

## Theoretical study on the mechanism of hydrogenation of carboxylic acids catalyzed by the Saito catalyst

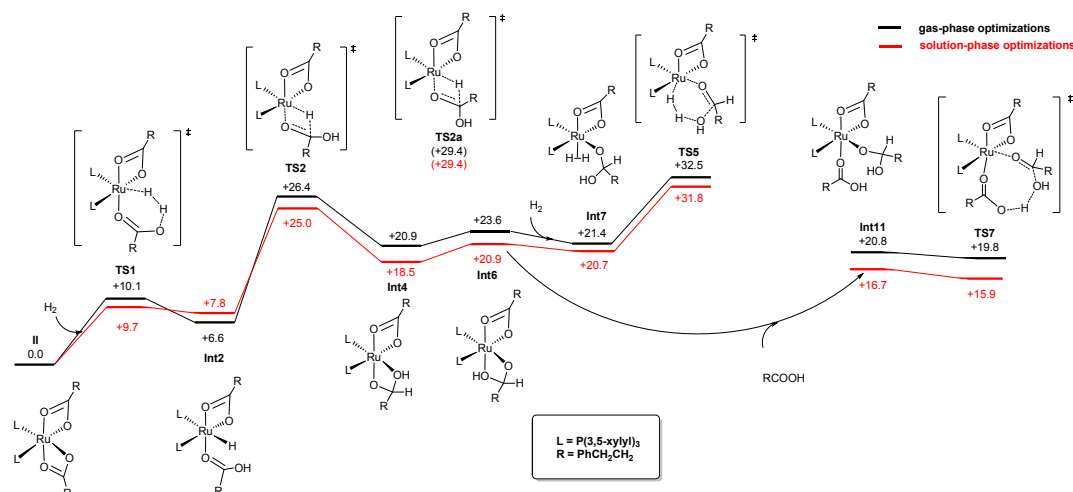
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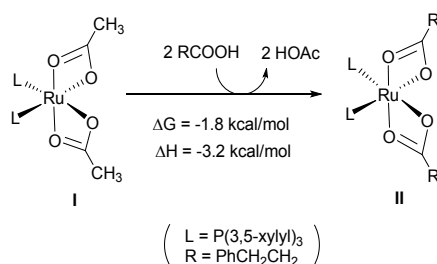
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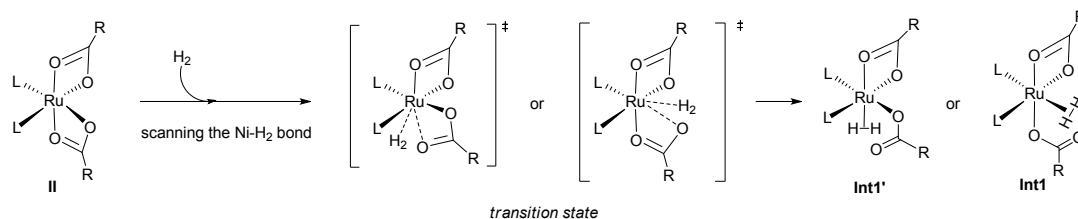


**Figure S1.** Computational results of gas-phase optimizations (M06/SDD-6-311+G(2d,p)(SMD)//B3LYP/Lan12DZ-6-31G(d) and solution-phase optimizations ( $\omega$ b97X-D/SDD-6-311+G(2d,p)(SMD)// $\omega$ b97X-D/Lan12DZ-6-31G(d)(SMD)

According to Figure S1, the energies of intermediates and transition states calculated by solution-phase optimizations are similar to those calculated by gas-phase optimizations. Besides, on the basis of solution-phase optimizations, the carboxylic acid-assisted protonation (TS7 = +15.9 kcal/mol) is more favorable than the H<sub>2</sub> heterolysis (TS5 = +31.8 kcal/mol), indicating the new mechanism assisted by carboxylic acid is preferred over the proposed mechanism. This is in accordance with the results of gas-phase optimizations.

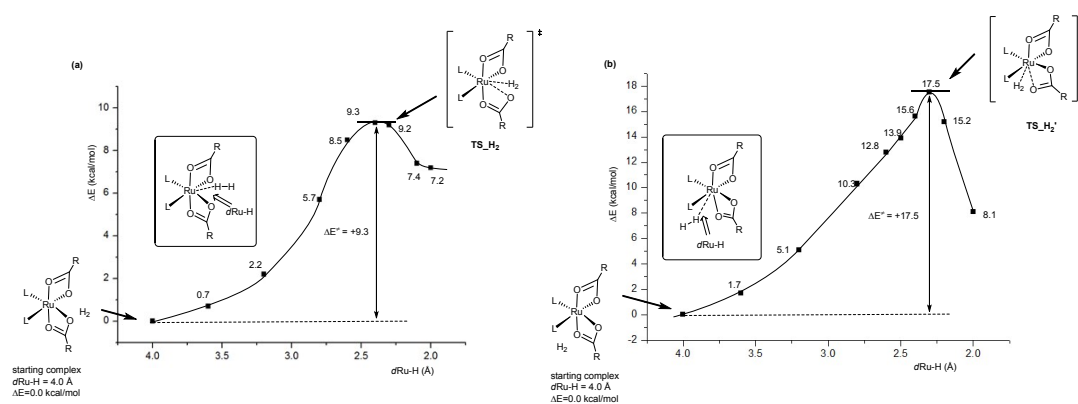


**Figure S2.** Ligand exchange between I and carboxylic acid.



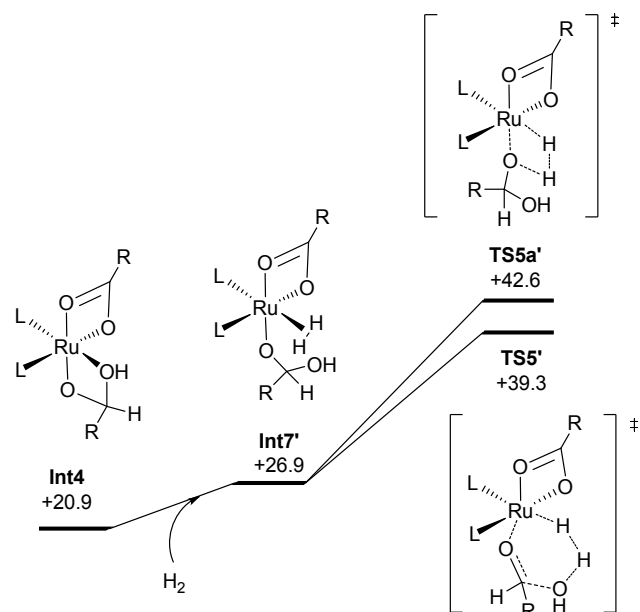
**Figure S3.** The proposed transition states for H<sub>2</sub> coordination

We failed in locating the intermediate resulting from the partial decooordination of the carboxylate ligand of **II**. This difficulty is attributed to the intrinsic preference of carboxylate ligand for the  $\kappa^2$ -coordinated mode. In this regard, the partial decooordination of carboxylate ligand and the coordination of H<sub>2</sub> molecule are expected to occur simultaneously (Figure S3).

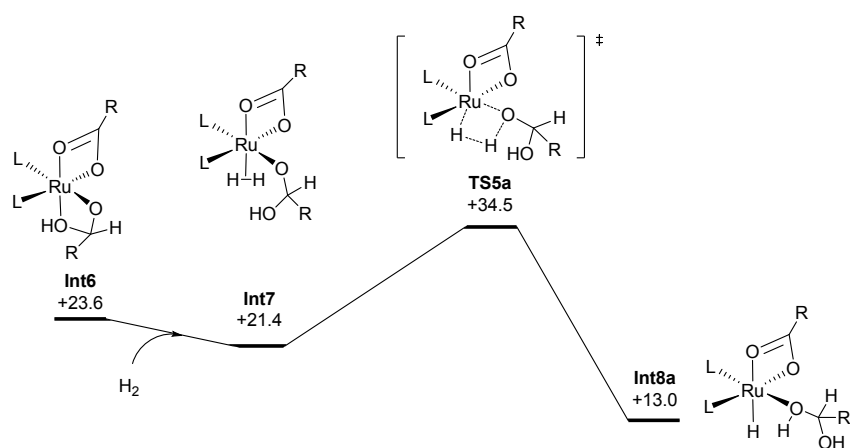


**Figure S4.** Estimated energy barriers for the H<sub>2</sub> coordination of **II**.

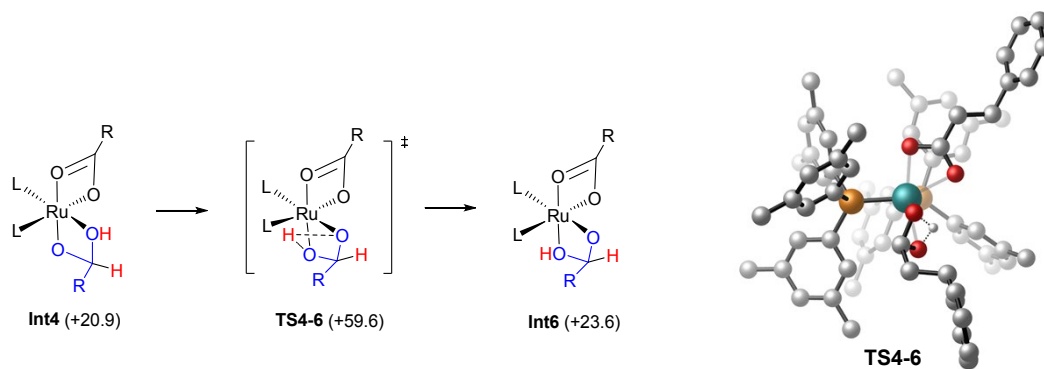
Note that the transition states connecting **II** and Int1/Int1' were failed to be located. In order to estimate the energy demand of this step, we performed partial optimizations by fixing the Ru-H<sub>2</sub> bond at different lengths (4.0–2.0 Å, Figure S4). The calculation results show that the partial dissociation of carboxylate ligand and the H<sub>2</sub> coordination need to overcome ~9.3 (**TS\_H2**) and ~17.5 kcal/mol (**TS\_H2'**) energy barrier for the generation of Int1 and Int1', respectively. The reason of the lower energy barrier of **TS\_H2** than **TS\_H2'** is the strong trans effect of the phosphine which leads to a facile dissociation of the Ru-O bond.



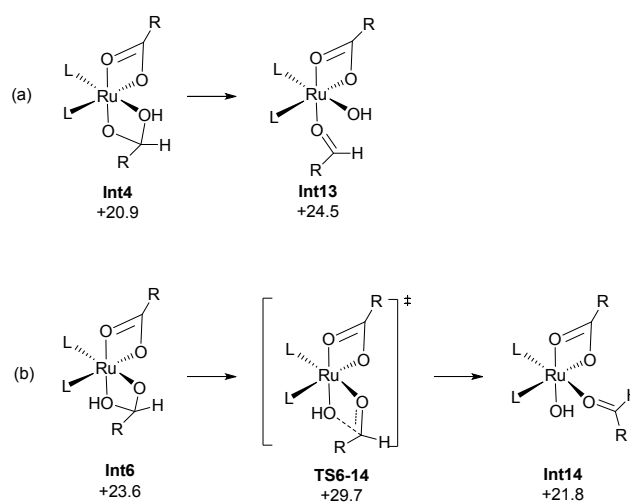
**Figure S5.** Energy profiles of H<sub>2</sub> heterolysis from **Int4**. Gibbs free energies (kcal/mol) are relative to **II**.



**Figure S6.** Energy profiles of the alternative H<sub>2</sub> heterolysis of **Int6**. Gibbs free energies (kcal/mol) are relative to **II**.

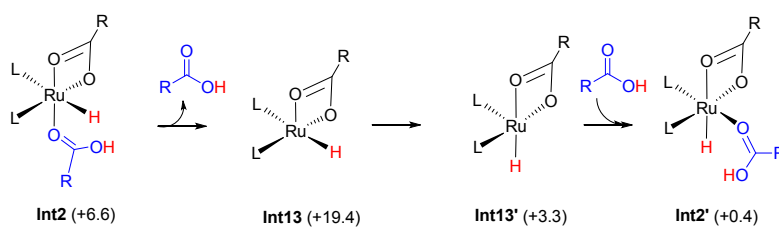


**Figure S7.** Direct proton transfer of **Int4**. Gibbs free energies (kcal/mol) are relative to **II**.

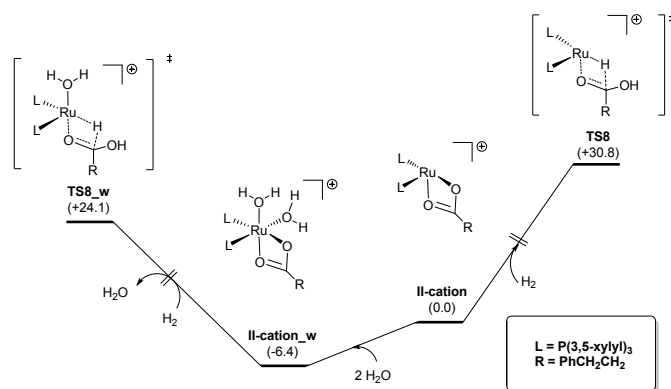


**Figure S8.** The C-OH bond cleavage of **Int4** and **Int6**. Gibbs free energies (kcal/mol) are relative to **II**.

Although the transition state of C-OH bond cleavage of **Int4** was not located, the results of constrained potential energy surface (PES) scan suggests that the C-OH bond cleavage of **Int4** needs to overcome the energy barrier of  $\sim 10$  kcal/mol. While the energy barrier for the C-OH bond cleavage of **Int6** is 6.1 kcal/mol.



