	0.91621800	-1.70035900
H	0.72894100	-0.23746600	-2.29052900
O	3.36659600	3.63619000	0.19506400
H	2.42559300	3.70904800	-0.09937000
H	1.87492200	1.74069300	-1.91083600
O	0.89027700	3.22245500	-0.78316500

H	0.09215900	3.74216600	-0.95219900
H	0.57263300	2.31898400	-0.47497500
O	5.31231500	-0.20737800	0.23785100
H	4.96948900	-1.01180500	-0.18914700
H	6.05915200	-0.47852400	0.78440100

TS5a-1

C	-1.02706400	3.42610800	-2.28430700
C	-0.74687300	2.09864100	-1.95627900
C	-1.47541600	1.42691300	-0.96202500
C	-2.50745200	2.12087200	-0.31695300
C	-2.78612400	3.45624300	-0.63576600
C	-2.04658200	4.11654300	-1.61947900
H	-0.44500900	3.92443700	-3.05489600
H	0.06979400	1.58534200	-2.45360700
H	-3.10162700	1.62327800	0.43999400
H	-3.58929000	3.97305800	-0.11729900
H	-2.26607500	5.15008100	-1.87184100
C	-1.15394600	-0.05763100	-0.66211300
C	0.30722300	-0.35710400	-0.32698300
H	-1.40068500	-0.60510400	-1.57470800
H	2.12825700	2.39097300	-1.02941400
C	0.58125600	-0.08927600	1.02636800
O	1.86111400	-0.02304000	1.54593900
C	-0.38676500	0.13100500	1.98522000
C	1.75327500	0.36223600	2.96340100
C	0.26457200	0.22988800	3.34672100
H	2.11008700	1.39429500	3.03825400
H	2.42187000	-0.29646300	3.52176800
H	0.06923300	-0.66980800	3.94459700
H	-0.06847800	1.08712300	3.94125900
C	-1.74313200	-0.33028700	1.75126800
O	-2.54724200	-0.54881400	2.66617400
N	-2.04658800	-0.59132300	0.39982000
C	-3.24670500	-1.26549300	0.02125700
C	-4.48937700	-0.94309300	0.59037200
C	-3.19221900	-2.28102100	-0.94854600
C	-5.64384900	-1.61453700	0.18332200
H	-4.54285300	-0.18844800	1.36353400
C	-4.35264900	-2.93645900	-1.36235400
H	-2.23420800	-2.57440800	-1.36706500
C	-5.58758100	-2.60719300	-0.79819300
H	-6.59549100	-1.35250600	0.63744000
H	-4.28515300	-3.71793000	-2.11426900

H	-6.49068900	-3.12129300	-1.11373900
Na	3.47858600	0.67601000	0.02238400
C	3.49391900	-1.95898200	-1.68142500
C	2.29770700	-1.83164200	-0.95008300
C	2.04307200	-2.78168200	0.05567100
C	2.95726700	-3.79883100	0.33798900
C	4.14715200	-3.90132600	-0.38639700
C	4.40900600	-2.97805900	-1.40168800
H	3.71397200	-1.25430600	-2.47518500
H	1.11355700	-2.72432900	0.61099600
H	2.73257500	-4.51561600	1.12269600
H	4.85670300	-4.69430900	-0.16895200
H	5.32361200	-3.05113200	-1.98360300
C	1.23509100	-0.80707900	-1.29414500
O	2.24342100	0.62111100	-1.87166500
H	0.77675500	-1.01727300	-2.26127100
O	2.44996500	2.92571200	-0.27493400
H	1.66643200	3.13182800	0.28407300
H	2.43083600	0.53404200	-2.81724500
O	0.24115000	3.27556500	1.38126600
H	-0.47488700	3.75107500	0.93519800
H	-0.11423400	2.37327600	1.51077200
O	4.95506700	2.35123900	0.47167000
H	5.78674500	2.82900300	0.39105100
H	4.21928500	2.95156200	0.21974900

TS5a''

C	-2.27721400	2.99420900	2.01336500
C	-1.80366700	1.93799900	1.23429800
C	-1.73955600	2.06567200	-0.16258600
C	-2.16192500	3.26389800	-0.74930900
C	-2.63098500	4.32174500	0.03182100
C	-2.68898500	4.18944100	1.41876100
H	-2.33247800	2.87727200	3.09286300
H	-1.51571700	1.00933700	1.72434500
H	-2.12126800	3.37230400	-1.83103900
H	-2.95518200	5.24279600	-0.44535700
H	-3.05858000	5.00726400	2.03183700
C	-1.17872300	0.96682600	-1.05478000
C	0.36448500	0.90689400	-1.09549800
H	-1.48373000	1.20809600	-2.08833000
C	0.94254900	-0.28349200	-1.80893200
O	2.12959200	-0.32181400	-2.19925000
C	0.04816000	-1.38656800	-1.97369300

C	0.51704700	-2.60180700	-2.76703400
C	1.03029500	-3.42543500	-1.67749000
H	1.27498500	-2.32695200	-3.50035700
H	-0.35461400	-3.08368800	-3.22804200
H	0.31425900	-3.88017700	-1.00236700
H	2.04163400	-3.81360000	-1.67484600
C	-1.26023600	-1.49457500	-1.37759600
O	-1.90968400	-2.55474600	-1.39136800
N	-1.76740200	-0.35983600	-0.70863200
C	-3.20646000	-0.39157300	-0.50283000
C	-3.72315800	-0.71645100	0.75238100
C	-4.06956600	-0.11073200	-1.56603100
C	-5.10687300	-0.75653900	0.93733300
H	-3.03869100	-0.92103300	1.57337500
C	-5.44991800	-0.14478700	-1.37288400
H	-3.66195600	0.12145900	-2.54642100
C	-5.97199600	-0.46922800	-0.11912500
H	-5.50847500	-1.01069900	1.91501200
H	-6.11635200	0.07365000	-2.20320400
H	-7.04794000	-0.49944300	0.03165100
C	3.29180500	-3.05281900	2.21815700
H	4.32887500	-3.10122300	2.56533900
H	2.82873800	-4.04027100	2.28395900
H	2.70794800	-2.31116800	2.77601500
S	3.29960800	-2.58703900	0.45785000
O	1.79878500	-2.40295600	0.07379600
C	3.95303700	-0.89971300	0.58172100
H	3.75880600	-0.43378200	-0.38752100
H	3.41639400	-0.37104000	1.37265900
H	5.02642800	-0.94771600	0.78655400
C	1.08064400	1.91741200	-0.53917300
C	2.50778500	2.28879200	-0.50097000
C	3.42622600	2.12765400	-1.55590500
C	2.94663300	2.96419500	0.65767100
C	4.73434700	2.59541700	-1.43332200
H	3.10678500	1.62137400	-2.45548700
C	4.25993500	3.40946000	0.78695400
H	2.23891800	3.13943600	1.46548000
C	5.16254200	3.22566200	-0.26280300
H	5.42416100	2.46750000	-2.26376600
H	4.57295600	3.91396400	1.69740100
H	6.18515700	3.58336400	-0.17471500
H	0.48429000	2.62797200	0.02716000
H	-1.83017300	-3.22851700	0.73839000

Na	0.07351400	-1.36298700	1.14583100
O	1.27934000	-0.66009100	3.07932400
O	-1.17200400	-3.35586200	1.44539900
H	-1.39172900	-2.68454900	2.15962800
H	1.36906100	0.29418800	3.22266300
O	-1.17491700	-1.16838900	2.95512200
H	0.25595900	-0.85832800	3.25240100
H	-1.73532400	-1.08192700	3.73621900

Int6a

C	-3.17090700	2.82574000	1.60941600
C	-2.42195400	1.83810600	0.97057800
C	-2.38155300	1.77370800	-0.43160100
C	-3.10251900	2.71887600	-1.16852200
C	-3.84999500	3.71031900	-0.52947900
C	-3.88748400	3.76512000	0.86331200
H	-3.19781400	2.85912300	2.69564000
H	-1.86957900	1.11354300	1.56431600
H	-3.07985100	2.67888600	-2.25539300
H	-4.40504700	4.43346800	-1.12125700
H	-4.47229000	4.53136900	1.36544100
C	-1.54326400	0.73892200	-1.16515800
C	-0.03154200	1.02932600	-1.17147600
H	-1.85512200	0.75448500	-2.22450300
C	0.79527000	-0.03847800	-1.83628800
O	1.92339900	0.23545400	-2.34172900
C	0.27554500	-1.35085300	-1.75695900
C	1.13331000	-2.50140900	-2.22688100
C	1.67604600	-3.32984100	-1.06811500
H	1.94999600	-2.10265000	-2.83699400
H	0.55777700	-3.20343100	-2.84590300
H	0.86782800	-3.79096900	-0.50305800
H	2.41588200	-4.08053400	-1.36741700
C	-0.97969400	-1.68808000	-1.13477900
O	-1.34587500	-2.86469300	-0.95181000
N	-1.77610900	-0.63129700	-0.62701100
C	-3.13084300	-1.00245200	-0.28266300
C	-3.42764400	-1.37149700	1.03166400
C	-4.13927700	-1.00740600	-1.24989200
C	-4.72767800	-1.74518300	1.37373300
H	-2.63792600	-1.35276800	1.77834900
C	-5.44051000	-1.37043600	-0.90238400
H	-3.90331000	-0.73610100	-2.27520500