**Figure S9.** The isomerization of **Int2** to **Int2'**.



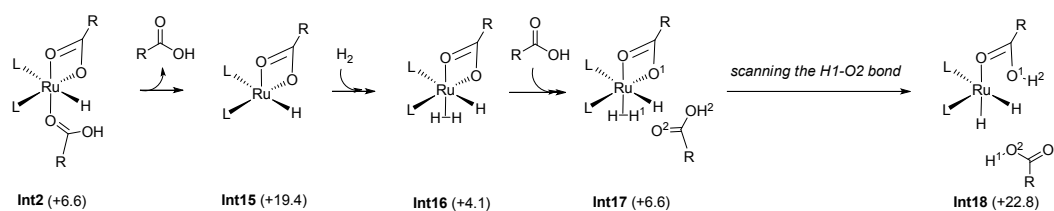
**Figure S10.** Energy profiles of hydride migration from the cationic Ru complex **II-cation**. Gibbs free energies are showed in kcal/mol.

Considering that several cationic ruthenium complexes were detected by experimental spectroscopy analysis, we also studied the cationic hydrogenation mechanism on the basis of the cationic catalyst  $(\text{P}(3,5\text{-xylyl})_3)_2\text{Ru}(\kappa^2\text{-OCOR})^+$  (**II-cation**). Note that due to the influence of solvation effect, it is inaccurate to compare the relative stability of species with different charges by relying on DFT calculations only.<sup>1</sup> Herein we focus on evaluating the reactivity of **II-cation**, as judged by the energy barrier of hydride migration and the second  $\text{H}_2$  heterolysis.

As shown in Figure S10, hydride migration via **TS8** from **II-cation** needs an energy barrier of 30.8 kcal/mol, which is 4.4 kcal/mol higher than that of the neutral mechanism. In an alternative pathway, we considered adding water molecule to stabilize **II-cation** and its hydride migration transition state. The calculated results show that the coordination of two water molecules indeed affords a thermodynamically stable intermediate **II-cation\_w**. However, hydride migration via **TS8\_w** still requires a high barrier of 30.5 kcal/mol. These results indicate that the neutral Ru-dicarboxylates complex **II** is more reactive than the cationic Ru-carboxylate **II-cation**. Therefore, the catalytic hydrogenation of carboxylic acids occurs via the neutral mechanism, and this is common for the detected metal species to lie off the catalytic cycle.<sup>2</sup>

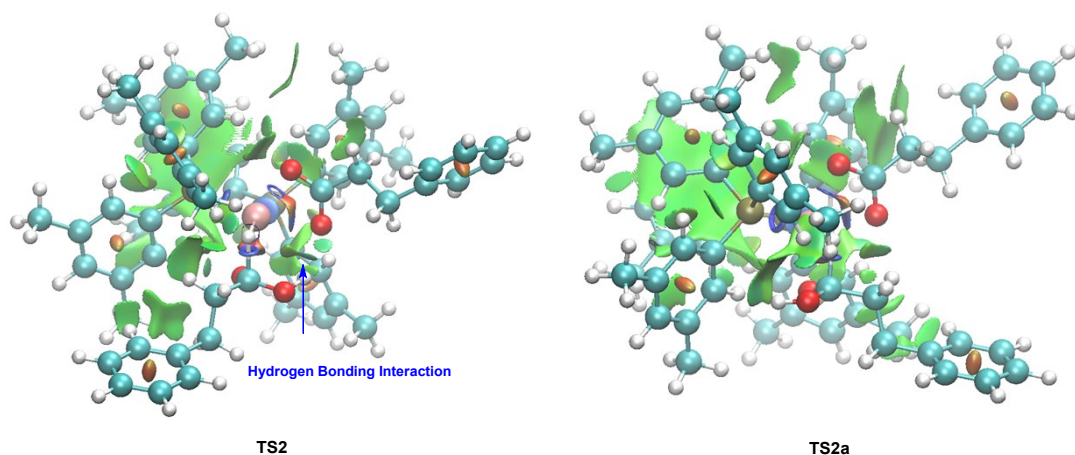
*References:*

1. R. E. Plata and D. A. Singleton, *J. Am. Chem. Soc.* **2015**, *137*, 3811-3826.
2. J. Halpern, *Inorg. Chim. Acta* **1981**, *50*, 11-19.

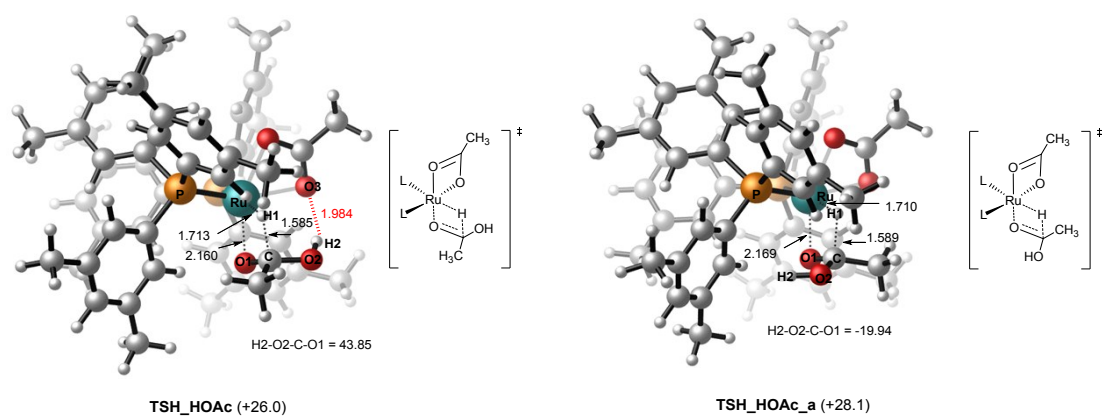


**Figure S11.** The ionic hydrogenation mechanism

As shown in Figure S11, carboxylic acid first dissociates from **Int2** to give the Ru-hydride intermediate **Int13**. Subsequent coordination of  $\text{H}_2$  and carboxylic acid result in the generation of **Int15**. From **Int15**, proton transfer from  $\text{H}_2$  to carboxylic acid will occur in the ionic hydrogenation mechanism. Unfortunately, the resultant ion pair involving the protonated carboxylic acid was not located after many trials, as the protonated carboxylic acid always returns back proton to the hydride during the geometry optimizations. Besides, the constrained potential energy surface (PES) scan along H1-O1 bond indicates that the H2 atom of carboxyl group would be transferred into the O2 atom of carboxylate ligand once H1 atom transfers to the O1 atom of carboxylic acid. These results suggest that the proton transfer from  $\text{H}_2$  to carboxylic acid is quite difficult for this carboxylic acid hydrogenation reaction.



**Figure S12.** Noncovalent interaction analysis of transition states **TS2** and **TS2a**.



**Figure S13.** Two types of hydride migration transition states of HOAc. Bond distances and angles are given in [Å] and [°], respectively. Gibbs free energies are relative to  $(P(3,5\text{-xylyl})_3)_2\text{Ru}(\kappa^2\text{-OAc})_2$ .



**Table S1. Thermal correction of Gibbs free energy (TCG, hartree) and total electronic energies (E, hartree) in toluene solvent for all species involved in this study**

Compounds	TCG	E	Compounds	TCG	E
<b>H<sub>2</sub></b>	-0.001342	-1.17008472813	<b>TS6</b>	1.089960	-3561.62010420
<b>H<sub>2</sub>O</b>	0.003474	-76.4222217383	<b>Int9</b>	1.090896	-3561.62038662
<b>HOAc</b>	0.034689	-229.036891346	<b>Int10</b>	1.25605	-4060.93672458
<b>A</b>	0.134636	-499.257035872	<b>Int8'</b>	1.091574	-3561.622739
<b>B</b>	0.154426	-425.209204062	<b>TS6'</b>	1.092407	-3561.613165
<b>hemiacetal</b>	0.157943	-500.437825916	<b>Int9'</b>	1.096149	-3561.631225
<b>aldehyde</b>	0.130783	-424.002387339	<b>Int7'</b>	1.116224	-3638.04433820
<b>I</b>	0.874629	-3095.25946371	<b>TS5'</b>	1.112522	-3638.02089745
<b>II</b>	1.076539	-3635.70467694	<b>TS5a'</b>	1.116164	-3638.01932706
<b>Int1</b>	1.092587	-3636.87804424	<b>Int11</b>	1.260257	-4136.14906057
<b>TS1</b>	1.090075	-3636.87355174	<b>TS7</b>	1.257674	-4136.14808832
<b>Int2</b>	1.091875	-3636.88086882	<b>Int12</b>	1.257558	-4136.16584416
<b>TS2</b>	1.091526	-3636.84900087	<b>TS4-6</b>	1.095113	-3636.79970729
<b>TS2a</b>	1.097134	-3636.84986442	<b>Int13</b>	1.093733	-3636.85432866
<b>Int3</b>	1.097637	-3636.85916327	<b>TS6-14</b>	1.097183	-3636.84941348
<b>Int4</b>	1.101150	-3636.86746631	<b>Int14</b>	1.094008	-3636.85879106
<b>Int1'</b>	1.091319	-3636.88594824	<b>Int15</b>	0.929798	-3137.57599354
<b>TS1'</b>	1.089234	-3636.88162537	<b>Int16</b>	0.948118	-3138.79021435
<b>Int2'</b>	1.092530	-3636.89145614	<b>Int17</b>	1.103432	-3638.06391308
<b>TS2'</b>	1.098418	-3636.85184994	<b>Int18</b>	1.108566	-3638.04323964
<b>Int4-acid</b>	1.260260	-4136.14905238	<b>II-cation</b>	0.926191	-3136.83374857
<b>TS3</b>	1.258031	-4136.14708883	<b>II- cation_w</b>	0.978684	-3289.73400066
<b>Int5</b>	1.259493	-4136.15060709	<b>TS8</b>	0.94569	-3137.97554747
<b>TS4</b>	1.256630	-4136.15005102	<b>TS8_w</b>	0.973472	-3214.43274285
<b>Int5-acid</b>	1.257571	-4136.15015585	<b>TSH_HOAc</b>	0.892254	-3096.4070008
<b>Int6</b>	1.097964	-3636.85998158	<b>TSH_HOAc_a</b>	0.895336	-3096.40676081
<b>Int7</b>	1.113663	-3638.05049621	<b>III<sup>a</sup></b>	1.000565	-3478.54939554
<b>TS5</b>	1.110645	-3638.02990747	<b>TSIII<sup>a</sup></b>	1.024022	-3479.69240299
<b>TS5a</b>	1.112927	-3638.02892813	<b>IV<sup>a</sup></b>	0.626175	-2701.11738115
<b>Int8</b>	1.086709	-3561.62843207	<b>TSIV<sup>a</sup></b>	0.645401	-2702.25925507
<b>In8a</b>	1.116572	-3638.06683892			

<sup>a</sup> The intermediate and transition states are calculated at the M06/6-311+G(d,p)(SDD)// $\omega$ B97X-D/6-31G(d)(LANL2DZ) level of theory.

**Table S2.** Thermal correction of Gibbs free energy (TCG, hartree) and total electronic energies (E, hartree) for some important species based on the solution-phase optimizations.