C	-5.73757500	-1.74208300	0.40999600
H	-4.95175500	-2.03385500	2.39741300
H	-6.22014100	-1.37081000	-1.65972000
H	-6.75069000	-2.02875000	0.67944300
C	4.27666100	-2.38613600	1.68039800
H	5.33809600	-2.15583700	1.81485200
H	4.07335000	-3.42247400	1.95790000
H	3.63169200	-1.68093400	2.22495500
S	3.91037700	-2.22383400	-0.08595000
O	2.30107800	-2.45378300	-0.02871600
C	4.06638000	-0.44400200	-0.34413900
H	3.43803600	-0.19583600	-1.21908700
H	3.70231100	0.07289500	0.54615200
H	5.12223000	-0.23310700	-0.53860500
C	0.45966100	2.12846100	-0.54964400
C	1.82346600	2.66560500	-0.34809400
C	2.82972000	2.73726000	-1.32831400
C	2.09302500	3.22877100	0.91746900
C	4.06509900	3.31617700	-1.03360200
H	2.63350700	2.31871400	-2.30559700
C	3.33525300	3.78730100	1.21577900
H	1.30800300	3.23028700	1.67162400
C	4.33097500	3.83141500	0.23729100
H	4.82432000	3.37164800	-1.81021600
H	3.51762400	4.20432200	2.20300500
H	5.29632900	4.27982100	0.45776100
H	-0.27948000	2.72789300	-0.02422900
H	-0.91126400	-3.16432500	1.24732200
Na	0.53379800	-0.92367000	0.99293600
O	2.18352400	-0.19880300	2.53761800
O	-0.11964800	-3.08275000	1.80920300
H	-0.30974600	-2.36455300	2.48647000
H	2.26303900	0.76808100	2.55862900
O	-0.17663000	-0.75845800	3.05103900
H	1.21678100	-0.41215300	2.97414500
H	-0.57243200	-0.57388300	3.91102600

TS6a

C	-0.10373800	1.08742000	3.52992200
C	0.16243800	0.93929300	2.16628000
C	1.38553600	1.36346200	1.63645700
C	2.32990200	1.93748700	2.49659900
C	2.06671000	2.08048800	3.85782800
C	0.84422300	1.65469800	4.38095500

H	-1.06676600	0.77109500	3.92474000
H	-0.59359200	0.49467600	1.52818300
H	3.28414600	2.27519300	2.09759800
H	2.81130700	2.53366200	4.50689700
H	0.63055200	1.77289400	5.43978000
C	1.75619400	1.19651500	0.15284100
C	2.64436400	-0.03045200	-0.05082100
H	2.34106500	2.07615100	-0.12822200
C	1.86050400	-1.29734100	-0.02903400
O	2.20510900	-2.34944700	0.55957900
C	0.65991000	-1.22903300	-0.77709100
C	0.10798200	-2.55186700	-1.30878100
C	0.00890900	-3.19276400	-0.02178200
H	0.75277200	-3.05421000	-2.03356900
H	-0.86141300	-2.29457100	-1.75091600
H	-0.69623900	-2.78894700	0.70055900
H	0.62380600	-4.03799600	0.26215200
C	-0.03985500	0.00157200	-1.10941200
O	-1.12136000	0.00471400	-1.73306000
N	0.57561600	1.17864600	-0.73628000
C	-0.04722000	2.43892400	-1.04346200
C	-1.27715600	2.79698100	-0.47905900
C	0.62025200	3.32694800	-1.89229800
C	-1.82683800	4.04695000	-0.77456100
H	-1.80340800	2.10669500	0.17790300
C	0.06743900	4.57673000	-2.17498000
H	1.56498200	3.02894800	-2.33931000
C	-1.15915400	4.93928200	-1.61714000
H	-2.77933300	4.32758800	-0.33148000
H	0.59141500	5.25998100	-2.83778400
H	-1.59277800	5.91098500	-1.83730400
C	-6.24905700	-0.98719800	0.42165600
H	-6.95539200	-1.24927500	1.21594600
H	-6.74109200	-0.35379500	-0.32024700
H	-5.36160700	-0.46548600	0.80872000
S	-5.74553500	-2.51689900	-0.44331300
O	-4.59847800	-2.14199400	-1.39401500
C	-4.98371800	-3.37612500	0.97770500
H	-4.63246500	-4.34222400	0.60418500
H	-4.13767500	-2.78976900	1.35903100
H	-5.74971200	-3.53968500	1.74285300
C	3.97238400	0.14894000	-0.23491600
C	5.10646300	-0.75840700	-0.45710900
C	5.15340200	-2.11578300	-0.08421600

C	6.24768400	-0.19942800	-1.06986700
C	6.29221600	-2.87741400	-0.33928000
H	4.29675400	-2.55495500	0.41148300
C	7.37893000	-0.96626600	-1.33176200
H	6.23682900	0.85172600	-1.35005500
C	7.40512600	-2.31394400	-0.96708200
H	6.31096900	-3.92180500	-0.03826100
H	8.24054300	-0.51189500	-1.81376900
H	8.28817300	-2.91659600	-1.16272900
H	4.27452400	1.19590400	-0.29394700
H	-3.75712800	2.31701200	-1.62586500
Na	-3.23936500	-0.33742200	-1.05548100
O	-2.30834300	-1.52053300	1.53082900
O	-4.43274600	1.70062600	-1.30075700
H	-4.16344000	1.51719200	-0.34700700
H	-1.70754900	-1.37991300	2.27747400
O	-3.49043800	0.68823400	0.93196700
H	-2.78245000	-0.61140400	1.38446300
H	-3.66647800	1.21350700	1.72389500

2'

C	-5.72418100	0.07562900	2.03138400
C	-4.42090300	-0.32371500	1.73247300
C	-4.05171200	-0.67493000	0.42029700
C	-5.03670900	-0.62242300	-0.58603400
C	-6.33807100	-0.22695600	-0.28771500
C	-6.68788100	0.12575100	1.02171300
H	-5.98631700	0.34441600	3.05048600
H	-3.67255500	-0.36054700	2.51979700
H	-4.78705800	-0.90147900	-1.60504900
H	-7.08496000	-0.19701800	-1.07575600
H	-7.70434000	0.43227900	1.25041800
C	-2.66594100	-1.08893200	0.17069200
C	-2.07941500	-1.28653700	-1.02682900
H	-2.04719800	-1.18022400	1.06010800
H	-2.60744800	-1.09168400	-1.95754800
C	-0.62772400	-1.54044700	-1.20623400
O	-0.02994000	-0.88124900	-2.07107400
C	0.08753900	-2.63388100	-0.48412400
C	-0.58999900	-3.58308900	0.50784500
C	-0.40762300	-4.03235700	-0.89646400
H	-1.59024100	-3.35608300	0.85476800
H	0.07299400	-3.99543000	1.26235400

H	0.39572400	-4.72161800	-1.13352000
H	-1.28290100	-4.07283300	-1.53778300
C	1.60960400	-2.53727300	-0.31959200
O	2.32483500	-3.49742600	-0.61240800
N	2.05091200	-1.37891000	0.24028800
H	1.34446700	-0.63412300	0.48139400
C	3.38714700	-1.04130700	0.55284400
C	3.57918100	0.10269400	1.35226100
C	4.50897300	-1.76185900	0.10535800
C	4.86536600	0.51887100	1.69070400
H	2.70825400	0.65285100	1.69427100
C	5.79107500	-1.33056000	0.45668900
H	4.36958300	-2.64886800	-0.49575700
C	5.98321700	-0.19459100	1.24610800
H	4.99284600	1.40234000	2.31086600
H	6.64863800	-1.89857500	0.10594500
H	6.98526400	0.12744500	1.51426200
Na	0.58332200	1.18413000	-1.34550700
H	0.42173200	0.68648200	0.67366100
C	-0.25753300	3.90823500	0.98818200
H	-0.06696600	4.51909600	1.87557600
H	-0.14663100	2.83977900	1.21461900
H	-1.24842800	4.11044000	0.57263300
S	1.01385300	4.27638600	-0.26705400
O	0.66244500	3.42327500	-1.50122500
C	0.48441100	5.96820300	-0.70127500
H	-0.55073500	5.93974100	-1.05023200
H	0.58917000	6.61351400	0.17526600
H	1.14088700	6.31489100	-1.50139800

TS1f

C	-5.97084900	0.80044300	1.96512400
C	-4.73581600	0.21612900	1.68156200
C	-4.32407500	-0.00721000	0.35398100
C	-5.19605100	0.37302400	-0.68597200
C	-6.42927100	0.95455800	-0.40375100
C	-6.82272600	1.17202200	0.92268200
H	-6.26694100	0.96349800	2.99722600
H	-4.07482500	-0.07021300	2.49546000
H	-4.91114200	0.20988700	-1.72060600
H	-7.08869500	1.23844400	-1.21883100
H	-7.78582800	1.62526700	1.13822300
C	-3.01685600	-0.63300100	0.12331100
C	-2.40962000	-0.83656400	-1.06328800