Compounds	TCG	E	Compounds	TCG	E
<b>H<sub>2</sub></b>	-0.001332	-1.17561185507	<b>TS2a</b>	1.130664	-3638.20481683
<b>H<sub>2</sub>O</b>	0.003862	-76.4366767971	<b>Int4</b>	1.132192	-3638.22371021
<b>A</b>	0.136806	-499.437981835	<b>Int6</b>	1.128486	-3638.216016
<b>II</b>	1.108162	-3637.05216729	<b>Int7</b>	1.146604	-3639.41143711
<b>TS1</b>	1.125231	-3638.23076183	<b>TS5</b>	1.14388	-3639.39105572
<b>Int2</b>	1.129202	-3638.23761659	<b>Int11</b>	1.296231	-4137.69165371
<b>TS2</b>	1.126966	-3638.20801768	<b>TS7</b>	1.293182	-4137.69001855

**Cartesian coordinates for all optimized geometries**

**H<sub>2</sub>**

H	0.00000000	0.00000000	0.37139400
H	0.00000000	0.00000000	-0.37139400

**H<sub>2</sub>O**

O	0.00000000	0.00000000	0.11942600
H	0.00000000	0.76261700	-0.47770500
H	0.00000000	-0.76261700	-0.47770500

**HOAc**

C	0.09248600	0.12560900	-0.00001900
O	0.77865800	-1.04664100	-0.00000200
O	0.64573600	1.20198000	0.00000300
C	-1.39759100	-0.10980200	-0.00000400
H	-1.68535400	-0.69175800	-0.88187400
H	-1.68536200	-0.69128500	0.88218900
H	-1.91751800	0.84841300	-0.00022900
H	1.72371000	-0.80292600	0.00004300

**A (phenylpropionic acid)**

C	2.94075900	0.00001800	-0.07328600
C	1.47293000	0.00049300	-0.44262400
C	0.55014700	-0.00093900	0.78671100
C	-0.91404600	-0.00048000	0.40039400
C	-1.60451400	1.20324800	0.20238500
C	-2.94456700	1.20668900	-0.18804400
C	-3.61934300	0.00051800	-0.38701500
C	-2.94487300	-1.20614300	-0.19003100
C	-1.60481200	-1.20369800	0.20040600
H	1.28053300	0.87414700	-1.07846600
H	1.28049000	-0.87165400	-1.08052100
H	0.78229400	-0.87762700	1.40132400
H	-1.08781900	2.14753800	0.36247200
H	-3.46270600	2.15138400	-0.33174400
H	-4.66359600	0.00088900	-0.68779800
H	-3.46325400	-2.15046600	-0.33529200
H	-1.08837200	-2.14839000	0.35892900
O	3.73058600	0.00163400	-1.17709200
O	3.39442100	-0.00158000	1.05004200
H	0.78229800	0.87433200	1.40333900
H	4.64999200	0.00118500	-0.84922300

**aldehyde**

H	-3.94470600	0.00511900	1.47042500
C	-3.34350100	0.00179800	0.53204300
C	-1.84631200	0.00274800	0.74062000
C	-1.03435600	-0.00247600	-0.56387200
C	0.45898200	-0.00130100	-0.31596000
C	1.16635000	-1.20406000	-0.18173100
C	2.53772400	-1.20577500	0.07857500
C	3.22765400	0.00114700	0.20911900
C	2.53612700	1.20689100	0.07563800
C	1.16480600	1.20274900	-0.18464100
H	-1.59566400	0.87697200	1.36155700
H	-1.59546100	-0.86635200	1.36862700
H	-1.32217600	-0.88052300	-1.15291500
H	0.63760100	-2.14905900	-0.28995500
H	3.06800600	-2.14989600	0.17360400
H	4.29603900	0.00210000	0.40774900
H	3.06522100	2.15190900	0.16834100
H	0.63481200	2.14678500	-0.29520800
O	-3.89076700	-0.00224900	-0.54884500
H	-1.32237600	0.87060300	-1.16021300

**hemiacetal**

H	-3.94470600	0.00511900	1.47042500
C	-3.34350100	0.00179800	0.53204300
C	-1.84631200	0.00274800	0.74062000
C	-1.03435600	-0.00247600	-0.56387200
C	0.45898200	-0.00130100	-0.31596000
C	1.16635000	-1.20406000	-0.18173100
C	2.53772400	-1.20577500	0.07857500
C	3.22765400	0.00114700	0.20911900
C	2.53612700	1.20689100	0.07563800
C	1.16480600	1.20274900	-0.18464100
H	-1.59566400	0.87697200	1.36155700
H	-1.59546100	-0.86635200	1.36862700
H	-1.32217600	-0.88052300	-1.15291500
H	0.63760100	-2.14905900	-0.28995500
H	3.06800600	-2.14989600	0.17360400
H	4.29603900	0.00210000	0.40774900
H	3.06522100	2.15190900	0.16834100
H	0.63481200	2.14678500	-0.29520800
O	-3.89076700	-0.00224900	-0.54884500
H	-1.32237600	0.87060300	-1.16021300

<b>B (phenylpropanol)</b>				H	-2.38702600	0.73521100	2.75542300
H	3.79185600	-0.58311500	1.34385500	C	-1.80895700	-0.96338300	3.93869800
C	3.25246900	-0.44211300	0.39290500	C	-1.28196300	-2.25786800	3.89905900
C	1.75652900	-0.33843100	0.66594700	H	-1.17407500	-2.81589800	4.82796900
C	0.91255800	-0.23728300	-0.62059900	C	-0.89671000	-2.85912000	2.69362500
C	-0.56731800	-0.08709300	-0.34045300	C	-1.05926600	-2.13757300	1.50694700
C	-1.12966200	1.17854700	-0.12027800	H	-0.79086400	-2.59842200	0.56017000
C	-2.48647300	1.32124500	0.17361400	C	-2.19026500	-0.31686000	5.25028600
C	-3.30939700	0.19546300	0.25130600	H	-1.42189000	0.39959700	5.56885500
C	-2.76405400	-1.07094500	0.03220700	H	-2.30272500	-1.05947700	6.04725400
C	-1.40578900	-1.20749300	-0.26045300	H	-3.13278200	0.23634000	5.16692600
H	1.44374600	-1.21469600	1.24921100	C	-0.30829900	-4.25155400	2.67094500
H	1.57442500	0.54260600	1.29414100	H	-0.43483600	-4.75672900	3.63424500
H	1.27559800	0.61548200	-1.20411500	H	0.76625200	-4.21926500	2.44930600
H	-0.49570700	2.06054500	-0.18494300	H	-0.77736500	-4.87289600	1.89909500
H	-2.90233200	2.31232900	0.33711400	C	-2.79119000	1.52868700	0.29208600
H	-4.36704900	0.30478400	0.47630200	C	-4.13270700	1.45642200	0.70381600
H	-3.39682500	-1.95346100	0.08446100	H	-4.62591400	0.49129400	0.77094800
H	-0.98962800	-2.19772400	-0.43575000	C	-4.85650900	2.60999500	1.01723100
H	1.08535500	-1.13499500	-1.22985400	C	-4.21611500	3.85261000	0.90939500
H	3.45609100	-1.32527100	-0.23641000	H	-4.77416000	4.75831000	1.14378800
O	3.67035100	0.75466600	-0.25724200	C	-2.88631000	3.95948700	0.49464100
H	4.60848000	0.66481000	-0.48125300	C	-2.18179600	2.78469000	0.18708000
<b>I</b>				H	-1.16403500	2.85350200	-0.17954700
C	-3.14282600	-1.08041700	-0.88824900	C	-6.30709300	2.52804600	1.43696200
C	-3.42360800	-0.94237700	-2.25438700	H	-6.97143500	2.90347900	0.64766400
H	-2.85084400	-0.24350600	-2.85332700	H	-6.50073400	3.12974000	2.33312100
C	-4.43481200	-1.69702500	-2.86302700	H	-6.60288500	1.49652400	1.65257700
C	-5.17041700	-2.59361300	-2.08213200	C	-2.21099700	5.30897700	0.38637100
H	-5.96246400	-3.17949900	-2.54679300	H	-1.72576900	5.59114900	1.33053700
C	-4.91308600	-2.75515900	-0.71621300	H	-2.92988100	6.09903900	0.14327300
C	-3.89759400	-1.99053500	-0.13025700	C	3.06730400	1.27687400	-0.64224600
H	-3.70053000	-2.11315400	0.92951500	C	3.36052100	1.35197900	-2.01028600
C	-4.70183100	-1.55843600	-4.34503300	H	2.83837200	0.70674800	-2.70823700
H	-5.73793300	-1.81409800	-4.59319700	C	4.32487400	2.24692500	-2.49288100
H	-4.05174700	-2.22522900	-4.92735000	C	4.99885000	3.06683200	-1.58340200
H	-4.50801100	-0.53794200	-4.69156500	H	5.75335400	3.76137700	-1.95054900
C	-5.70072100	-3.75159000	0.10516700	C	4.72898700	3.01411500	-0.21071300
H	-5.64711200	-3.52145400	1.17447500	C	3.76253500	2.11192500	0.24761000
H	-5.31568400	-4.77159100	-0.02869200	H	3.55846100	2.06453400	1.31201900
H	-6.75746900	-3.76618000	-0.18562300	C	4.60683400	2.33330400	-3.97599100
C	-1.59689800	-0.84124100	1.51443600	H	5.57771300	2.80008500	-4.17436800
C	-1.96532500	-0.26447600	2.73357600	H	3.84234200	2.93171800	-4.48911600
				H	4.60251800	1.34189500	-4.44195000

C	5.45481400	3.92569500	0.75365300	H	0.77610200	-3.93709200	-3.58396400
H	6.52312500	3.99330000	0.51675300	H	0.57226500	-2.81120300	-4.94782100
H	5.35948500	3.57364500	1.78613000	O	1.32406200	-0.70521000	-3.23265300
H	5.05226000	4.94696900	0.71732500	O	0.00342200	-2.02598000	-2.07530700
C	2.86446800	-1.50082300	0.10482000	C	-0.71341400	2.10482300	-2.93462900
C	4.22618000	-1.40829700	0.43591900	C	-1.04830800	3.33967100	-3.73400400
H	4.68131200	-0.43327400	0.58057500	H	-0.24366300	4.07496400	-3.65709000
C	5.01772600	-2.55233800	0.57384300	H	-1.22631300	3.07711400	-4.77971100
C	4.42404400	-3.80531300	0.37150400	O	-1.20627400	0.97652800	-3.23855800
H	5.03397700	-4.70268200	0.46760700	O	0.05475100	2.19480500	-1.91613800
C	3.07300900	-3.93176600	0.03685500	H	2.17414700	-3.01464100	-4.22632100
C	2.30043000	-2.76745700	-0.09262700	H	-1.96602600	3.78758900	-3.33314400
H	1.26133600	-2.84849600	-0.38880400				
C	6.49010400	-2.44163100	0.90069400	<b>II</b>			
H	7.10825400	-2.58348100	0.00421400	C	1.61970500	-0.23316200	2.93295800
H	6.79844800	-3.20139000	1.62831500	C	1.37187200	1.10482500	3.25403900
H	6.73491400	-1.45784800	1.31375500	H	1.05498500	1.79223200	2.48041500
C	2.45182700	-5.29477300	-0.17546900	C	1.54090000	1.57605300	4.56570400
H	2.05248900	-5.70512100	0.76180700	C	1.97251100	0.68509600	5.54918400
H	3.18517100	-6.01359000	-0.55707300	H	2.10951400	1.04389800	6.56848900
H	1.62049800	-5.24649400	-0.88660500	C	2.23517300	-0.66198500	5.25811500
C	1.55403000	0.54863200	1.69454300	C	2.05241700	-1.10778900	3.94771200
C	1.93323800	-0.24154600	2.78476200	H	2.25141700	-2.14982400	3.71656800
H	2.38289100	-1.21505300	2.61774000	C	1.24055000	3.02071100	4.89504300
C	1.75197300	0.20750500	4.09968200	H	1.62511100	3.29575600	5.88278600
C	1.19145200	1.47233000	4.30470800	H	0.15904200	3.20915800	4.89496600
H	1.06283200	1.83722500	5.32262200	H	1.68360600	3.69802800	4.15602400
C	0.79533300	2.28385200	3.23398300	C	2.69862100	-1.60582800	6.34524200
C	0.97822500	1.80565800	1.93235900	H	2.93566900	-2.59500200	5.94078000
H	0.69207400	2.43205500	1.09216200	H	1.92828100	-1.73835800	7.11597700
C	0.19164500	3.65006600	3.47008500	H	3.59508000	-1.22622000	6.85118000
H	0.83193700	4.44553700	3.06785900	C	0.95155700	-2.59539600	1.49999100
H	0.04965000	3.84583700	4.53795000	C	1.70246000	-3.67917800	1.03911900
H	-0.78357800	3.74046400	2.97671500	H	2.59226500	-3.50673600	0.44166500
C	2.14049200	-0.67162800	5.26608500	C	1.34169500	-4.99708600	1.35915200
H	3.10105000	-1.16971400	5.09135100	C	0.21806800	-5.20799800	2.16152000
H	1.39276700	-1.45936100	5.42730000	H	-0.05389200	-6.22579400	2.43771200
H	2.22137500	-0.09602900	6.19430200	C	-0.56005100	-4.14085800	2.63340200
Ru	0.01800700	0.06917000	-1.55764200	C	-0.18194900	-2.84028900	2.29300100
P	-1.82553400	-0.00452900	-0.12129100	H	-0.75214000	-2.00245700	2.68648900
P	1.81421300	0.02467800	-0.06310500	C	2.15558900	-6.15837800	0.83683200
H	-1.43461100	5.30386600	-0.38581200	H	1.90152400	-6.37248400	-0.20966100
C	0.80642300	-1.84975400	-3.05531800	H	1.97184300	-7.07057700	1.41433500
C	1.10344500	-2.98381000	-4.00449200	H	3.22996000	-5.94501200	0.87283000