H	-2.47625400	-0.90742400	1.02565100
H	-2.84897700	-0.48397400	-1.99330300
C	-1.01654800	-1.31795800	-1.21205500
O	-0.30649500	-0.75401000	-2.06101400
C	-0.48417200	-2.50835900	-0.48224500
C	-1.33074000	-3.40205700	0.42625200
C	-1.10852300	-3.82414700	-0.98168400
H	-2.32221300	-3.07688500	0.71558800
H	-0.77100800	-3.91475300	1.20241500
H	-0.37577900	-4.59583100	-1.19239000
H	-1.94039400	-3.74202500	-1.67508900
C	1.02771800	-2.59413800	-0.21830700
O	1.62001800	-3.65958500	-0.42059600
N	1.57444300	-1.46587600	0.30225800
H	0.89487600	-0.51737200	0.60161100
C	2.93998700	-1.32672700	0.62999800
C	3.26851800	-0.42179300	1.65986100
C	3.98331100	-1.98308700	-0.05300500
C	4.60176000	-0.17676000	1.99219400
H	2.46679100	0.07302000	2.19749000
C	5.31198200	-1.73227800	0.29405800
H	3.74379700	-2.70130400	-0.82625800
C	5.63386500	-0.82951200	1.31254600
H	4.83216000	0.51876700	2.79517500
H	6.10345900	-2.25503700	-0.23668100
H	6.67099300	-0.64622300	1.57814000
Na	1.25460000	0.66638000	-1.25906800
H	0.36151000	0.51300700	0.74730600
C	0.60963800	3.81586200	0.69274400
H	0.71994500	4.47789300	1.55656900
H	0.34547100	2.80061700	1.01082100
H	-0.13578400	4.20022000	-0.00855200
S	2.21975800	3.66858100	-0.15342800
O	1.97638900	2.77300900	-1.38214600
C	2.32438900	5.36271000	-0.82406700
H	1.45243400	5.55137800	-1.45506300
H	2.37624700	6.07505800	0.00396500
H	3.23749300	5.41539300	-1.41966700
Int1f			
C	-6.43492800	1.32006500	0.58377500
C	-5.17357500	0.75872100	0.78237000
C	-4.59160800	-0.08096500	-0.18747600
C	-5.32011600	-0.34685900	-1.36518100

C	-6.57995600	0.21130000	-1.56182300
C	-7.14258900	1.04796800	-0.58941500
H	-6.86325700	1.96834500	1.34243100
H	-4.62170700	0.97426100	1.69335400
H	-4.90142500	-0.99652000	-2.12715100
H	-7.12820300	-0.00542300	-2.47409400
H	-8.12561900	1.48183400	-0.74770400
C	-3.26403000	-0.63531600	0.08037500
C	-2.49567300	-1.36381600	-0.76140500
H	-2.86280300	-0.40587300	1.06535900
H	-2.81583500	-1.60504200	-1.77160800
C	-1.15076900	-1.84603600	-0.42830200
O	-0.47809900	-2.42161100	-1.30512000
C	-0.59401300	-1.61763300	0.95437800
C	-1.18796000	-2.36266600	2.12093800
C	0.18062700	-2.74569700	1.61869100
H	-2.00640900	-3.04990500	1.92476500
H	-1.25330000	-1.79446500	3.04427100
H	1.03765800	-2.46561900	2.22518200
H	0.28636700	-3.67874000	1.07100700
C	-0.05873700	-0.18295300	1.20763200
O	-0.25201300	0.32721500	2.32751300
N	0.58231900	0.29617400	0.12749600
C	1.17218400	1.56435600	0.12083100
C	1.51172700	2.09678200	-1.14739300
C	1.50546400	2.34411400	1.25748500
C	2.15090600	3.32805800	-1.28269300
H	1.23766600	1.52758800	-2.03323500
C	2.15314300	3.57386700	1.11181400
H	1.23450700	1.97638000	2.23809200
C	2.48508100	4.07977200	-0.14974200
H	2.38178500	3.70569000	-2.27603100
H	2.39376600	4.14893600	2.00319700
H	2.97797800	5.04266200	-0.24937300
Na	1.56606300	-1.40737400	-1.12870400
C	5.03030000	0.85496200	-0.32108400
H	5.81640300	1.23029200	0.34006100
H	4.09107100	1.37123100	-0.11246300
H	5.30375400	0.97773700	-1.37185800
S	4.77131700	-0.91492400	0.02981700
O	3.78669500	-1.43318800	-1.03500400
C	6.40358500	-1.52664200	-0.51115000
H	6.56325900	-1.24379200	-1.55447000
H	7.17809100	-1.10691600	0.13635600

H	6.38522200	-2.61360200	-0.41472800
TS2f			
C	-4.71218500	0.29086000	-1.64989600
C	-3.45650300	-0.26894600	-1.41475000
C	-3.17409500	-0.91059300	-0.19756900
C	-4.17973800	-0.96061100	0.78146600
C	-5.43974600	-0.40826100	0.54671800
C	-5.70908000	0.22075200	-0.67174300
H	-4.91271400	0.78571100	-2.59589300
H	-2.68518500	-0.20134700	-2.17490500
H	-3.97157700	-1.44619700	1.73173500
H	-6.20791400	-0.46640800	1.31263600
H	-6.68697100	0.65599300	-0.85714900
C	-1.85382400	-1.53249900	0.07827400
C	-1.12624900	-2.18344900	-0.97549500
H	-1.82781500	-2.00582400	1.05560000
H	-1.50289400	-2.18554300	-1.99237800
C	0.20534600	-2.52644800	-0.73175000
O	1.08837900	-2.91892700	-1.56053900
C	0.67551400	-2.11701200	0.67091900
C	0.43896500	-2.99375700	1.87847100
C	1.83572400	-2.82079900	1.32350400
H	-0.06071000	-3.94504400	1.71661600
H	0.20440500	-2.50955500	2.82290100
H	2.53388200	-2.22415400	1.90457000
H	2.26842300	-3.66303200	0.78882400
C	0.55893300	-0.59778100	0.75690600
O	1.62746200	0.07885600	0.73141200
N	-0.68867800	-0.13845800	0.72671500
C	-0.99289000	1.22669600	0.55803200
C	-0.57858600	1.93578700	-0.58395500
C	-1.79095000	1.88192800	1.50925300
C	-0.94671100	3.27041800	-0.75990200
H	0.02570200	1.42933400	-1.32977300
C	-2.15828200	3.21623400	1.32863000
H	-2.11682700	1.33188100	2.38651200
C	-1.73722500	3.91816100	0.19500100
H	-0.62220300	3.80419900	-1.64948100
H	-2.77626600	3.70838800	2.07459100
H	-2.02563500	4.95582700	0.05460000
Na	2.73640400	-1.42900400	-0.97803200
C	4.75407400	0.95549900	1.35394000
H	4.96652800	1.89514100	1.87185900

H	5.50190400	0.20829600	1.62718100
H	3.74101400	0.60288300	1.56557100
S	4.91658000	1.23074100	-0.44597300
O	4.49639200	-0.08747500	-1.12313000
C	3.51101600	2.38273600	-0.63627100
H	2.60762100	1.91968700	-0.22828800
H	3.75251400	3.31282100	-0.11353300
H	3.41082200	2.58022600	-1.70551800

Int2f

C	-3.43773400	-1.18165800	-2.58970200
C	-2.34792700	-1.21668200	-1.71956400
C	-2.53882600	-1.27783100	-0.33146800
C	-3.84707500	-1.31559100	0.16216100
C	-4.94425800	-1.28759700	-0.70529100
C	-4.74249700	-1.21710400	-2.08463800
H	-3.27180800	-1.13533900	-3.66283600
H	-1.33454700	-1.20974700	-2.11082200
H	-4.01008900	-1.36769300	1.23580500
H	-5.95262900	-1.32124300	-0.30222300
H	-5.59176900	-1.19579200	-2.76185300
C	-1.34975800	-1.34243900	0.62138900
C	-0.37286500	-2.41023900	0.20032700
H	-1.76201900	-1.53148500	1.62851100
H	-0.74594700	-3.22729800	-0.40719800
C	0.92672400	-2.40154000	0.61806400
O	1.86344000	-3.25255200	0.32037700
C	1.31035400	-1.20780500	1.49254400
C	1.53421200	-1.45098600	2.98912700
C	2.69509700	-1.13507700	2.09278100
H	1.40823300	-2.47481900	3.32864300
H	1.20109500	-0.68172600	3.68042100
H	3.14653200	-0.15407100	2.18761800
H	3.35911400	-1.96227500	1.85796800
C	0.63487800	0.09189700	1.15165800
O	1.21214600	1.18657700	1.27337700
N	-0.65848800	0.00158200	0.71192200
C	-1.45233200	1.20354100	0.73107400
C	-1.67062600	1.93303400	-0.44032900
C	-2.01658200	1.64166900	1.93384300
C	-2.44771500	3.09305800	-0.41013200
H	-1.23879200	1.58171200	-1.37112600
C	-2.79584800	2.80019900	1.96368800
H	-1.83404000	1.07790300	2.84390900

C	-3.01297500	3.52922200	0.79126000
H	-2.61609600	3.65224900	-1.32618400
H	-3.22945200	3.13385700	2.90214800
H	-3.61985500	4.42978400	0.81342900
Na	3.16046000	-2.02434200	-0.86948300
C	4.18908500	2.03626600	0.03262500
H	4.24631700	3.12850500	0.00859400
H	5.14369300	1.62640200	0.36844700
H	3.35792900	1.70152000	0.66126700
S	3.93373100	1.44596800	-1.67525700
O	3.82828400	-0.08946700	-1.59620600
C	2.23109500	2.06876000	-1.88972100
H	1.61547800	1.75798200	-1.04150800
H	2.27412700	3.15986600	-1.95538000
H	1.86166300	1.65787300	-2.83122300