C	-1.78238800	-4.39662700	3.48586000	C	-3.37293700	-1.21291200	0.79323600
H	-1.64108700	-5.26438000	4.13990700	H	-2.52074100	-1.35294700	1.44879200
H	-2.66517300	-4.60031700	2.86435500	C	-6.76943500	-0.49453000	-1.76983400
H	-2.01942300	-3.53288400	4.11564800	H	-7.21132100	0.48777900	-1.55740600
C	3.16192900	-0.93323800	0.56274200	H	-7.55850400	-1.24135000	-1.62157600
C	4.27489200	-0.70634000	1.38816100	H	-6.48831400	-0.50575700	-2.82760400
H	4.13146600	-0.47450600	2.43806500	C	-4.87102300	-1.61053600	2.79107100
C	5.57686600	-0.76549300	0.87981800	H	-4.63197600	-2.65951000	3.00970300
C	5.75415200	-1.06474100	-0.47813500	H	-5.90784900	-1.43847500	3.09809000
H	6.76382900	-1.11787500	-0.88311700	H	-4.22344800	-0.99413800	3.42542600
C	4.66701700	-1.29117400	-1.32716000	C	-0.95162400	-2.59520500	-1.50023400
C	3.37300000	-1.21305300	-0.79328500	C	-1.70261600	-3.67899000	-1.03946800
H	2.52080900	-1.35296500	-1.44887800	H	-2.59238300	-3.50654200	-0.44196500
C	6.76951400	-0.49501100	1.76984600	C	-1.34198300	-4.99687300	-1.35968200
H	7.20957000	0.48857200	1.55948900	C	-0.21839700	-5.20778000	-2.16213700
H	7.55976900	-1.24012700	1.61946400	H	0.05345800	-6.22556100	-2.43848000
H	6.48895800	-0.50911200	2.82774000	C	0.55979500	-4.14066100	-2.63389600
C	4.87104600	-1.61055500	-2.79116700	C	0.18181500	-2.84008800	-2.29331100
H	4.63158700	-2.65939400	-3.00998900	H	0.75206100	-2.00225300	-2.68671600
H	5.90795600	-1.43885700	-3.09810400	C	1.78212900	-4.39637100	-3.48637600
C	-1.61958600	-0.23277100	-2.93290300	H	2.01773300	-3.53350000	-4.11790400
C	-1.37159500	1.10522800	-3.25384900	H	1.64175700	-5.26556200	-4.13869800
H	-1.05454700	1.79249700	-2.48016900	H	2.66545800	-4.59762100	-2.86484400
C	-1.54084800	1.57666800	-4.56539700	C	-2.15591400	-6.15818500	-0.83746400
C	-1.97281500	0.68590600	-5.54891000	H	-3.23023200	-5.94442400	-0.87257800
H	-2.11016900	1.04490500	-6.56809600	H	-1.90117800	-6.37299000	0.20872500
C	-2.23550600	-0.66119500	-5.25800600	H	-1.97288700	-7.07011800	-1.41561900
C	-2.05262100	-1.10719900	-3.94767800	Ru	0.00010800	0.60372400	0.00005900
H	-2.25184700	-2.14920800	-3.71660000	P	1.41405000	-0.82815900	1.18273000
C	-1.24061200	3.02139500	-4.89453900	P	-1.41397000	-0.82797400	-1.18275000
H	-1.62449600	3.29631600	-5.88257800	H	4.22374800	-0.99379400	-3.42545300
H	-0.15915700	3.21011800	-4.89362800	C	-1.96850000	1.99866700	0.84117100
H	-1.68441100	3.69862300	-4.15587800	C	-3.08039700	2.84027300	1.42890100
C	-2.69843800	-1.60503100	-6.34535800	C	-4.15157400	3.22528800	0.38647600
H	-3.58791800	-1.21993700	-6.85930500	C	-5.28395500	4.02548200	0.99300700
H	-2.94633800	-2.59093500	-5.93940800	C	-6.40220300	3.38078800	1.54085800
H	-1.92336400	-1.74647800	-7.10979300	C	-7.43600700	4.11087700	2.12931100
C	-3.16185500	-0.93296700	-0.56277100	C	-7.36887600	5.50488500	2.18015200
C	-4.27480200	-0.70590700	-1.38815200	C	-6.26174800	6.16028700	1.63739400
H	-4.13139800	-0.47395300	-2.43803200	C	-5.23078400	5.42510200	1.04967900
C	-5.57678600	-0.76503400	-0.87981500	H	-3.52384300	2.28958800	2.26408800
C	-5.75408300	-1.06440000	0.47810700	H	-2.63226900	3.75135000	1.84936400
H	-6.76374700	-1.11749900	0.88312300	H	-3.66808800	3.79152500	-0.41610200
C	-4.66694800	-1.29100100	1.32710300	H	-6.46087700	2.29477100	1.49960900

H	-8.29627600	3.59159500	2.54455900
H	-8.17422600	6.07564800	2.63505500
H	-6.20244100	7.24544300	1.66686000
H	-4.37398300	5.94302000	0.62329900
O	-1.51810600	2.23017000	-0.32525600
O	-1.46608800	1.04117900	1.52103700
H	-4.54508000	2.30862900	-0.06840400
C	1.96868100	1.99868700	-0.84101800
C	3.08057300	2.84031100	-1.42872400
C	4.15161200	3.22553900	-0.38624400
C	5.28396800	4.02578000	-0.99276300
C	6.40234300	3.38114200	-1.54041900
C	7.43611800	4.11127300	-2.12887000
C	7.36882900	5.50526700	-2.17990400
C	6.26157500	6.16061400	-1.63733800
C	5.23064000	5.42538600	-1.04962300
H	3.52414700	2.28956100	-2.26380200
H	2.63241100	3.75129400	-1.84935400
H	3.66800200	3.79181400	0.41623200
H	6.46114200	2.29513900	-1.49901500
H	8.29648800	3.59203800	-2.54396600
H	8.17415600	6.07606200	-2.63480900
H	6.20214400	7.24575800	-1.66695400
H	4.37373700	5.94326100	-0.62339400
O	1.51821400	2.23022000	0.32537700
O	1.46631700	1.04117800	-1.52088800
H	4.54516600	2.30896200	0.06876500

**Int1**

C	-0.05457500	3.54119100	-1.56920700
C	-1.44754100	3.68405500	-1.69817300
H	-2.11024600	3.05137400	-1.11457000
C	-1.99537900	4.61545000	-2.58234000
C	-1.12735700	5.40689200	-3.34968000
H	-1.54560100	6.13258100	-4.04571500
C	0.25872100	5.28428700	-3.24537100
C	0.78615500	4.34802000	-2.34059200
H	1.86370000	4.25690200	-2.25145900
C	-3.49353100	4.77794500	-2.70751300
H	-4.02517100	3.99744200	-2.15448400
H	-3.81509700	4.72913100	-3.75494500
H	-3.82432700	5.74833600	-2.31455500
C	1.18240800	6.11961800	-4.10306000
H	1.53612500	5.55165900	-4.97380800

H	2.06998300	6.43862000	-3.54494400
H	0.67832900	7.01596900	-4.47946400
C	0.18315600	3.23710500	1.23695000
C	0.31304900	4.63857200	1.26341700
H	0.62656500	5.16803600	0.36920400
C	0.03183900	5.37003400	2.41803300
C	-0.39141300	4.67781400	3.56308900
H	-0.62246600	5.23899300	4.46740700
C	-0.52917900	3.28988700	3.57061800
C	-0.23757100	2.58109600	2.39343400
H	-0.33953800	1.50476000	2.39080600
C	0.16566300	6.87610700	2.43853400
H	-0.79365600	7.35899600	2.66340400
H	0.51275400	7.25899100	1.47387200
H	0.87770200	7.20487100	3.20605300
C	-0.96615100	2.55443100	4.81670800
H	-1.71507600	1.78832300	4.58655000
H	-1.39247700	3.23959400	5.55683400
H	-0.11924000	2.03960000	5.28847200
C	2.40079000	2.44426800	-0.47941700
C	2.99732800	1.98762400	-1.66838400
H	2.38280900	1.55531900	-2.45223600
C	4.37484000	2.09911300	-1.87063100
C	5.15904200	2.66841900	-0.85458700
H	6.23410200	2.76071100	-1.00216800
C	4.59510200	3.12194300	0.33966400
C	3.20703900	3.00002900	0.51791400
H	2.76324400	3.35326000	1.44336100
C	5.00605900	1.62738500	-3.16160200
H	5.45493900	2.46234300	-3.71502600
H	4.26619900	1.15268400	-3.81288400
H	5.80749000	0.90174200	-2.97374700
C	5.44749000	3.74983200	1.41986300
H	5.21376800	4.81517500	1.54344500
H	6.51373500	3.66979800	1.18485400
C	0.10590400	-2.84554000	0.69150800
C	-0.61010800	-3.46590600	-0.34193200
H	-1.36099900	-2.90644200	-0.88798500
C	-0.36465100	-4.80069200	-0.68768600
C	0.61882100	-5.50951900	0.01165200
H	0.81747200	-6.54696600	-0.25390400
C	1.35194700	-4.91638400	1.04560500
C	1.08056000	-3.58338900	1.38047600
H	1.64636700	-3.12563900	2.18432700

C	-1.16762400	-5.46309500	-1.78491300	P	-0.28649300	-1.08213000	1.14794400
H	-1.39293500	-4.75909800	-2.59287500	H	5.27950000	3.27036200	2.39159800
H	-2.12755000	-5.83725300	-1.40395000	C	-3.03669200	-0.21002100	-1.06186300
H	-0.63262600	-6.31657900	-2.21494600	C	-4.53400400	-0.40060800	-1.18516700
C	2.44009700	-5.68384600	1.76277100	C	-4.94944700	-1.44011500	-2.24285700
H	2.18124200	-6.74333000	1.86951700	C	-6.45249000	-1.60460900	-2.32524100
H	2.62533300	-5.27707200	2.76252200	C	-7.12221400	-2.51859100	-1.49957600
H	3.38733100	-5.63414100	1.20923600	C	-8.51086600	-2.64988400	-1.55067000
C	-1.79505200	-1.27700400	2.20760900	C	-9.25706900	-1.86603100	-2.43331400
C	-2.06607500	-2.48296400	2.87620800	C	-8.60328800	-0.95305500	-3.26305300
H	-1.39367000	-3.32721200	2.75984900	C	-7.21430000	-0.82584200	-3.20733700
C	-3.19639400	-2.62253100	3.68692300	H	-4.90546000	-0.70216500	-0.19556100
C	-4.06250500	-1.52881800	3.82321100	H	-4.98537100	0.57631300	-1.39203000
H	-4.94977800	-1.62996600	4.44666200	H	-4.55106900	-1.13540900	-3.21770000
C	-3.82223700	-0.31614900	3.17170500	H	-6.54683800	-3.13801600	-0.81426400
C	-2.68144100	-0.20273600	2.36184400	H	-9.00953800	-3.36871600	-0.90527500
H	-2.50937800	0.72109600	1.82183300	H	10.33801400	-1.96970600	-2.47769700
C	-3.49342800	-3.92891400	4.38846200	H	-9.17396500	-0.34272000	-3.95848900
H	-2.66157100	-4.63325900	4.29028100	H	-6.71145900	-0.11706100	-3.86229100
H	-4.38663600	-4.41125200	3.97081700	O	-2.58023200	0.85479100	-0.52351100
H	-3.68195100	-3.77636600	5.45811200	O	-2.22101300	-1.09444000	-1.46521900
C	-4.76102900	0.85816800	3.33751700	H	-4.47444600	-2.39637900	-2.00061500
H	-4.41489300	1.53801700	4.12773600	C	1.63428600	-0.89715300	-2.56227400
H	-5.76970000	0.52974100	3.60975500	C	2.69710300	-1.96384100	-2.84137600
H	-4.82953500	1.44484800	2.41533000	C	3.65993300	-2.25525700	-1.67564000
C	1.06577900	-0.71530300	2.35779000	C	4.64695700	-3.35686500	-1.99958400
C	0.86976700	-0.75157900	3.74552000	C	4.27781700	-4.70543700	-1.87668800
H	-0.11924500	-0.94264400	4.15026600	C	5.17158500	-5.72755000	-2.19953200
C	1.93944800	-0.55573800	4.62770600	C	6.45701500	-5.42009300	-2.65230300
C	3.21684800	-0.35029300	4.09377200	C	6.83812900	-4.08333000	-2.77923800
H	4.05909600	-0.21840200	4.77128500	C	5.93937800	-3.06461500	-2.45529700
C	3.44420700	-0.32156100	2.71302700	H	2.15527800	-2.88399800	-3.10180100
C	2.35255000	-0.48536200	1.84968800	H	3.24454500	-1.66607000	-3.74157300
H	2.50602100	-0.46628900	0.77433000	H	4.20093400	-1.33583600	-1.41885800
C	4.84312100	-0.16854600	2.16186300	H	3.27798700	-4.95115600	-1.52414100
H	4.85638500	0.47069400	1.27403200	H	4.86544900	-6.76577100	-2.09549800
H	5.25702100	-1.14261600	1.86876100	H	7.15502100	-6.21506400	-2.90170000
H	5.52124500	0.26302400	2.90617600	H	7.83675900	-3.83210700	-3.12835100
C	1.71815700	-0.55960200	6.12375300	H	6.24535700	-2.02481000	-2.55442500
H	1.58945900	0.46004300	6.51211300	O	1.17921400	-0.23293700	-3.50956200
H	2.56978000	-1.00005900	6.65415700	O	1.26898800	-0.79188600	-1.32528800
H	0.82066700	-1.12574700	6.39428000	H	3.06530600	-2.52775800	-0.79852400
Ru	-0.50314000	0.25283500	-0.82316600	H	-0.87549300	1.08876900	-2.45345700
P	0.56304500	2.30092100	-0.32309600	H	-0.25265000	0.65862300	-2.72054100



**TS1**

C	0.17956100	3.61464000	-1.42213700	H	3.49158100	1.33754800	0.64639300
C	-1.12617900	3.63647800	-1.91588300	C	4.07818200	2.06928700	-4.67505000
H	-1.76465700	2.76902000	-1.78759900	H	3.79497600	3.08249600	-4.98552100
C	-1.63053000	4.77622700	-2.56615400	H	3.42906500	1.37244600	-5.21948400
C	-0.80228600	5.88884500	-2.70952900	H	5.10890900	1.89432900	-5.00011300
H	-1.18514500	6.77563200	-3.21285600	C	6.04540900	0.82593300	-0.17933400
C	0.51300000	5.89732100	-2.21759700	H	6.98744000	1.21694900	-0.57953300
C	0.98814800	4.75583400	-1.57276300	H	6.12846200	-0.26953100	-0.17197900
H	2.00326900	4.75562400	-1.18591600	C	-0.17136000	-2.70936300	1.09489100
C	-3.04263700	4.77600200	-3.10673800	C	-0.63139300	-3.36272400	-0.05777500
H	-3.76233700	4.46221900	-2.34134400	H	-1.18948800	-2.80637100	-0.80166200
H	-3.14599700	4.07878500	-3.94827700	C	-0.39038600	-4.72730800	-0.25868000
H	-3.33684900	5.76956000	-3.46076500	C	0.33186000	-5.43396600	0.71020100
C	1.38632400	7.12016000	-2.38698700	H	0.52832200	-6.49474800	0.55947900
H	1.54606500	7.35570800	-3.44698400	C	0.80145700	-4.81129700	1.87192600
H	2.36894500	6.97578400	-1.92667800	C	0.53741100	-3.44758800	2.05492000
H	0.92882400	8.00551300	-1.92772300	H	0.89918000	-2.96329800	2.95605800
C	1.01265200	2.93521000	1.17326800	C	-0.92461700	-5.42506200	-1.48970400
C	2.16342900	3.62308600	1.58766200	H	-1.02132700	-4.73067400	-2.33053400
H	3.05211700	3.62586400	0.96493400	H	-1.92028600	-5.85022300	-1.30398200
C	2.18986300	4.31781400	2.80141700	H	-0.27339200	-6.24977700	-1.80020700
C	1.03116400	4.34080100	3.58880000	C	1.60307000	-5.58389800	2.89580100
H	1.03818900	4.89172200	4.52811500	H	1.28787600	-6.63211400	2.94458000
C	-0.13609400	3.68208500	3.19371400	H	1.49771900	-5.15136800	3.89653000
C	-0.12477700	2.97339100	1.98564100	H	2.67369600	-5.57802000	2.65065400
H	-1.02339000	2.45499800	1.66455900	C	-2.18166500	-0.93653000	2.20115600
C	3.44698200	5.02000900	3.26305400	C	-2.61121700	-2.06448500	2.91942000
H	3.21881600	5.98041900	3.73925400	H	-1.99693200	-2.95908200	2.93704000
H	4.12906900	5.21067600	2.42800700	C	-3.82590700	-2.06205600	3.61133600
H	3.99261600	4.41595100	4.00055700	C	-4.61276100	-0.90204600	3.58211700
C	-1.39277300	3.74209600	4.03216000	H	-5.56185200	-0.89071800	4.11624800
H	-2.15631100	4.37267500	3.55812600	C	-4.21507000	0.23650500	2.87670000
H	-1.19319500	4.15770700	5.02540400	C	-2.99490300	0.20383500	2.18424700
H	-1.83246800	2.74623000	4.16197100	H	-2.70169000	1.06229300	1.59109000
C	2.52075600	1.94320000	-1.18680900	C	-4.29469600	-3.28848800	4.36165000
C	2.69306800	2.11853900	-2.56568300	H	-3.49777500	-4.03398200	4.44510400
H	1.85520700	2.43825300	-3.17800300	H	-5.14236000	-3.76686400	3.85369500
C	3.92924900	1.88751200	-3.18204500	H	-4.62906300	-3.03583900	5.37505200
C	5.00521100	1.48578000	-2.38598600	C	-5.06867500	1.48484800	2.85895600
H	5.97725000	1.32284600	-2.84875700	H	-4.69393000	2.23529300	3.56796600
C	4.86487200	1.28657000	-1.00598100	H	-6.10590400	1.26529300	3.13264100
C	3.61201900	1.50465000	-0.41966900	H	-5.06873500	1.95088900	1.86749800
				C	0.63442400	-0.43696800	2.65898500
				C	0.21429500	-0.02052600	3.92430900

H	-0.84570900	0.05322500	4.14602600	C	5.24950800	-5.96429700	-1.90475200
C	1.14264700	0.29383700	4.92887100	C	6.48038400	-5.56717300	-2.43051700
C	2.50195600	0.15082900	4.64915400	C	6.73798400	-4.20843100	-2.62712200
H	3.23038900	0.36691500	5.42945500	C	5.76988100	-3.25783500	-2.30052800
C	2.95462500	-0.27309300	3.39056200	H	2.20832700	-3.04971600	-3.16451300
C	2.01145100	-0.54571000	2.39655600	H	3.32642300	-1.73337700	-3.44252800
H	2.34431300	-0.87625300	1.41593300	H	3.93264500	-1.72208500	-1.00070200
C	4.43441000	-0.44978700	3.13707100	H	3.32954600	-5.32262100	-1.16262100
H	4.62516400	-0.84063700	2.13349600	H	5.04099700	-7.01918100	-1.74382100
H	4.87976700	-1.14781400	3.85699000	H	7.23383300	-6.30907200	-2.68190000
H	4.97591500	0.49979600	3.23738000	H	7.69501900	-3.88868900	-3.03208900
C	0.67316700	0.78885000	6.27750600	H	5.97750500	-2.20055100	-2.45535500
H	0.49860200	1.87301100	6.25763800	O	0.97559500	-0.64940800	-3.39814400
H	1.41483500	0.59145900	7.05891500	O	1.24330400	-0.95992700	-1.18919600
H	-0.26841300	0.31409100	6.57473100	H	2.77461700	-3.00814700	-0.69899100
Ru	-0.49471600	0.22571100	-0.83139800	H	-0.55154000	0.83724900	-2.48682600
P	0.81514500	2.13239200	-0.48855200	H	0.04113100	0.20718700	-2.83308400
P	-0.55132400	-0.89948700	1.31539900				
H	5.95997000	1.15174700	0.86207000				
C	-3.02439400	-0.10767100	-1.20112800	<b>Int2</b>			
C	-4.51924500	-0.22965200	-1.41145400	C	0.05693000	3.84844900	-1.06528000
C	-4.91242100	-1.26053700	-2.48695100	C	-1.18503800	3.83787700	-1.70261400
C	-6.41334400	-1.39013000	-2.63787500	H	-1.71720300	2.90028500	-1.81402000
C	-7.13829300	-2.29921300	-1.85444700	C	-1.76055600	5.02847000	-2.17930600
C	-8.52586600	-2.39933500	-1.96768500	C	-1.06504200	6.22535600	-2.01020700
C	-9.21583500	-1.58874100	-2.87154700	H	-1.50455100	7.15252900	-2.37582200
C	-8.50675900	-0.68028100	-3.65993600	C	0.18588800	6.26687500	-1.37331700
C	-7.11913900	-0.58427300	-3.54200000	C	0.73006500	5.07299800	-0.90091100
H	-4.96086400	-0.51176800	-0.44518000	H	1.69080700	5.09929400	-0.39469700
H	-4.91503800	0.76339600	-1.65059400	C	-3.10950500	4.99537200	-2.86177000
H	-4.46379400	-0.96627600	-3.44341200	H	-3.87023200	4.54012500	-2.21594300
H	-6.60701900	-2.93934000	-1.15280700	H	-3.07563800	4.40072200	-3.78356600
H	-9.06750500	-3.11487900	-1.35401400	H	-3.45031200	6.00183600	-3.12639900
H	10.29579000	-1.66799800	-2.96438100	C	0.92216700	7.57801900	-1.21244800
H	-9.03313500	-0.04893800	-4.37143400	H	1.27578700	7.96142300	-2.17877300
H	-6.57311600	0.12150900	-4.16490600	H	1.79525900	7.46757000	-0.56134700
O	-2.53875500	0.98034500	-0.73855300	H	0.27565600	8.35056800	-0.77860200
O	-2.24294100	-1.07425300	-1.45281300	C	1.21020400	2.83915000	1.31250900
H	-4.47056000	-2.22626900	-2.22167100	C	2.42584400	3.43211700	1.69039800
C	1.55231600	-1.18275200	-2.40416900	H	3.23328000	3.52414400	0.97054500
C	2.66996700	-2.17610000	-2.68495500	C	2.62076500	3.91798300	2.98766400
C	3.46961500	-2.61101200	-1.44508700	C	1.56918600	3.81575400	3.90818000
C	4.52847400	-3.64214700	-1.77268800	H	1.70884900	4.19585000	4.91906700
C	4.28469000	-5.00886500	-1.57910500	C	0.34441100	3.24086800	3.56008900
				C	0.18320600	2.75159200	2.25721900

H	-0.76244800	2.29733400	1.97327300	H	-2.10655100	-3.27949300	2.48682500
C	3.93976300	4.53609300	3.39552800	C	-3.93861000	-2.42610000	3.21430600
H	3.79187600	5.49002200	3.91574600	C	-4.67948900	-1.24243500	3.34134200
H	4.57973000	4.72266000	2.52695500	H	-5.65559100	-1.27646300	3.82349700
H	4.49464800	3.88076500	4.08013400	C	-4.20195500	-0.02122600	2.85736200
C	-0.78628600	3.13864700	4.55778900	C	-2.95075100	0.00474500	2.22364600
H	-1.67478500	3.68135800	4.21142300	H	-2.59113000	0.93581800	1.79794000
H	-0.50102100	3.55250500	5.53058200	C	-4.48825900	-3.73502900	3.73580200
H	-1.08350600	2.09370700	4.70791100	H	-3.75751700	-4.54333200	3.63269100
C	2.44592200	2.23483200	-1.28419800	H	-5.39311700	-4.03368600	3.19096700
C	2.56818000	2.76799000	-2.57344800	H	-4.76214200	-3.66228700	4.79565000
H	1.72525400	3.28394600	-3.02359700	C	-5.00379500	1.25094300	3.01720300
C	3.75957700	2.64984000	-3.30202300	H	-4.65746000	1.83372800	3.88144500
C	4.84383100	1.99582100	-2.70974100	H	-6.06708400	1.03897400	3.17124800
H	5.77932400	1.91075300	-3.26067700	H	-4.90816400	1.89381700	2.13545200
C	4.75545000	1.44786200	-1.42316300	C	0.60472100	-0.73340700	2.71868600
C	3.54505500	1.55906000	-0.72992100	C	0.17015900	-0.76814700	4.05072800
H	3.46573100	1.12387000	0.26172900	H	-0.87401200	-0.96371600	4.27363900
C	3.85543400	3.20414500	-4.70547400	C	1.06574800	-0.57071000	5.10892200
H	3.34121400	4.16791900	-4.79040600	C	2.41556500	-0.35189800	4.81150000
H	3.38968800	2.52522500	-5.43204300	H	3.12311400	-0.20914400	5.62683700
H	4.89751900	3.34708500	-5.01033600	C	2.88065800	-0.31502600	3.49234900
C	5.95720000	0.78530800	-0.78656000	C	1.96101700	-0.50209600	2.45355600
H	6.61889700	1.52648800	-0.31813500	H	2.30521900	-0.48635200	1.42224900
H	6.55759500	0.24370400	-1.52653700	C	4.33969700	-0.05474600	3.19408900
C	-0.13788600	-2.79942700	0.85596900	H	4.70785500	-0.70373700	2.39079400
C	-0.76591200	-3.36441500	-0.26589900	H	4.96599600	-0.22471400	4.07622900
H	-1.45170600	-2.76243700	-0.85372300	H	4.49636400	0.98346100	2.87273700
C	-0.52268500	-4.69181700	-0.63808200	C	0.58325400	-0.58327300	6.54209900
C	0.37952000	-5.44967700	0.11934600	H	0.41280500	0.43616500	6.91367800
H	0.57654900	-6.48312800	-0.16406600	H	1.31659300	-1.05092900	7.20889000
C	1.02869300	-4.91176200	1.23642700	H	-0.36110700	-1.12851300	6.64155500
C	0.75397800	-3.58571400	1.59910300	Ru	-0.43262200	0.37745300	-0.83196400
H	1.24998300	-3.17045700	2.47012400	P	0.80679200	2.27192500	-0.41240300
C	-1.24060300	-5.30023200	-1.82253500	P	-0.52235300	-1.02426200	1.27474300
H	-1.55838700	-4.53057200	-2.53315000	H	5.66176900	0.07668500	-0.00561000
H	-2.14144600	-5.84256400	-1.50473900	C	-2.96403300	0.05228500	-1.17852800
H	-0.60462500	-6.01634300	-2.35533400	C	-4.46877500	-0.03817200	-1.33610600
C	2.02521900	-5.73605600	2.02106800	C	-4.92168000	-1.01974200	-2.43325600
H	1.68597500	-6.77167700	2.13943500	C	-6.42941500	-1.11150300	-2.53658800
H	2.19167700	-5.31822100	3.01929000	C	-7.15093100	-2.00993000	-1.73759300
H	2.99861700	-5.77070200	1.51353900	C	-8.54337400	-2.07556900	-1.80637700
C	-2.18295900	-1.15888600	2.08758800	C	-9.24248700	-1.24033100	-2.68046000
C	-2.68954100	-2.36906500	2.58825900	C	-8.53729900	-0.34190000	-3.48352600