TS3f

C	2.59662900	-2.78803400	1.52458300
C	1.65532100	-2.06847700	0.78790300
C	1.99294300	-1.48794800	-0.44359200
C	3.29705400	-1.65265800	-0.92115600
C	4.24554700	-2.37630200	-0.19006800
C	3.89902900	-2.94547000	1.03621600
H	2.31684700	-3.23015200	2.47741400
H	0.64369900	-1.94897400	1.16575500
H	3.57535300	-1.20608600	-1.87230900
H	5.25312300	-2.49189600	-0.57960700
H	4.63293900	-3.50767100	1.60667800
C	0.95476000	-0.73768200	-1.27321400
C	-0.23282900	-1.62214800	-1.55955000
H	1.45974100	-0.43352000	-2.21034900
H	-0.05908900	-2.68688100	-1.68477800
C	-1.43096300	-1.05560900	-1.95123900
O	-2.50646700	-1.73743700	-2.28376600
C	-1.55946800	0.38237800	-1.85913200
C	-3.80984300	0.19815300	-1.94805900
C	-2.75748500	1.02827200	-2.52515600
H	-4.01462600	0.29512100	-0.88647200
H	-4.44344200	-0.46184400	-2.52468800
H	-2.72740000	1.00713600	-3.61809400
H	-2.78740000	2.06401000	-2.16676300
C	-0.70558300	1.13786100	-0.98971000
O	-0.99954200	2.27142600	-0.54672000
N	0.51153300	0.52710500	-0.58915800

C	1.57539400	1.44878500	-0.26669100
C	2.19786800	1.40687000	0.98406300
C	2.02191900	2.37287000	-1.22116100
C	3.25351500	2.27449400	1.27871900
H	1.86403800	0.68479000	1.72080600
C	3.07202800	3.24288100	-0.92590900
H	1.53088600	2.41713800	-2.18848800
C	3.69335200	3.19587700	0.32600000
H	3.73146400	2.22703100	2.25329600
H	3.40346700	3.95889600	-1.67280500
H	4.51227300	3.87159500	0.55565000
Na	-2.56440800	-2.15979700	-0.07704800
C	-3.31634000	1.70534600	1.78230800
H	-3.23707300	2.53899800	2.48664700
H	-4.35480300	1.60393500	1.45974100
H	-2.63930900	1.85823000	0.93339200
S	-2.90077000	0.17832700	2.69250900
O	-3.05929400	-0.99578600	1.70474900
C	-1.10773300	0.47081100	2.84987700
H	-0.66730000	0.57897900	1.85550700
H	-0.95393900	1.37767500	3.44116100
H	-0.68764800	-0.38896000	3.37549900

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C	5.36105300	-3.62767400	-0.15815700
C	4.42935100	-2.75318700	-0.71824300
C	3.05784600	-2.85916600	-0.41609600
C	2.64895200	-3.88337600	0.46220800
C	3.57819200	-4.75816400	1.01911900
C	4.93932200	-4.63413300	0.71368100
H	6.41396400	-3.52291400	-0.40300700
H	4.76172300	-1.96953800	-1.39392800
H	1.59705500	-4.00317600	0.70176600
H	3.24241700	-5.54383000	1.69015400
H	5.66087200	-5.31918400	1.14916700
C	2.13073200	-1.90372200	-1.03092800
C	0.80994800	-1.77997600	-0.78086200
H	2.58814500	-1.24294900	-1.76357500
H	0.30325900	-2.43085500	-0.07438200
C	-0.11466600	-0.88418600	-1.50165500
O	-1.32306600	-1.17686000	-1.52249700
C	0.40987000	0.23232000	-2.36927000
C	0.25523900	-0.05149100	-3.86904200
C	-0.61345900	0.97351000	-3.22383600

H	-0.18962700	-1.00596000	-4.13243400
H	1.08762400	0.28042900	-4.48007800
H	-0.39252000	2.01800000	-3.41872500
H	-1.65443500	0.73390900	-3.03557900
C	1.63076600	1.06707800	-1.98975800
O	2.44406600	1.41302800	-2.85551000
N	1.68815600	1.41601500	-0.67909100
H	0.87944100	1.08741500	-0.06438700
C	2.67308400	2.18803600	-0.03901400
C	2.59294700	2.27472200	1.36617300
C	3.70668300	2.87338700	-0.70558900
C	3.51621100	3.03091000	2.08465100
H	1.79856800	1.73823700	1.87598100
C	4.62639900	3.62460600	0.03173600
H	3.77818600	2.80675100	-1.78199500
C	4.54287700	3.71380700	1.42317500
H	3.43680800	3.08167600	3.16765000
H	5.41931000	4.14683300	-0.49742100
H	5.26529100	4.30030900	1.98332100
Na	-2.51643600	0.22865300	0.14815800
H	-0.29756800	0.64977200	0.73516500
C	-1.13169000	3.75690600	1.55273100
H	-0.35947800	4.53088900	1.57441700
H	-0.72389800	2.80296000	1.89310400
H	-2.00623200	4.04520600	2.14220600
S	-1.64811700	3.46236200	-0.17373100
O	-2.84605400	2.50553700	-0.11015700
C	-2.38498000	5.10838100	-0.48631000
H	-3.16994100	5.29823200	0.25006900
H	-1.60295100	5.87149200	-0.43907900
H	-2.81575200	5.07755800	-1.48882000
C	-0.14573600	-1.32007200	3.23622600
H	0.48925200	-1.05539500	4.08688500
H	0.32992500	-1.02932400	2.29724900
H	-0.39751900	-2.38398200	3.24772700
S	-1.68497100	-0.34252200	3.30103400
O	-2.61620300	-0.91606900	2.22318000
C	-2.33432700	-1.01784700	4.87584300
H	-2.42897000	-2.10376400	4.79536500
H	-1.66474100	-0.74120600	5.69534000
H	-3.31753400	-0.56956300	5.03070700
C	-3.73221900	-3.15750900	-0.09045100
H	-4.00311700	-4.19959700	-0.28447500
H	-3.80366900	-2.93071200	0.97528000

H	-2.72751700	-2.92577200	-0.45220200
S	-4.93658500	-2.06574500	-0.93351900
O	-4.52198100	-0.62820100	-0.61872600
C	-4.37909700	-2.38788800	-2.64826500
H	-3.32847400	-2.09920000	-2.72838600
H	-4.52613200	-3.44570200	-2.88493500
H	-4.99718000	-1.77096300	-3.30351500

TS1g

C	6.42897100	-2.21236800	-0.08571100
C	5.25188100	-1.67541700	-0.60757100
C	3.99301500	-2.18362300	-0.23255400
C	3.95212500	-3.25742200	0.68014900
C	5.12682400	-3.79470800	1.19906200
C	6.37070700	-3.27428700	0.81963600
H	7.38867100	-1.80175000	-0.38518100
H	5.29845000	-0.84587500	-1.30800200
H	2.99766400	-3.67895700	0.97938900
H	5.07645800	-4.62390200	1.89900900
H	7.28480300	-3.69656500	1.22673900
C	2.79591300	-1.56907600	-0.81220300
C	1.50898500	-1.85406800	-0.51677600
H	2.99870500	-0.80388600	-1.55809800
H	1.24816200	-2.61551800	0.21374000
C	0.33640200	-1.24827000	-1.17297700
O	-0.77728300	-1.76322200	-0.98573400
C	0.51557000	-0.10707800	-2.13809000
C	0.56266900	-0.54770600	-3.60080700
C	-0.63147400	0.19371600	-3.08984600
H	0.45782800	-1.61070700	-3.79865500
H	1.28848200	-0.01555300	-4.20708500
H	-0.74264500	1.23300600	-3.38160800
H	-1.55804800	-0.34967300	-2.93660700
C	1.39632000	1.09747900	-1.77530400
O	2.15402900	1.57392400	-2.63787300
N	1.22226900	1.54096600	-0.51280100
H	0.27181700	1.11879400	0.13809600
C	1.86581200	2.65584200	0.04645700
C	1.77348700	2.80021100	1.44879000
C	2.55941800	3.64670200	-0.68153100
C	2.34424800	3.89331100	2.09830500
H	1.24622100	2.03990700	2.01510400
C	3.13152500	4.73391000	-0.01583300
H	2.65234600	3.54261200	-1.75360700

C	3.02996700	4.87237400	1.37126100
H	2.26013100	3.97655900	3.17927600
H	3.66688100	5.48179100	-0.59584500
H	3.48245900	5.72055500	1.87714200
Na	-2.55170200	-0.26499800	0.00241100
H	-0.62361600	0.81218700	0.73869900
C	-2.08659600	3.73874300	0.74492000
H	-1.52204700	4.66818600	0.63084500
H	-1.49312000	3.00336000	1.29100000
H	-3.04953400	3.90987700	1.23367500
S	-2.37530900	3.00407200	-0.90093700
O	-3.30813200	1.80363300	-0.68819800
C	-3.45581800	4.32175800	-1.56645400
H	-4.32475800	4.43788300	-0.91377000
H	-2.88790300	5.25335200	-1.64085600
H	-3.77592000	3.99938200	-2.55896100
C	-0.26395000	-0.82548800	3.41895800
H	0.25595000	-0.33989800	4.24994700
H	0.22584400	-0.58920600	2.47288200
H	-0.33184200	-1.90583100	3.57208100
S	-1.94862300	-0.13649200	3.27297900
O	-2.68623700	-1.00275800	2.24160300
C	-2.58069100	-0.71137500	4.89351900
H	-2.48071600	-1.79775200	4.95992600
H	-2.02793900	-0.21551200	5.69660900
H	-3.63475700	-0.43127600	4.93948800
C	-3.07816300	-3.83255800	0.44486000
H	-3.12911100	-4.92499900	0.47876400
H	-3.40131800	-3.40044100	1.39393000
H	-2.07261000	-3.48006300	0.20344900
S	-4.24902500	-3.22938800	-0.82692400
O	-4.14582600	-1.70370100	-0.83707000
C	-3.31515700	-3.80806400	-2.29219200
H	-2.32342100	-3.35011400	-2.27321600
H	-3.25373700	-4.90005300	-2.27493500
H	-3.87204300	-3.48101900	-3.17241700

Int1g

C	7.36705200	-0.66608300	-0.48962300
C	6.11497200	-0.51501400	0.10667900
C	5.20981700	0.46686800	-0.34107800
C	5.60441600	1.29845400	-1.40910500
C	6.85434700	1.14879500	-2.00332800
C	7.74188700	0.16597100	-1.54705200

H	8.04705200	-1.43301300	-0.13046600
H	5.82243000	-1.16771000	0.92479200
H	4.93047500	2.06621300	-1.77567500
H	7.14046900	1.79873700	-2.82538500
H	8.71568100	0.05176200	-2.01440900
C	3.91022700	0.57198200	0.32618400
C	2.88776900	1.39265900	-0.00096400
H	3.77054000	-0.10700200	1.16467500
H	2.94990700	2.07909100	-0.84162700
C	1.60029000	1.43669100	0.70993100
O	0.72862100	2.24003900	0.33411300
C	1.36494200	0.51411600	1.87537900
C	2.03722800	0.80731900	3.19475400
C	0.55115100	1.00833300	3.05576600
H	2.66491900	1.69214900	3.26230000
H	2.38753600	-0.06827500	3.73404700
H	-0.10315300	0.28534800	3.53453100
H	0.16130600	2.02101300	3.00878600
C	1.17588600	-0.95928900	1.45745600
O	1.62581400	-1.85115600	2.20758600
N	0.50873700	-1.03985500	0.29367100
C	0.32233100	-2.25800600	-0.36350600
C	-0.30223800	-2.19496900	-1.63585400
C	0.69936000	-3.54517000	0.10448600
C	-0.54137000	-3.33914100	-2.39384300
H	-0.58701700	-1.21884600	-2.01914100
C	0.45787100	-4.68480800	-0.66839900
H	1.18179200	-3.62463800	1.06904700
C	-0.16568800	-4.60227900	-1.91718300
H	-1.01525900	-3.24518000	-3.36865500
H	0.76598400	-5.65456900	-0.28282800
H	-0.34503200	-5.49525500	-2.50961300
Na	-1.29353800	0.70856000	0.11767300
C	-2.96582900	-3.44269300	0.87538300
H	-2.80683300	-4.33663900	1.48431600
H	-2.29865600	-3.46438400	0.01257500
H	-4.00919300	-3.35588300	0.56069800
S	-2.51344100	-1.97350100	1.85977400
O	-2.91974200	-0.74996200	1.01980200
C	-3.82239600	-2.12623700	3.12914300
H	-4.80102100	-2.13774700	2.64243400
H	-3.65847700	-3.03929700	3.70818200
H	-3.73674000	-1.25349300	3.77906000
C	-4.41874800	0.34480500	-3.73188200

H	-5.39199300	-0.14015500	-3.84917100
H	-3.72482800	-0.02522500	-4.48887500
H	-4.50999500	1.43141900	-3.80617800
S	-3.71458900	-0.09522300	-2.10117300
O	-2.43796100	0.74819000	-1.97773400
C	-4.97809600	0.71864200	-1.06274900
H	-5.06705900	1.76892700	-1.34986800
H	-5.92832900	0.19108900	-1.18899800
H	-4.62321400	0.63168200	-0.03479400
C	-1.43780700	3.96811300	-1.38808200
H	-1.38409800	4.97044200	-1.82339400
H	-1.96559700	3.28315500	-2.05522100
H	-0.44537100	3.57375900	-1.15891900
S	-2.43323000	4.05377900	0.14751500
O	-2.55897800	2.62562800	0.68627500
C	-1.18519400	4.89140300	1.19186200
H	-0.29035500	4.26589300	1.22459500
H	-0.97104100	5.87850400	0.77184500
H	-1.62201300	4.99739300	2.18679100

TS2g

C	4.40859300	-3.60142000	0.87079800
C	3.23023900	-2.96791100	0.47925500
C	3.18784800	-2.17735000	-0.68354400
C	4.37222900	-2.02466500	-1.42521300
C	5.55413900	-2.65499600	-1.03520600
C	5.57568500	-3.44873200	0.11421100
H	4.41996400	-4.21306400	1.76880500
H	2.33439100	-3.08893200	1.07966300
H	4.36152500	-1.39941800	-2.31376600
H	6.45714000	-2.52194600	-1.62381700
H	6.49411500	-3.94012700	0.42240500
C	1.95762000	-1.50960200	-1.15020100
C	0.66531000	-1.90877600	-0.75071200
H	2.06397700	-1.07234000	-2.13669800
H	0.51643400	-2.72412500	-0.05028100
C	-0.41441200	-1.05995700	-1.04173300
O	-1.61097900	-1.24519500	-0.64088700
C	-0.06543000	0.22480400	-1.77172800
C	-0.02880300	0.20069900	-3.30577300
C	-1.13783000	0.90295900	-2.57474200
H	-0.23840500	-0.74857200	-3.79215500
H	0.72764100	0.80909200	-3.79476300
H	-1.13740100	1.98493900	-2.56999800

H	-2.11710500	0.43507200	-2.57192100
C	1.00227000	1.12014900	-1.11250200
O	0.85047300	2.36335500	-1.17006000
N	2.01489200	0.47302500	-0.51033700
C	3.18829900	1.12550500	-0.11329900
C	3.83548500	0.69593100	1.06258400
C	3.80116500	2.14697700	-0.87166800
C	5.04499100	1.26146000	1.46802100
H	3.37839700	-0.09584100	1.64743000
C	5.00922300	2.70920800	-0.46034300
H	3.30872000	2.50478400	-1.76825300
C	5.64124200	2.27354100	0.71008300
H	5.52349500	0.90844300	2.37802400
H	5.46082400	3.49673200	-1.05869900
H	6.58233700	2.71564700	1.02459300
Na	-2.95161200	0.44456300	0.28091400
C	-1.50529700	4.72754300	-1.04393500
H	-1.06625900	5.66463900	-0.68843800
H	-2.22305700	4.93404600	-1.84044400
H	-0.73003900	4.02796600	-1.36986200
S	-2.44345500	3.97366500	0.33164000
O	-2.98801800	2.64072500	-0.20539200
C	-1.01158600	3.57326300	1.39536100
H	-0.23753600	3.09114800	0.79150700
H	-0.64362900	4.50385600	1.83820400
H	-1.38455000	2.89924300	2.16965600
C	0.38061000	-0.38844000	2.86516300
H	0.93981100	-1.15629900	3.40783500
H	0.71899400	0.60056100	3.17973100
H	0.50198900	-0.49919500	1.78450100
S	-1.38314400	-0.51519800	3.32529000
O	-2.13257400	0.49658600	2.44564900
C	-1.71732300	-2.16219900	2.60409000
H	-1.55859400	-2.11690100	1.52079400
H	-1.06724600	-2.90034700	3.08254500
H	-2.76156700	-2.39347100	2.82497300
C	-4.24455000	-2.54753400	-1.95458400
H	-4.38152600	-3.58767300	-2.26442800
H	-3.18340200	-2.31257100	-1.83447800
H	-4.71722100	-1.85955600	-2.66067600
S	-4.98282000	-2.31629000	-0.30200200
O	-4.84046600	-0.82951300	0.04098600
C	-6.73625000	-2.53145900	-0.77286300
H	-6.99300900	-1.78975300	-1.53333500

H	-6.89122100	-3.54871400	-1.14314700
H	-7.33210000	-2.36517300	0.12643700

Int2g

C	-3.38240900	2.74488200	1.62830100
C	-2.88415500	1.58002000	1.04470500
C	-3.11227800	1.30037600	-0.31098700
C	-3.84938200	2.21941100	-1.06558600
C	-4.33836100	3.39843300	-0.49023900
C	-4.10810600	3.66515900	0.86036300
H	-3.21327200	2.93425200	2.68554200
H	-2.31814800	0.87331900	1.64595100
H	-4.04866700	2.00988800	-2.11440900
H	-4.90980100	4.09799600	-1.09448000
H	-4.49855800	4.57119700	1.31527800
C	-2.51937500	0.04859800	-0.98105600
C	-1.05152500	0.22491900	-1.25720500
H	-3.05284100	-0.06526000	-1.93542800
H	-0.80287700	0.98227100	-1.99591800
C	-0.04658000	-0.44291800	-0.61844400
O	1.22737100	-0.25024000	-0.81334800
C	-0.44028700	-1.50807500	0.38000700
C	0.52856000	-2.66783200	0.59137400
C	0.38426100	-1.63945000	1.66445600
H	1.42088000	-2.62686300	-0.02425700
H	0.07645600	-3.63957400	0.75689600
H	-0.16700700	-1.91840100	2.55715700
H	1.18809500	-0.92014300	1.78770300
C	-1.88860600	-1.89244600	0.52079600
O	-2.22810000	-2.83940100	1.23609300
N	-2.81738000	-1.16623600	-0.19248800
C	-4.19622300	-1.57467800	-0.14126600
C	-4.93078100	-1.49334800	1.04575700
C	-4.81267400	-2.04517600	-1.30551300
C	-6.27284900	-1.87618500	1.06419200
H	-4.44471000	-1.14305700	1.94886800
C	-6.15857800	-2.41935400	-1.28731400
H	-4.23272100	-2.12807800	-2.22018300
C	-6.89263500	-2.33579800	-0.10161300
H	-6.83533800	-1.81377100	1.99144800
H	-6.62793400	-2.78538000	-2.19618700
H	-7.93799700	-2.63062700	-0.08474300
Na	3.11828900	0.66841800	-0.16075100
C	1.03718400	2.65298300	2.05942700