C	-7.14455900	-0.28048600	-3.40996200	H	-2.24330500	-0.88911100	-4.04701900
H	-4.88028400	-0.34729500	-0.36505400	C	-2.44087900	4.47268100	-3.46693800
H	-4.85535400	0.96975600	-1.52379000	H	-1.55625000	4.85204100	-2.94259700
H	-4.49925200	-0.70159900	-3.39387000	H	-3.31760100	4.77102300	-2.87708100
H	-6.61297800	-2.66822000	-1.05818700	H	-2.50563200	4.98269400	-4.43372500
H	-9.08223700	-2.78317400	-1.18108800	C	-3.00460200	0.34408600	-6.34164400
H	10.32653700	-1.29249300	-2.73843300	H	-3.95002400	0.73004600	-6.74177100
H	-9.07086600	0.30907800	-4.17164200	H	-3.09323900	-0.74384100	-6.25784700
H	-6.60197300	0.41848600	-4.04344200	H	-2.22947500	0.55503500	-7.09006300
O	-2.45469300	1.09446000	-0.64217900	C	-0.98194500	-1.84961100	-2.08547900
O	-2.20183500	-0.89281800	-1.54293300	C	-1.72141000	-3.03409000	-2.05504800
H	-4.49375800	-2.00424800	-2.21805500	H	-2.62898100	-3.09353100	-1.46306000
C	1.65807200	-1.07560000	-2.44247500	C	-1.32088200	-4.15603600	-2.79814300
C	2.74352400	-2.06794400	-2.77952400	C	-0.16371500	-4.06602600	-3.57395900
C	3.45604500	-2.64973000	-1.54744100	H	0.14398100	-4.92398900	-4.17013200
C	4.43022600	-3.74834100	-1.91886900	C	0.60534500	-2.89340200	-3.61656900
C	4.03155300	-5.09228800	-1.89181000	C	0.18490300	-1.79194500	-2.86793000
C	4.91356700	-6.10931000	-2.26208600	H	0.75249600	-0.86585400	-2.91596400
C	6.21313800	-5.79778500	-2.66642800	C	-2.13416600	-5.42928900	-2.75329300
C	6.62381700	-4.46330000	-2.69547500	H	-1.84973200	-6.11562200	-3.55786500
C	5.73851000	-3.45004900	-2.32419400	H	-3.20697400	-5.22395900	-2.84798100
H	2.27627300	-2.86768200	-3.36908900	H	-1.98869900	-5.95293500	-1.80000600
H	3.45297500	-1.57714600	-3.45716700	C	1.86269000	-2.83049000	-4.45350300
H	3.97761800	-1.83808600	-1.02764600	H	2.12956800	-1.79721200	-4.69756200
H	3.02131900	-5.33900700	-1.57156300	H	1.74739900	-3.38231600	-5.39342600
H	4.58651400	-7.14561500	-2.23113600	H	2.71570500	-3.27194000	-3.92097500
H	6.90187500	-6.58832100	-2.95240700	C	-3.16481600	-0.70041800	-0.50720600
H	7.63547900	-4.21126800	-3.00338700	C	-4.28020700	-0.93695100	-1.32774300
H	6.06804400	-2.41291300	-2.34369100	H	-4.18230700	-0.86982600	-2.40694300
O	1.05037600	-0.54915300	-3.48263300	C	-5.52964300	-1.24653700	-0.78182400
O	1.35049300	-0.80171300	-1.27221000	C	-5.65189300	-1.31845100	0.61282900
H	2.70291500	-3.03337300	-0.85236600	H	-6.62132900	-1.55775000	1.04839500
H	-0.46893400	1.06669900	-2.34026800	C	-4.56435500	-1.07768400	1.45833900
H	0.35333400	0.09349300	-3.10809800	C	-3.32272600	-0.76308900	0.88345000
				H	-2.48381800	-0.51438200	1.52456900
<b>TS2</b>				C	-6.73109800	-1.47554100	-1.67131800
C	-1.94324100	0.76348900	-2.68207200	H	-6.43620600	-1.59091300	-2.71912500
C	-1.99155400	2.15586100	-2.56305800	H	-7.43269600	-0.63271600	-1.61796800
H	-1.70427000	2.62243700	-1.62683200	H	-7.28534400	-2.37420900	-1.37524800
C	-2.37863200	2.97133400	-3.63610800	C	-4.71359700	-1.16979300	2.96158600
C	-2.71124800	2.36651000	-4.84967800	H	-4.64000900	-2.21018900	3.30586000
H	-3.00482300	2.99037600	-5.69265700	H	-5.68513000	-0.78789200	3.29466000
C	-2.66744000	0.97521300	-5.00927100	C	1.52891900	-1.11172400	2.82577100
C	-2.28537300	0.18769900	-3.91934300	C	1.95511000	0.13385600	3.30290600

H	2.14428300	0.93811900	2.60011300	H	-3.34113400	-3.98848400	1.67513800
C	2.15560000	0.35732400	4.67138700	C	1.42515300	-6.48644500	-0.50627000
C	1.92641600	-0.69344600	5.56321000	H	1.30399700	-6.41641800	-1.59549900
H	2.07835800	-0.52927500	6.62908200	H	1.04253500	-7.46394400	-0.19382600
C	1.50840000	-1.95373900	5.11762400	H	2.50089000	-6.46105600	-0.29896700
C	1.31694700	-2.15091900	3.74570000	Ru	0.13586200	0.65650200	0.12774600
H	1.00298200	-3.12927400	3.39836500	P	-1.48830200	-0.29775000	-1.20774100
C	2.59181600	1.71984400	5.16128400	P	1.32619600	-1.31558700	0.98592100
H	1.80099500	2.46551800	5.00822900	H	-3.92984700	-0.60242100	3.47358500
H	3.47729800	2.07539000	4.62078500	C	2.30992800	1.84522200	-0.59153300
H	2.83225200	1.70503800	6.22942200	C	3.58202400	2.50703700	-1.07641700
C	1.25873700	-3.07346800	6.10333400	C	3.95591900	3.78324200	-0.29745200
H	2.08849300	-3.17749000	6.81287800	C	5.26624300	4.37875400	-0.76787900
H	1.12976000	-4.03361400	5.59329200	C	6.48513400	3.94576700	-0.22663200
H	0.35215300	-2.88973700	6.69505400	C	7.69820100	4.46473100	-0.68148400
C	3.08726900	-1.59334900	0.45771600	C	7.71305000	5.43136700	-1.68939900
C	4.06257400	-2.06013400	1.35269700	C	6.50675100	5.87363400	-2.23584900
H	3.79605600	-2.25624500	2.38660100	C	5.29631900	5.35044100	-1.77746900
C	5.38184400	-2.27428900	0.94012300	H	4.38755800	1.76568900	-0.97826600
C	5.71591400	-2.01570900	-0.39524400	H	3.47752400	2.71193400	-2.14698300
H	6.74169200	-2.17365100	-0.72592700	H	3.14953400	4.51862300	-0.40699700
C	4.76777000	-1.55350600	-1.31336500	H	6.48098300	3.19728600	0.56333900
C	3.45290800	-1.34411200	-0.87223500	H	8.63157300	4.11840900	-0.24469300
H	2.71365700	-0.96007500	-1.56550300	H	8.65635200	5.83973200	-2.04240100
C	6.43292500	-2.74836600	1.91871800	H	6.50691300	6.62982800	-3.01686100
H	5.97783600	-3.18877100	2.81157700	H	4.36003200	5.70376000	-2.20481300
H	7.07060600	-1.91845300	2.25134700	O	1.60706200	1.15833300	-1.39894600
H	7.09154200	-3.49974300	1.46782800	O	1.95110000	1.93448900	0.63172800
C	5.14958900	-1.29710700	-2.75454100	H	4.01116200	3.53640300	0.76779300
H	5.07113100	-2.21136300	-3.35820400	C	-1.10814800	2.25398600	1.46864500
H	6.18301500	-0.94303100	-2.83824800	C	-2.49773100	2.83853100	1.24958200
H	4.49576900	-0.54801600	-3.21286200	C	-3.18958500	3.12409000	2.60454900
C	0.59936900	-3.01584100	0.86059100	C	-4.55410100	3.75459700	2.42448700
C	1.27242800	-4.08038400	0.25142300	C	-4.74300300	5.12786400	2.62901600
H	2.25680000	-3.92313000	-0.17769800	C	-5.99476700	5.71794800	2.44174000
C	0.69988500	-5.35753500	0.18955900	C	-7.08282800	4.93976000	2.04375400
C	-0.55785800	-5.55728100	0.76773900	C	-6.90822100	3.56948100	1.83425600
H	-1.00171800	-6.55145100	0.74501200	C	-5.65591600	2.98407100	2.02318900
C	-1.26110300	-4.51033100	1.37702600	H	-2.41340000	3.76569000	0.67476200
C	-0.67315700	-3.24131200	1.40641200	H	-3.09256100	2.12630600	0.67345900
H	-1.20619200	-2.42199200	1.88005600	H	-3.27542600	2.17938300	3.15476200
C	-2.61722100	-4.74269400	2.00483200	H	-3.89945600	5.73955000	2.94191700
H	-2.56587500	-4.68476200	3.10008600	H	-6.11929300	6.78476300	2.61004700
H	-3.01384300	-5.72983200	1.74560300	H	-8.05888900	5.39567200	1.89952300

H	-7.75006900	2.95454900	1.52561900
H	-5.52915000	1.91666800	1.85436600
O	-0.23863300	3.23336300	1.87002800
O	-0.97860100	1.05533800	1.93469200
H	-2.54894700	3.78430600	3.19887800
H	-0.69965100	2.13235200	-0.06021100
H	0.66053600	2.84929500	1.86280700

**TS2a**

C	0.75780600	-0.95678700	2.88594200
C	1.88809700	-0.12861200	2.91371800
H	2.27306100	0.28082900	1.98598800
C	2.54105500	0.15764800	4.12000100
C	2.03907600	-0.39113100	5.30398000
H	2.54276600	-0.17468300	6.24510300
C	0.90951700	-1.21810800	5.30867800
C	0.28271900	-1.49989600	4.08991000
H	-0.57929600	-2.15871500	4.08493000
C	3.75550200	1.05797200	4.13886900
H	3.46636300	2.11690700	4.10863800
H	4.40102200	0.87372000	3.27278200
H	4.35267600	0.90847100	5.04480300
C	0.37221000	-1.78456900	6.60399100
H	-0.25728900	-2.66282500	6.42637000
H	-0.24052100	-1.04607800	7.13860600
H	1.18231600	-2.08014400	7.28059700
C	-1.59797900	-2.15162600	1.72882700
C	-1.90780400	-3.48631600	1.44451300
H	-1.19373500	-4.10611600	0.91196900
C	-3.12919300	-4.04678800	1.84110100
C	-4.03458900	-3.25057200	2.54972000
H	-4.97743500	-3.68303900	2.88126900
C	-3.75651000	-1.91039600	2.84633900
C	-2.53802100	-1.37248400	2.41962400
H	-2.31151500	-0.33542200	2.64850700
C	-3.46241300	-5.47823900	1.48790900
H	-4.23898300	-5.88506000	2.14440700
H	-2.58165200	-6.12581500	1.56238500
H	-3.83133200	-5.55042200	0.45604300
C	-4.73894000	-1.06324800	3.62398200
H	-5.71229800	-1.55729400	3.71104800
H	-4.89466000	-0.09140600	3.14116100
H	-4.37818600	-0.86533100	4.64206300
C	1.03318700	-2.82175500	0.70680900

C	1.92188500	-3.46743000	1.57889100
H	2.02462800	-3.11909100	2.60119300
C	2.68958700	-4.55890100	1.15568700
C	2.54675600	-5.00750200	-0.16274700
H	3.13506500	-5.85959400	-0.50071600
C	1.66557600	-4.38890100	-1.05703900
C	0.91841300	-3.29037600	-0.61036800
H	0.25233600	-2.78329100	-1.29891300
C	3.67125500	-5.22166400	2.09603400
H	4.67393800	-4.78489900	1.99623400
H	3.76293000	-6.29400300	1.89044400
H	3.36760800	-5.10075100	3.14112500
C	1.51140800	-4.90544000	-2.47023700
H	0.69551400	-5.63734700	-2.54189500
H	2.42351100	-5.40299100	-2.81702800
C	-2.17845100	1.63570100	-2.63118100
C	-1.54445100	2.87328500	-2.81939700
H	-0.98079700	3.32251900	-2.00907400
C	-1.63751100	3.56150900	-4.03304600
C	-2.38188300	2.99254600	-5.07362500
H	-2.46344600	3.52222900	-6.02184600
C	-3.02615100	1.76256000	-4.92012700
C	-2.92311400	1.09743500	-3.68990500
H	-3.43583900	0.14951300	-3.57082500
C	-0.92903300	4.88394100	-4.22288100
H	-0.73427900	5.37321700	-3.26307600
H	-1.51748800	5.57001500	-4.84284700
H	0.03950900	4.74637600	-4.72214400
C	-3.80295400	1.14639100	-6.06221800
H	-3.15176900	0.53578000	-6.70229200
H	-4.25587500	1.91360600	-6.69996100
H	-4.60270200	0.49283800	-5.69742200
C	-3.32416600	1.80007700	-0.00805500
C	-4.49698400	2.28425600	-0.61304400
H	-4.68399800	2.08133000	-1.66365400
C	-5.42731300	3.03506800	0.11008100
C	-5.16181100	3.31403200	1.45973100
H	-5.87375500	3.91198400	2.02686600
C	-4.00130600	2.85935100	2.08961000
C	-3.08632100	2.09833600	1.34049500
H	-2.16057000	1.76670000	1.80027500
C	-6.69176800	3.54636200	-0.54262100
H	-6.70594900	3.32341800	-1.61386100
H	-6.79165600	4.63217700	-0.42416600

H	-7.58450300	3.09117600	-0.09466300
C	-3.73013900	3.16347300	3.54605800
H	-2.66204200	3.32486300	3.72700700
H	-4.04339800	2.33116500	4.19034400
H	-4.27254500	4.05522100	3.87731500
C	-2.92546800	-0.79456100	-1.29813000
C	-4.20079900	-1.10223100	-0.81906200
H	-4.72418600	-0.40122000	-0.17689100
C	-4.83359200	-2.30601100	-1.16679000
C	-4.16656300	-3.19043200	-2.01638400
H	-4.65931900	-4.11532500	-2.31323100
C	-2.88229400	-2.91251700	-2.50812300
C	-2.26808500	-1.71418300	-2.13542400
H	-1.28142300	-1.47353100	-2.52348000
C	-2.18354100	-3.89472900	-3.42060400
H	-1.37170800	-3.41554100	-3.97699200
H	-2.87919900	-4.33222900	-4.14611300
H	-1.74626500	-4.72562600	-2.85129700
C	-6.20817500	-2.62818700	-0.62754400
H	-6.87429900	-1.75901200	-0.67926900
H	-6.15298100	-2.93126300	0.42583800
H	-6.67642400	-3.44614400	-1.18520400
Ru	0.11298200	0.63070900	-0.19483800
P	0.00790700	-1.36192100	1.23522000
P	-2.06476400	0.80866700	-0.95659500
H	1.28087500	-4.09463500	-3.16914300
H	0.41097300	2.15458700	-0.89831400
C	2.14240100	-0.31022500	-1.44919500
C	3.30113300	-0.82549000	-2.27644200
C	4.51206100	-1.25955800	-1.42680300
C	5.66035700	-1.76258000	-2.27539500
C	5.81147300	-3.13051400	-2.54138400
C	6.85018000	-3.59562700	-3.35006600
C	7.75982400	-2.69585700	-3.90887500
C	7.62331200	-1.33010300	-3.65013000
C	6.58359300	-0.87089400	-2.84036100
H	2.93937200	-1.65014300	-2.89874300
H	3.60042500	-0.02437800	-2.96734000
H	4.83112300	-0.40755800	-0.81740600
H	5.10866700	-3.83572200	-2.10221000
H	6.95160900	-4.66134800	-3.54022100
H	8.57093700	-3.05561600	-4.53655500
H	8.33024200	-0.62181400	-4.07503600
H	6.48796600	0.19415200	-2.63803600

O	0.94735200	-0.44762700	-1.87735900
O	2.33948600	0.27722400	-0.33818700
H	4.19158500	-2.04230400	-0.72983000
C	0.38516700	2.97357900	0.48081800
C	1.79639800	3.53238300	0.35141100
C	2.15094900	4.41336700	1.57310700
C	3.52628700	5.03350500	1.44910200
C	4.68211300	4.27314100	1.68159400
C	5.95144900	4.83599700	1.54577000
C	6.08924100	6.17525200	1.17294900
C	4.94800700	6.94356000	0.93768600
C	3.67984800	6.37516500	1.07474000
H	-1.40537600	3.61488400	0.51449200
H	2.48989500	2.69327400	0.26643700
H	1.86305600	4.12388000	-0.56745200
H	1.39709500	5.20191300	1.67602100
H	4.58428500	3.23035600	1.97485400
H	6.83372800	4.22954100	1.73482000
H	7.07735700	6.61589300	1.06934500
H	5.04318200	7.98764000	0.64995500
H	2.79482000	6.98133700	0.89279100
O	0.08737500	2.11565300	1.39357700
O	-0.54732200	3.94150000	0.18088800
H	2.09165600	3.79114200	2.47438600

**Int3**

C	-1.04346400	-0.51810800	-3.15597400
C	-1.59616300	0.75758900	-3.35315500
H	-2.03682700	1.28171800	-2.50935800
C	-1.60464100	1.35329900	-4.62072700
C	-1.03965000	0.65019700	-5.69012900
H	-1.03706100	1.10438700	-6.67975600
C	-0.48182800	-0.62367700	-5.52370600
C	-0.49140300	-1.20057200	-4.24866200
H	-0.06618000	-2.18981400	-4.11436300
C	-2.23616700	2.71105700	-4.82886700
H	-2.05271100	3.37301000	-3.97594200
H	-3.32501900	2.62818600	-4.94528500
H	-1.84705200	3.19930800	-5.72847900
C	0.13980600	-1.35117600	-6.69459500
H	-0.41635800	-1.17010600	-7.62120200
H	0.17068300	-2.43224000	-6.52328800
H	1.17216400	-1.01801800	-6.86620900
C	-0.41228100	-2.89153500	-1.55292100

C	-1.18472000	-4.02927900	-1.30970000	H	-1.89272700	4.09484300	4.31117400
H	-2.22681800	-3.92960900	-1.02576400	C	-0.65863000	-0.44004000	6.81567200
C	-0.63164500	-5.31577800	-1.41584600	H	-0.21546800	0.11860400	7.64842400
C	0.71039400	-5.44013400	-1.77732800	H	-0.18953400	-1.42890500	6.78505500
H	1.14378000	-6.43458400	-1.87557700	H	-1.71992300	-0.58734800	7.05673300
C	1.51647900	-4.31556900	-2.01452700	C	2.46700100	-0.77632400	1.99821000
C	0.94795700	-3.04638300	-1.88689400	C	3.05139000	-0.11274700	3.08482000
H	1.56651500	-2.16719100	-2.04533100	H	2.43684400	0.48620700	3.74801100
C	-1.48229000	-6.53249300	-1.13115000	C	4.42783300	-0.20099300	3.33321500
H	-0.94971100	-7.45887100	-1.36958400	C	5.21423700	-0.97857000	2.47845500
H	-2.41128300	-6.51922200	-1.71391100	H	6.28403800	-1.05742700	2.66505900
H	-1.76701600	-6.57194400	-0.07211700	C	4.66106700	-1.65395600	1.38267700
C	2.96750100	-4.48135300	-2.40766900	C	3.28735800	-1.53376500	1.14595300
H	3.46745600	-3.51215500	-2.49859100	H	2.85746500	-2.02302300	0.27871300
H	3.06352500	-4.99794400	-3.37137700	C	5.04505700	0.55260100	4.48998200
H	3.51823800	-5.07764400	-1.66952700	H	4.39753900	0.52982800	5.37352200
C	-2.86612300	-1.29804200	-1.09312100	H	5.20572200	1.60883700	4.23608000
C	-3.70262300	-2.04071300	-1.94539800	H	6.01633900	0.13134000	4.76995300
H	-3.28064000	-2.55720300	-2.80387200	C	5.52497000	-2.50822500	0.48207900
C	-5.07662300	-2.12315500	-1.71123800	H	5.51676600	-3.55972300	0.80000600
C	-5.60839100	-1.43342900	-0.61018700	H	6.56803200	-2.17445200	0.49326600
H	-6.67873600	-1.49212900	-0.41728700	H	5.17015600	-2.47881700	-0.55362600
C	-4.80798700	-0.65813800	0.23245500	C	-0.02364800	-2.31957200	1.93921900
C	-3.42736300	-0.59306900	-0.02396100	C	0.77781500	-3.46188100	2.04110900
H	-2.79222700	0.05158100	0.57552900	H	1.85343100	-3.38509600	1.93145400
C	-5.97457700	-2.94147800	-2.61179600	C	0.21671200	-4.71864900	2.30577500
H	-5.43917200	-3.28637400	-3.50212900	C	-1.16629500	-4.81184600	2.48632400
H	-6.84288700	-2.36110100	-2.94599000	H	-1.60920100	-5.78116900	2.71013300
H	-6.36184500	-3.82823500	-2.09296900	C	-1.99546300	-3.68623200	2.40055100
C	-5.41117700	0.11770600	1.38250700	C	-1.40933900	-2.44783600	2.12144300
H	-4.77404400	0.07457800	2.27269300	H	-2.04192400	-1.56815400	2.07060500
H	-6.39909600	-0.27083700	1.65189900	C	-3.48504900	-3.79428600	2.63740900
C	0.01837700	0.28420700	3.11692000	H	-3.75446900	-3.43323700	3.63889700
C	-0.22003800	1.66143200	3.06323600	H	-3.82725400	-4.83173900	2.56065000
H	-0.14780200	2.19326700	2.12328100	H	-4.04864200	-3.19411200	1.91476000
C	-0.58362600	2.37054000	4.21770000	C	1.09683400	-5.94551100	2.37618100
C	-0.71301600	1.67442900	5.42312400	H	1.34794300	-6.30445900	1.36936100
H	-0.99343800	2.21852700	6.32456800	H	0.60135700	-6.76613200	2.90568100
C	-0.48888700	0.29362400	5.50383200	H	2.04155400	-5.73274200	2.88918700
C	-0.11669900	-0.39081200	4.34288900	Ru	0.33321900	0.36315700	-0.40636900
H	0.07570600	-1.45769900	4.40257000	P	-1.05091300	-1.16322900	-1.41493000
C	-0.83257600	3.86080000	4.14731700	P	0.65231100	-0.61589300	1.62734600
H	-0.54984800	4.25556200	3.16762400	H	-5.53309000	1.17863700	1.12957000
H	-0.26313300	4.39782000	4.91623800	C	2.78754900	1.04561500	-0.88521300



C	4.21140400	1.45226900	-1.19872800	C	2.30618400	1.12297800	2.21903700
C	4.40567600	2.97236300	-1.36689100	H	2.56110300	1.03887000	1.16861200
C	5.85387600	3.34334700	-1.60661400	C	3.11955400	1.88819200	3.06430700
C	6.71125300	3.61497600	-0.53113200	C	2.78753600	1.97270200	4.42109600
C	8.05507300	3.92629700	-0.74386800	H	3.41736400	2.56136400	5.08679400
C	8.56658200	3.97239400	-2.04246300	C	1.67014400	1.31426800	4.94472900
C	7.72377900	3.70622700	-3.12343500	C	0.87564400	0.55046600	4.08074100
C	6.38070000	3.39501200	-2.90458900	H	0.01789500	0.02678500	4.48886400
H	4.83437400	1.08869100	-0.36914400	C	4.32039300	2.62490400	2.51413200
H	4.53699900	0.90897500	-2.09183000	H	4.04990300	3.63570600	2.18056900
H	3.78730700	3.32098400	-2.20339700	H	4.74591200	2.10419900	1.65000200
H	6.31739300	3.58837900	0.48290700	H	5.10655700	2.73135800	3.26996500
H	8.70104300	4.13932900	0.10420900	C	1.31371400	1.43803400	6.40935500
H	9.61155900	4.21906800	-2.21089600	H	0.76059900	0.56134000	6.76311600
H	8.11049400	3.74592200	-4.13869600	H	0.68066800	2.31693400	6.59227100
H	5.72863300	3.19531800	-3.75264000	H	2.20827700	1.54883100	7.03230600
O	2.35110300	-0.08827500	-1.26409500	C	-1.31946100	-0.94673500	2.60964700
O	2.02633400	1.81689300	-0.20906000	C	-1.49499900	-2.17220300	3.26920400
H	4.02882300	3.47354000	-0.46967500	H	-0.78417600	-2.97676600	3.11425300
C	-0.97898900	2.87638700	-0.40090300	C	-2.56834200	-2.37326600	4.14394900
C	-2.27480300	3.68942600	-0.55890900	C	-3.46981800	-1.32020500	4.34989800
C	-3.08480600	3.82477800	0.74234100	H	-4.30171100	-1.46040500	5.03854600
C	-4.40097600	4.54640200	0.54172300	C	-3.32043200	-0.08588700	3.70852200
C	-4.60270300	5.84219400	1.03520400	C	-2.23634300	0.08769100	2.83596700
C	-5.81404500	6.51008300	0.83971800	H	-2.09583700	1.04647100	2.34585700
C	-6.85223700	5.89088400	0.14233800	C	-2.75204500	-3.69514200	4.85551400
C	-6.66689000	4.59991500	-0.35896900	H	-3.01715900	-3.54853600	5.90908500
C	-5.45438500	3.93871800	-0.16090200	H	-1.83922800	-4.29798100	4.81736200
H	-2.01579000	4.68374800	-0.94326800	H	-3.55631800	-4.28748600	4.39995000
H	-2.89215900	3.19635400	-1.32006000	C	-4.29333000	1.04352600	3.95973200
H	-3.26156100	2.81879900	1.13930200	H	-5.03793500	0.76670100	4.71320900
H	-3.79913500	6.33186400	1.58113100	H	-4.82422900	1.32211600	3.04225700
H	-5.94600200	7.51472700	1.23427700	H	-3.77472900	1.94241000	4.31519500
H	-7.79639400	6.40769900	-0.00930100	C	1.06122100	-2.21376000	1.54537400
H	-7.46863100	4.10687600	-0.90366700	C	2.18187800	-2.45539700	2.35306600
H	-5.31778400	2.93569100	-0.56084600	H	2.54904100	-1.67824900	3.01570000
O	-0.10013100	3.63884200	0.44095200	C	2.83841900	-3.69278600	2.32670000
O	-1.25446200	1.60882700	0.07452200	C	2.34316200	-4.69412700	1.48274400
H	-2.48026000	4.35571000	1.48446700	H	2.83518400	-5.66585500	1.46654400
H	-0.49665000	2.82845400	-1.40485200	C	1.22823800	-4.48103100	0.66296800
H	0.78146400	3.23407400	0.34700600	C	0.59795600	-3.23149200	0.69922000
				H	-0.25922200	-3.05396000	0.05726600
				C	4.06106100	-3.93860800	3.18271000
				H	4.98464400	-3.83515300	2.59775700
<b>Int4</b>							
C	1.17864200	0.45137500	2.71467900				