H	0.24324100	3.18606600	2.58947600
H	1.86193400	2.43026400	2.73922400
H	0.65362500	1.73546600	1.60698300
S	1.71274900	3.73884000	0.75102300
O	2.77893500	2.91579800	0.01626300
C	0.23808600	3.75215000	-0.32638400
H	-0.03037400	2.72499500	-0.58794700
H	-0.58600900	4.24396100	0.19781000
H	0.50701500	4.32293700	-1.21748900
C	2.74093500	0.75472900	-3.59916200
H	2.32644200	0.57273700	-4.59500800
H	3.27520800	1.70696300	-3.58729200
H	1.96335400	0.72013000	-2.82758800
S	3.97069700	-0.54644000	-3.22964900
O	4.47322000	-0.26385700	-1.79912300
C	2.78797600	-1.93240500	-3.08469200
H	2.06332500	-1.66718900	-2.30547800
H	2.30516900	-2.08797000	-4.05385200
H	3.36606200	-2.81907900	-2.81615300
S	5.04745000	-1.12930300	2.15720800
O	3.98169600	-0.07886000	1.82326100
C	4.98744000	-2.37046700	0.81638400
H	5.22228200	-1.84062100	-0.11080500
H	5.73116000	-3.14656800	1.01882100
H	3.98076800	-2.79249400	0.75978500
C	4.31942800	-2.16217600	3.47853400
H	4.97812400	-3.01235600	3.67656900
H	4.24344000	-1.53549300	4.36902300
H	3.32646400	-2.49365600	3.16485800

TS3g

C	3.89778300	3.09810500	-0.46059800
C	3.37849100	1.80251900	-0.47794200
C	3.09785800	1.12774200	0.71805000
C	3.34328100	1.78406400	1.92986000
C	3.85037200	3.08808100	1.95311900
C	4.13134800	3.75022200	0.75592700
H	4.13293600	3.59651300	-1.39770400
H	3.20673200	1.29369900	-1.42142700
H	3.14607300	1.26615600	2.86630500
H	4.03935900	3.57774200	2.90478600
H	4.54190000	4.75610900	0.76911800
C	2.46304100	-0.26754900	0.72434800
C	0.96579600	-0.10984000	0.60819100

H	2.71401400	-0.71746800	1.70511500
H	0.50841700	0.68046100	1.19410700
C	0.18640800	-1.02712300	-0.06129300
O	-1.13337000	-1.01544100	-0.06426500
C	0.83282800	-2.08760400	-0.77818600
C	-0.04281800	-3.14953900	-1.39186500
C	-1.11065700	-2.35141400	-1.99210800
H	-0.40611700	-3.91584000	-0.69671100
H	0.58562900	-3.63568500	-2.15226700
H	-0.85048600	-1.65391700	-2.78112000
H	-2.15936700	-2.44585800	-1.73966200
C	2.24400900	-2.08242700	-1.04733300
O	2.78978300	-2.87681600	-1.83347800
N	3.02824100	-1.12218600	-0.34549200
C	4.45037500	-1.27376100	-0.37852400
C	5.12714500	-1.32620600	-1.60855900
C	5.20186600	-1.34776500	0.80370800
C	6.51482200	-1.45465700	-1.64762300
H	4.55605800	-1.28268400	-2.52691000
C	6.59383100	-1.46568300	0.75930500
H	4.70609000	-1.31816000	1.76767800
C	7.25978500	-1.52215500	-0.46558400
H	7.01707800	-1.49811700	-2.61035800
H	7.15361900	-1.51883200	1.68932200
H	8.34147300	-1.61575400	-0.50058500
Na	-2.90593800	0.31950000	0.01747000
C	-0.35069100	2.32324700	-1.92846000
H	0.40422400	2.92715500	-2.43967600
H	-1.04300700	1.90054500	-2.65947400
H	0.11580800	1.53232900	-1.33038300
S	-1.33401000	3.40949900	-0.83594100
O	-2.24091500	2.48883000	-0.00700900
C	0.01766500	3.92567600	0.27872200
H	0.53083700	3.04605300	0.67160900
H	0.71534700	4.55894100	-0.27526200
H	-0.44568000	4.49727300	1.08511800
C	-1.81304600	-0.67510600	3.41725500
H	-1.31334600	-1.28223800	4.17753300
H	-2.07451700	0.29968500	3.83372700
H	-1.18855900	-0.56927800	2.52561100
S	-3.38230300	-1.48908800	2.95786700
O	-4.01891600	-0.61080500	1.86171300
C	-2.65558500	-2.92756600	2.09758200
H	-2.02954800	-2.55374000	1.27858100

H	-2.07647500	-3.51330800	2.81741600
H	-3.48795600	-3.52581800	1.72099000
S	-6.15294100	0.45745700	-1.03197500
O	-4.70255600	0.12294200	-1.40126100
C	-6.74652400	-0.92208400	0.00691000
H	-6.11092600	-0.91836200	0.89684400
H	-7.79273800	-0.74574700	0.27303800
H	-6.63039700	-1.86230200	-0.53874400
C	-7.13015000	0.08793200	-2.53138600
H	-8.19534400	0.18030200	-2.30199100
H	-6.84604500	0.82219700	-3.28732800
H	-6.88497200	-0.91948000	-2.87695000

Int3h

C	-2.36494800	4.02960900	-0.65142100
C	-2.30418900	2.73841700	-1.18925800
C	-1.95389400	1.64322700	-0.39336000
C	-1.67863500	1.86320500	0.96459900
C	-1.74833800	3.14569700	1.50960800
C	-2.08708000	4.23799800	0.70028800
H	-2.63850300	4.86710900	-1.28746000
H	-2.53487500	2.58086200	-2.24057900
H	-1.41405700	1.01854800	1.59542100
H	-1.54582800	3.29500000	2.56718600
H	-2.14239100	5.23680400	1.12390800
C	-1.80155000	0.25034800	-1.02165700
H	-2.27914800	0.31167900	-2.01282000
H	2.96379900	-1.27805600	2.30879000
C	0.24732300	-1.28606300	-0.83333800
O	1.47836000	-1.59606900	-1.05581900
C	-2.03421000	-1.96350600	0.21391500
O	-2.74284300	-2.76105100	0.83241700
N	-2.54712100	-0.76559000	-0.24623300
C	-3.96690300	-0.55588800	-0.11621400
C	-4.54151600	-0.32101100	1.13626900
C	-4.77811800	-0.58384900	-1.25499800
C	-5.91652000	-0.10976900	1.24654100
H	-3.91024200	-0.31863800	2.01757200
C	-6.15348200	-0.36298600	-1.14435100
H	-4.33558000	-0.79218100	-2.22459200
C	-6.72639000	-0.12462300	0.10700100
H	-6.35545300	0.06727800	2.22432000
H	-6.77565100	-0.38870100	-2.03455900

H	-7.79604000	0.04291200	0.19487100
Na	3.23497700	-0.42875500	-0.59925400
O	1.68764800	1.14423000	0.51987400
O	3.36171700	-0.52166000	1.86008300
H	2.63267500	0.11873300	1.70999900
H	1.45258500	2.06657900	0.68177900
H	0.87917800	0.73839200	0.07965800
C	8.00771600	0.55176000	-0.95416100
H	8.83734100	0.90471000	-0.33552100
H	7.96519900	1.12263200	-1.88335200
H	8.10123300	-0.51483700	-1.17268600
S	6.43384500	0.84458000	-0.07632200
O	5.36039800	0.17439900	-0.94534400
C	6.71719000	-0.27105500	1.34125800
H	6.96975700	-1.26833100	0.97166400
H	7.52201500	0.13627400	1.95964300
H	5.77865900	-0.30051100	1.89992900
C	-0.34081500	-0.08883900	-1.19522400
H	0.18959000	0.55099500	-1.89828500
C	-0.59446400	-2.27625800	-0.07469800
C	-0.31046200	-3.75884900	-0.33922300
C	0.09920000	-3.16184000	0.96144900
H	0.46417400	-3.94713300	-1.07475100
H	-1.17679800	-4.41128900	-0.34509100
H	-0.48616000	-3.40973400	1.84065300
H	1.15637900	-2.96007800	1.10304500

TS3h

C	-4.39989000	3.33451300	-0.06654500
C	-3.69239500	2.40013200	-0.82906100
C	-2.76169600	1.54049700	-0.23388000
C	-2.55660600	1.63106800	1.14985800
C	-3.26765600	2.55601400	1.91728200
C	-4.18976400	3.41557400	1.31172800
H	-5.11865900	3.99126400	-0.54882700
H	-3.86643800	2.33728600	-1.90092500
H	-1.85785200	0.95268200	1.62964400
H	-3.10891800	2.59904600	2.99158300
H	-4.74464500	4.13285700	1.90974600
C	-1.93979800	0.60938400	-1.12012500
H	-2.52565400	0.43610200	-2.04315700
H	1.19685000	-2.04165400	0.74542100
C	0.40654400	0.51113500	-1.99434600
O	1.52946500	0.98506900	-2.46878000

C	0.25125600	-0.91469000	-1.92252500
C	2.47617200	-1.17081700	-2.31901400
C	1.21571300	-1.78186800	-2.71037500
H	2.78307600	-1.27169000	-1.28202400
H	3.14955500	-0.68585000	-3.01468800
H	1.03486700	-1.78785300	-3.78893500
H	1.09957800	-2.79278600	-2.29972000
C	-0.60748300	-1.50125700	-0.93000100
O	-0.40780800	-2.64424100	-0.46014100
N	-1.68316700	-0.70975000	-0.47414200
C	-2.77356600	-1.38969000	0.16174000
C	-2.56790300	-2.08228200	1.36346500
C	-4.05791800	-1.36619900	-0.39899900
C	-3.62866200	-2.73940700	1.98717200
H	-1.57550400	-2.11032100	1.79589000
C	-5.11975200	-2.01425800	0.23654300
H	-4.23345400	-0.84347500	-1.33279600
C	-4.91106100	-2.70641400	1.43101800
H	-3.45112200	-3.27605200	2.91509600
H	-6.10954600	-1.98086700	-0.21025800
H	-5.73619300	-3.21339200	1.92289200
Na	2.84108000	1.51500500	-0.76154900
O	1.15389600	1.42326300	0.80906900
O	1.87475800	-1.47363900	1.15901200
H	1.48589300	-0.58180300	1.17677300
H	0.83136400	1.96415700	1.54046700
H	0.40070200	1.38579400	0.12600300
C	7.13678000	0.48084900	1.30111400
H	7.58831500	-0.02848200	2.15669600
H	7.40576300	1.53852900	1.31156700
H	7.44716000	0.02222800	0.35908000
S	5.31917300	0.38706800	1.43824000
O	4.79795100	0.98522300	0.11702600
C	5.13099700	-1.41853000	1.29540300
H	5.60969500	-1.75662400	0.37252400
H	5.59165300	-1.88516300	2.17103500
H	4.05519200	-1.62287200	1.27894100
C	-0.62159700	1.28439000	-1.44937900
H	-0.64454000	2.35479200	-1.63376000

Int4h

C	0.32273300	3.57622800	-0.09281000
C	-0.22399400	2.50719400	-0.80599300
C	-1.09388900	1.58916900	-0.19248100

C	-1.41976300	1.78866000	1.15483300
C	-0.86551500	2.85385400	1.87855800
C	0.01121400	3.74885400	1.26113400
H	0.98563500	4.27736100	-0.59300500
H	0.02292000	2.38306700	-1.85834500
H	-2.10983700	1.10840600	1.64078300
H	-1.13072600	2.98565100	2.92433000
H	0.43530700	4.57749700	1.82090300
C	-1.65166400	0.41523800	-1.03062500
H	-2.24285700	0.87114200	-1.82820100
H	3.51061300	-1.67404600	3.37819000
C	-0.15373400	-1.47252200	-0.92152300
O	0.92496500	-2.28374600	-1.25169300
C	-0.71137200	-1.83722000	0.33112900
C	0.80415200	-3.50365800	-0.44820000
C	-0.07688700	-3.14930600	0.77084100
H	1.81999000	-3.81958500	-0.19975700
H	0.33608200	-4.26270000	-1.08469000
H	-0.83373900	-3.91815600	0.95871900
H	0.52774100	-3.06795400	1.68523000
C	-2.09230500	-1.48861100	0.57085900
O	-2.82929400	-2.06655400	1.38340600
N	-2.58210100	-0.42925800	-0.24331500
C	-3.97831100	-0.14230400	-0.30057800
C	-4.75140000	-0.00542900	0.86413700
C	-4.60852100	0.01102300	-1.54733300
C	-6.11290700	0.29092200	0.77533900
H	-4.28860600	-0.15855000	1.83015700
C	-5.96619400	0.32435100	-1.62914600
H	-4.03724000	-0.13831000	-2.45879800
C	-6.72843000	0.46678400	-0.46676500
H	-6.69400200	0.38853800	1.68843900
H	-6.43039900	0.43802500	-2.60515200
H	-7.78671400	0.70340200	-0.52848300
Na	2.01075000	-0.07100500	-0.70806700
O	1.26445800	-0.13720300	1.53058600
O	3.62447200	-1.18997000	2.55214700
H	2.73781400	-0.84470700	2.31348000
H	0.90446600	0.69099800	1.88115700
H	0.45013900	-0.68489200	1.27347100
C	6.67141200	1.00086500	-1.55806700
H	7.65943100	1.11584400	-1.10411000
H	6.39553000	1.91473400	-2.08713300
H	6.64654500	0.14816600	-2.24092300

S	5.43153000	0.74928900	-0.24194700
O	4.12249100	0.45035000	-0.99357300
C	6.03167100	-0.85109700	0.38796000
H	6.06507400	-1.56921000	-0.43559300
H	7.02406900	-0.70469800	0.82447300
H	5.32106100	-1.16490500	1.15847600
C	-0.53974000	-0.40367200	-1.67353600
H	-0.29238400	-0.29683900	-2.72387600

Int5h

C	4.45690900	-3.83688200	-0.20823700
C	3.37129900	-2.96824500	-0.11571500
C	3.20407900	-1.93007500	-1.04584800
C	4.15005100	-1.79555000	-2.06788200
C	5.23512800	-2.67018400	-2.16975500
C	5.39299100	-3.69378800	-1.23722800
H	4.57283200	-4.63248000	0.52400100
H	2.64554100	-3.08917000	0.68242300
H	4.03760000	-0.99306800	-2.79452900
H	5.95616400	-2.54662800	-2.97426700
H	6.23701000	-4.37528100	-1.30841400
C	2.00806800	-0.96842600	-0.99102100
C	0.66197900	-1.66344800	-1.12358000
H	2.13895300	-0.28706300	-1.83973500
H	0.43733400	-2.16503100	-2.05853100
C	0.07673200	-2.02850900	0.05509500
O	-1.02979700	-2.85167100	0.14395800
C	0.44719000	-1.53820800	1.33101700
C	-1.23414000	-3.15013200	1.55202000
C	-0.55211800	-2.02119700	2.34959500
H	-0.76903100	-4.12218700	1.75901800
H	-2.31286000	-3.23500500	1.71295300
H	-1.27729400	-1.24410200	2.64749700
H	-0.10419600	-2.40599700	3.27355800
C	1.35346300	-0.48027600	1.44478100
O	1.54031300	0.22216700	2.47968200
N	2.02331700	-0.08651600	0.23165900
C	3.14200200	0.80764200	0.32334000
C	4.12669500	0.67213200	1.31150200
C	3.27282000	1.83136700	-0.62552800
C	5.20919000	1.54948700	1.34732800
H	4.02929300	-0.10847100	2.05542500
C	4.36669800	2.69671600	-0.59607400
H	2.50885800	1.95087800	-1.39047100

C	5.34009000	2.56179800	0.39430100
H	5.96184600	1.43350700	2.12313300
H	4.45031300	3.48217200	-1.34330300
H	6.19037200	3.23796600	0.42439900
Na	-1.76183600	1.86060200	1.00804100
C	-2.08500400	6.31837400	-0.97403800
H	-1.51990100	6.90492000	-1.70448800
H	-2.17469400	6.87503300	-0.03854300
H	-3.07909700	6.06775000	-1.35482800
S	-1.18094600	4.77578700	-0.59877900
O	-2.12001600	3.96523500	0.29791300
C	-1.27086100	4.02891700	-2.26237200
H	-2.31546900	3.98085900	-2.58481200
H	-0.67157500	4.62404700	-2.95849300
H	-0.85854000	3.02106300	-2.16010700
C	-4.45323000	-2.70909300	-0.79911300
C	-4.69534100	-1.43386400	-0.26239100
C	-6.01302400	-0.98246300	-0.07628400
C	-7.07806900	-1.80306400	-0.42774900
C	-6.83392600	-3.07455700	-0.96342500
C	-5.52574000	-3.52810800	-1.14830100
H	-3.42698100	-3.04581900	-0.92801100
H	-6.17457100	0.00671200	0.34121600
H	-8.09956800	-1.46079000	-0.28761300
H	-7.67009000	-3.71306100	-1.23620400
H	-5.34424400	-4.51581000	-1.56205700
C	-3.54509400	-0.59408100	0.09654900
O	-3.62847300	0.52503500	0.59981900
H	-2.55765400	-1.04144900	-0.10970100
O	-0.37237500	1.19605000	-0.73594700
H	0.51852200	1.12712300	-0.32251300
H	-0.44306700	0.26977600	-1.07462000
O	-0.75624100	1.45508300	2.97237200
H	0.14087000	1.00829500	2.87717200
H	-1.15485800	1.04481900	3.75255300

TS4h

C	-2.90857100	3.79598200	0.71367300
C	-2.62207300	2.42747000	0.73328700
C	-2.40653200	1.72251600	-0.45891200
C	-2.51053200	2.42184600	-1.67094100
C	-2.80377300	3.78751900	-1.69649000
C	-2.99962000	4.48364600	-0.49977000
H	-3.07469600	4.32179900	1.65026400

H	-2.57322900	1.90769400	1.68402300
H	-2.36527800	1.88795200	-2.60752300
H	-2.89601000	4.30233500	-2.64943900
H	-3.23947300	5.54332000	-0.51332700
C	-2.03095900	0.23417600	-0.49287800
C	-0.50700300	0.03728200	-0.45542000
H	-2.37945300	-0.14539000	-1.45661800
H	0.02315900	1.32848400	-0.49197100
C	-0.05781800	-0.20785000	0.88527600
O	1.29153200	-0.20064800	1.20066400
C	-0.84364800	-0.42005700	1.97116700
C	1.40583000	-0.67776100	2.58471900
C	0.00531600	-0.52104200	3.21324700
H	2.18969400	-0.08647000	3.06204000
H	1.71650300	-1.72662000	2.53489700
H	-0.26178600	-1.37997000	3.83562600
H	-0.06416500	0.37558700	3.84544900
C	-2.25910000	-0.71320100	1.83895700
O	-2.95051100	-1.13611800	2.77402200
N	-2.77287200	-0.54320000	0.54366000
C	-4.13133000	-0.88886100	0.25701900
C	-5.19145500	-0.42218400	1.04660400
C	-4.41374000	-1.69870700	-0.85290600
C	-6.50701300	-0.76035300	0.72477500
H	-4.97922600	0.18690800	1.91600900
C	-5.73205600	-2.02207000	-1.18004700
H	-3.59654300	-2.08755600	-1.45386400
C	-6.78609600	-1.55526500	-0.39055500
H	-7.31809300	-0.39492100	1.34862400
H	-5.93150800	-2.65107900	-2.04327000
H	-7.81205800	-1.81150200	-0.63880500
Na	2.93114800	0.39365800	-0.41653600
C	6.66983000	1.78453700	-0.39705800
H	7.51513600	2.37887200	-0.03831200
H	5.80905400	2.42172800	-0.61754100
H	6.94580700	1.19601100	-1.27611700
S	6.12234300	0.66177400	0.93395000
O	4.98257000	-0.18098500	0.34711500
C	7.57484000	-0.44620400	0.94962200
H	7.69793300	-0.88494800	-0.04365100
H	8.46073100	0.12305400	1.24434300
H	7.37220100	-1.22940400	1.68223100
C	0.13145800	-3.04962600	-0.72594800
C	0.84076800	-2.04632900	-1.40574700

C	2.09968500	-2.36177600	-1.93665900
C	2.64449300	-3.64080700	-1.78056900
C	1.93286900	-4.62905700	-1.09658900
C	0.67150700	-4.32836300	-0.57208700
H	-0.84526800	-2.82492600	-0.30592000
H	2.64038500	-1.59968300	-2.49042700
H	3.62234800	-3.86468200	-2.19893400
H	2.35336200	-5.62339500	-0.97484800
H	0.10819800	-5.08845200	-0.03743700
C	0.22427000	-0.67449000	-1.62252900
O	1.29253600	0.16856500	-2.12178800
H	-0.48441900	-0.76277800	-2.46370800
O	0.95698300	2.05948600	-1.08759700
H	1.67222500	1.45580700	-2.04655500
H	1.30305600	2.94225300	-0.93740600
O	1.59442500	4.63591000	-0.73858400
H	2.39499800	5.15775900	-0.64718200
H	0.92882800	4.96049100	-0.12766000

Int6h

C	-2.32486200	3.45631300	-0.91385900
C	-2.21382500	2.17209000	-0.37023000
C	-1.81856200	1.08863400	-1.16644200
C	-1.56663900	1.32950200	-2.52804700
C	-1.68195400	2.60844500	-3.07603900
C	-2.05786000	3.68325800	-2.26516400
H	-2.64690900	4.27925600	-0.27928700
H	-2.46291100	2.00497200	0.67161500
H	-1.31591300	0.49295700	-3.18002100
H	-1.50425000	2.76023600	-4.13805600
H	-2.16759300	4.67831400	-2.68891500
C	-1.65340300	-0.34623800	-0.61493100
C	-0.19229700	-0.73980600	-0.41056700
H	-2.06440200	-1.00412000	-1.38727000
H	0.91000400	0.42407900	-2.38241300
C	0.25369000	-0.48120000	0.86751100
O	1.59113600	-0.61572000	1.25199400
C	-0.53551400	-0.07826200	1.94195600
C	1.61563000	-0.62952500	2.71076100
C	0.31091400	0.04295500	3.18266400
H	2.53239700	-0.11352900	3.01601500
H	1.67412300	-1.67671400	3.02895700
H	-0.12753700	-0.48199600	4.03839900
H	0.49330500	1.08021600	3.51072800

C	-1.95662900	-0.23783900	1.89880300
O	-2.70501600	-0.15628000	2.88128000
N	-2.46623800	-0.56200900	0.60385100
C	-3.83535700	-0.92043400	0.43570600
C	-4.87439300	-0.19058200	1.03500900
C	-4.16693500	-2.02857400	-0.36060300
C	-6.20281000	-0.56171000	0.83026500
H	-4.63131600	0.64663300	1.67515300
C	-5.49782600	-2.38253900	-0.57689600
H	-3.37289400	-2.62940200	-0.79626100
C	-6.52598000	-1.65072800	0.01882300
H	-6.99302200	0.01442000	1.30576700
H	-5.72815200	-3.24395700	-1.19921600
H	-7.56416200	-1.92929300	-0.14168200
Na	2.98257400	0.11824700	-0.43898600
C	0.97598100	3.31595700	1.50532300
H	0.30707000	4.17919700	1.43889800
H	1.38430700	3.24892000	2.51634200
H	0.44250600	2.39279300	1.25112300
S	2.37981200	3.59172500	0.37856500
O	3.18456700	2.27288400	0.33418500
C	1.45247800	3.64260700	-1.18565900
H	0.84378400	2.74026400	-1.28270700
H	0.81121500	4.52747800	-1.19575400
H	2.18889600	3.70412700	-1.99044700
C	1.10402500	-3.44956600	-0.21183700
C	1.50875600	-2.51469000	-1.17503400
C	2.71232800	-2.73972500	-1.86019800
C	3.50495600	-3.85432000	-1.56509500
C	3.09787400	-4.76985300	-0.59421700
C	1.88850200	-4.56553900	0.07569400
H	0.16965400	-3.28610700	0.31656400
H	3.02561300	-2.04497000	-2.63215500
H	4.43170400	-4.01266900	-2.11192900
H	3.70898800	-5.64028300	-0.36978900
H	1.55496900	-5.27693900	0.82690100
C	0.60540100	-1.32707500	-1.51281400
O	1.50446300	-0.31712400	-2.17643700
H	-0.08278300	-1.65633700	-2.30557600
O	5.11849600	-0.63289400	-0.33194200
H	5.18712000	-1.58126500	-0.14401700
H	5.37347000	-0.15794800	0.49628300
O	5.19892100	1.07729500	1.79497600
H	4.73588300	0.76953800	2.58870600

H	4.57052600	1.70324200	1.36714000
TS5h			
C	-1.56127400	3.06389700	1.95289700
C	-1.77991500	1.78020900	1.45443000
C	-1.70486200	1.52254400	0.07599500
C	-1.42557400	2.59362300	-0.78355200
C	-1.20781700	3.88235300	-0.28789400
C	-1.27112400	4.12122200	1.08485600
H	-1.62483600	3.24179800	3.02356200
H	-2.00971700	0.96939100	2.13809400
H	-1.38486400	2.41799300	-1.85687300
H	-1.00451000	4.69879300	-0.97689100
H	-1.11186700	5.12290500	1.47592500
C	-1.87041200	0.10693700	-0.50478000
C	-0.63598000	-0.77328200	-0.27205900
H	-1.97227200	0.23630100	-1.58692700
H	0.89483000	1.35676000	-0.23095000
C	-0.73486500	-1.53370900	0.91231000
O	0.35470700	-2.14911900	1.53499800
C	-1.89664900	-1.77299000	1.59616300
C	-0.20776300	-3.11094700	2.48848100
C	-1.62585900	-2.61435300	2.81392700
H	0.47568000	-3.15347600	3.34052800
H	-0.22210200	-4.08765100	1.99095300
H	-2.33276100	-3.44286300	2.92572200
H	-1.65253000	-2.03823100	3.75179100
C	-3.18567500	-1.34523800	1.10727300
O	-4.25676900	-1.68463700	1.61640000
N	-3.12910500	-0.53529900	-0.04546900
C	-4.34106600	-0.09011100	-0.65740400
C	-5.35537400	0.52607300	0.08783100
C	-4.51520400	-0.25479800	-2.03822800
C	-6.51735500	0.96796700	-0.54333600
H	-5.23153000	0.63992800	1.15738900
C	-5.67232700	0.20350200	-2.66763000
H	-3.74584900	-0.76153300	-2.61500800
C	-6.68037700	0.81627600	-1.92186000
H	-7.29787500	1.44069700	0.04758400
H	-5.79072400	0.06681900	-3.73970300
H	-7.58623700	1.16746300	-2.40904300
Na	3.09995500	-0.09821800	0.78376400
C	3.65569400	3.57306100	0.82919300
H	3.56927200	4.60517600	0.47649100

H	4.01369300	3.56258000	1.86130600
H	2.69642900	3.05329700	0.75201000
S	4.90074000	2.69805900	-0.18109500
O	4.93561200	1.25450400	0.34767500
C	3.94440200	2.66679400	-1.73656200
H	3.00452900	2.12295500	-1.55714500
H	3.76920900	3.69732600	-2.06196000
H	4.55903600	2.15129700	-2.47936100
C	1.22259200	-3.02925200	-1.20129700
C	1.48396200	-1.66890100	-1.42966800
C	2.69020800	-1.33359200	-2.07150100
C	3.61852000	-2.31458000	-2.43075900
C	3.35814100	-3.66123400	-2.15907700
C	2.15158300	-4.01079900	-1.54907000
H	0.27361600	-3.31924800	-0.76662200
H	2.88961200	-0.28995600	-2.28827000
H	4.53292800	-2.02852100	-2.94691300
H	4.07407400	-4.42843800	-2.44186100
H	1.92331300	-5.05578000	-1.35625100
C	0.46494800	-0.60338900	-1.13634300
O	1.59180600	0.77864300	-0.58187200
H	0.19730500	-0.06594600	-2.04609600
O	4.94896100	-1.54700500	0.62154400
H	5.44666900	-0.74319000	0.37901200
H	4.78517800	-2.00840100	-0.21949000
O	2.24661800	-0.57631200	2.83939800
H	1.48322300	-1.08240400	2.47495200
H	2.80053600	-1.23958000	3.27929500