H	4.05853900	-4.95007300	3.60505800	H	-3.70019900	-5.54304900	-0.87616800
H	4.11888000	-3.22567500	4.01152300	C	-2.70329600	-4.04676200	-2.05577800
C	0.72810600	-5.56593100	-0.26403400	C	-2.33825900	-2.69410600	-2.12138500
H	-0.35794400	-5.50992700	-0.39157500	H	-1.81993600	-2.33737700	-3.00470400
H	0.97970500	-6.56354900	0.11258600	C	-2.34959300	-4.98603000	-3.18700700
C	-2.20400000	0.35005400	-2.98539400	H	-1.27537700	-5.21176300	-3.19536800
C	-1.12757800	-0.03307900	-3.80225300	H	-2.59289200	-4.54709500	-4.16151700
H	-0.26280000	-0.51893100	-3.36002800	H	-2.88651300	-5.93644300	-3.10124400
C	-1.14470000	0.20779900	-5.18029400	C	-4.50000000	-4.14606300	1.31769900
C	-2.25750200	0.84920100	-5.73598600	H	-5.52478800	-4.41891000	1.03306600
H	-2.28234800	1.03704300	-6.80851800	H	-4.56083700	-3.38965100	2.10525000
C	-3.33554800	1.26044800	-4.94620200	H	-4.03719100	-5.04398000	1.74549800
C	-3.29828700	1.00095500	-3.57005800	Ru	0.04024700	0.44433900	-0.51563600
H	-4.13755100	1.31316000	-2.95813100	P	0.16259800	-0.59163100	1.55533500
C	0.03274100	-0.18708500	-6.04312800	P	-2.11236400	-0.02791100	-1.16287700
H	0.76203300	0.63115100	-6.11259100	H	1.17705500	-5.47027300	-1.26190700
H	-0.28026500	-0.43136900	-7.06436800	H	-1.16769900	3.21333900	-1.51046500
H	0.55800900	-1.05505900	-5.63071900	C	2.20535400	-0.71080900	-1.44603100
C	-4.50962600	1.99089000	-5.55884400	C	3.38734100	-1.46298700	-2.02448500
H	-4.68957600	1.66731300	-6.59003900	C	4.57134800	-1.54030300	-1.03459900
H	-4.33403800	3.07485300	-5.58492900	C	5.72501400	-2.35545600	-1.57738500
H	-5.42851300	1.82532800	-4.98622500	C	5.77447300	-3.74282600	-1.37937200
C	-3.57315900	0.88782200	-0.48745600	C	6.81853300	-4.50623600	-1.90385400
C	-4.89418800	0.43896700	-0.66215100	C	7.83551100	-3.89231700	-2.63830500
H	-5.08295900	-0.51699900	-1.14175700	C	7.79997000	-2.51127600	-2.84140500
C	-5.97801800	1.20599400	-0.22637900	C	6.75350400	-1.75230000	-2.31436200
C	-5.71953600	2.44436600	0.38164700	H	3.05403000	-2.46438200	-2.31171600
H	-6.55774400	3.05313800	0.71848600	H	3.71196500	-0.95023100	-2.94044900
C	-4.41728600	2.91532800	0.56807800	H	4.89668100	-0.52110000	-0.80194200
C	-3.34356000	2.11946500	0.13588800	H	4.98619100	-4.22466500	-0.80397800
H	-2.31614000	2.44456700	0.29837500	H	6.84057400	-5.58011000	-1.73542100
C	-7.39910000	0.71862900	-0.40030800	H	8.65114200	-4.48443700	-3.04496400
H	-7.43290700	-0.22347500	-0.95659500	H	8.59018300	-2.02303000	-3.40627000
H	-8.01078400	1.45063500	-0.94207700	H	6.73580200	-0.67556900	-2.47108300
H	-7.88561500	0.54984400	0.56899000	O	1.03663400	-1.20866600	-1.54273500
C	-4.15878000	4.26271900	1.20427000	O	2.37663600	0.40563800	-0.85626500
H	-5.03132900	4.61895900	1.76212900	H	4.21444200	-1.98123300	-0.09615400
H	-3.92265200	5.01928100	0.44433300	C	-0.17674500	3.05429600	-1.04600800
H	-3.30543400	4.22328200	1.89009100	C	0.57896000	4.38663300	-1.00018000
C	-2.64586400	-1.80719300	-1.08311800	C	1.99333500	4.28657400	-0.39601100
C	-3.32834500	-2.29716800	0.04452900	C	2.65319000	5.63840200	-0.22878000
H	-3.57737500	-1.62720200	0.86082600	C	2.45693100	6.38926500	0.93988700
C	-3.71875200	-3.63680400	0.12776500	C	3.03622700	7.65040800	1.09047200
C	-3.39539800	-4.49884300	-0.92977200	C	3.82645000	8.18567100	0.07106400

C	4.03232700	7.44890700	-1.09713200	H	0.42838700	-7.16274400	-2.65874400
C	3.45060300	6.18827800	-1.24235600	H	-0.71397900	-6.83073100	-1.34410000
H	0.61671500	4.81218900	-2.01168300	C	1.91427800	-2.75533400	-4.68803600
H	-0.02109700	5.07247900	-0.38855900	H	1.87400300	-3.46687700	-5.52037500
H	1.91065300	3.77936100	0.57025100	H	2.97228400	-2.63046300	-4.41956500
H	1.84399700	5.97664300	1.73874200	H	1.55346600	-1.78792700	-5.05270700
H	2.87378000	8.21336800	2.00636300	C	-2.43770700	-2.40487900	0.43462200
H	4.28082900	9.16614300	0.18750700	C	-3.82316700	-2.31776700	0.26851700
H	4.64973900	7.85397000	-1.89515300	H	-4.23519000	-1.73454800	-0.54819100
H	3.61957000	5.61864200	-2.15414500	C	-4.70124200	-2.97428100	1.14555600
O	0.44031300	2.11651800	-2.03887900	C	-4.16478200	-3.72584400	2.19166700
O	-0.23607500	2.41430800	0.15248200	H	-4.83733200	-4.24229500	2.87454900
H	2.62988100	3.65434800	-1.03047400	C	-2.78020100	-3.82506200	2.39221300
H	1.40043000	2.07170000	-1.85802700	C	-1.93029800	-3.15622700	1.50926400
<b>Int1'</b>				H	-0.85649200	-3.21835900	1.66445600
C	-2.32720200	-0.84119000	-2.02971000	C	-6.19642200	-2.85434900	0.95460300
C	-2.51404600	0.52690900	-2.23949100	H	-6.54138700	-1.83091700	1.14986200
H	-2.04429500	1.24049400	-1.57640100	H	-6.74066200	-3.52233900	1.62988700
C	-3.30503300	0.98627800	-3.30704900	H	-6.49053400	-3.09978600	-0.07288400
C	-3.90531300	0.05261500	-4.15134400	C	-2.22853900	-4.60981800	3.56068700
H	-4.51606000	0.40276900	-4.98248500	H	-1.17437600	-4.86566800	3.41169200
C	-3.73764300	-1.32869300	-3.96247900	H	-2.78424700	-5.54150600	3.71749200
C	-2.94068500	-1.76073800	-2.90281100	C	2.77450700	-0.19624400	2.39689100
H	-2.78935800	-2.82702000	-2.75837900	C	2.09960300	0.68062000	3.25165400
C	-3.50181100	2.47077400	-3.51630200	H	1.21095500	1.19533300	2.90699400
H	-3.94372500	2.68386900	-4.49533000	C	2.56239900	0.91777500	4.55622100
H	-2.55125300	3.01145800	-3.44543500	C	3.71620200	0.26219800	4.98755200
H	-4.16876900	2.89398300	-2.75346300	H	4.07904100	0.43619900	5.99962700
C	-4.40454700	-2.31696900	-4.89280200	C	4.41956500	-0.61936700	4.15218800
H	-4.11296700	-3.34566100	-4.65817800	C	3.93636300	-0.84173600	2.86141500
H	-4.13886700	-2.12409600	-5.93963300	H	4.46698800	-1.53418100	2.21430100
H	-5.49842100	-2.25685900	-4.82387000	C	1.81674400	1.87590100	5.45680900
C	-0.32955700	-2.77361500	-1.58561900	H	2.16903500	1.81119600	6.49159200
C	-0.38679500	-4.14135400	-1.30619400	H	0.74011300	1.67194900	5.44708000
H	-0.98199600	-4.50278600	-0.47384200	H	1.94807900	2.91354800	5.12380700
C	0.29744100	-5.07032700	-2.10526500	C	5.66254200	-1.32186800	4.65093000
C	1.02681200	-4.60439800	-3.20164100	H	6.41143400	-0.60528200	5.01059700
H	1.53946500	-5.32109100	-3.84168000	H	6.12569000	-1.92247400	3.86157400
C	1.10385700	-3.23817100	-3.50655900	H	5.43370700	-1.99319100	5.48858600
C	0.42202300	-2.33566500	-2.68787600	C	3.32111600	0.41345300	-0.41066700
H	0.44230100	-1.27659300	-2.93337500	C	4.46234200	1.06163700	0.08775800
C	0.25270000	-6.54374200	-1.77236100	H	4.68798900	1.02043200	1.14795400
H	1.02533700	-6.80004400	-1.03504500	C	5.31781100	1.77284000	-0.76043100
				C	5.01867600	1.82061600	-2.12926800

H	5.68144300	2.36698500	-2.79888100	H	1.21860900	3.82352600	-1.82869100
C	3.88844000	1.18902000	-2.65606600	H	0.06156400	4.53640500	-0.71012200
C	3.04139200	0.49498300	-1.78074800	H	1.80134200	4.68455600	1.06658400
H	2.14408000	0.02972900	-2.17402600	H	3.91141900	5.11769800	-1.95408100
C	6.52992900	2.49303900	-0.21322900	H	4.51095100	7.31190400	-2.93829000
H	6.37455400	3.57971600	-0.19979000	H	3.43456800	9.39232000	-2.09727700
H	7.41994600	2.30231600	-0.82453800	H	1.75946200	9.25400300	-0.26196000
H	6.75058700	2.18047100	0.81217900	H	1.16812100	7.05897800	0.71792300
C	3.57199400	1.25254000	-4.13337900	O	0.69122800	2.26312400	0.99059000
H	3.67613000	0.26848000	-4.60867900	O	0.24755100	1.62501800	-1.06186000
H	4.23993600	1.94439400	-4.65652600	H	2.97819700	3.91475600	0.01342000
H	2.54090600	1.58418400	-4.30372200	C	-2.51704300	1.29325400	1.87581600
C	2.62319200	-2.28267500	0.47388100	C	-3.78192500	2.14461900	1.97985900
C	3.49091800	-2.72938000	-0.52584500	C	-4.93246200	1.58748600	1.11109500
H	3.90479000	-2.02302200	-1.23869800	C	-6.17834100	2.44411200	1.17561500
C	3.85966400	-4.08043800	-0.61252700	C	-7.14831200	2.23549800	2.16639500
C	3.35368100	-4.97594700	0.33258300	C	-8.28131900	3.04679100	2.24697100
H	3.65399400	-6.02177400	0.28776600	C	-8.46573400	4.08640200	1.33302800
C	2.47927200	-4.55897000	1.34591600	C	-7.50894000	4.30574900	0.33983500
C	2.12117600	-3.21005900	1.40174800	C	-6.37820900	3.49099600	0.26466300
H	1.47355400	-2.86999100	2.20656400	H	-4.08347500	2.19445700	3.02980100
C	1.93207700	-5.54986200	2.34847800	H	-3.54304000	3.16226100	1.64646000
H	1.67394900	-5.06203800	3.29453800	H	-4.57768400	1.50730700	0.07829900
H	2.65636400	-6.34298000	2.56475400	H	-7.01302200	1.42576700	2.88078800
H	1.02221900	-6.03668700	1.97160600	H	-9.02185800	2.86484200	3.02195800
C	4.77719500	-4.55218800	-1.71684800	H	-9.34856100	4.71762100	1.39228500
H	5.54252900	-3.80396000	-1.95116500	H	-7.64485600	5.10938000	-0.37976700
H	4.21186500	-4.74048400	-2.63941100	H	-5.63808000	3.66659600	-0.51386200
H	5.28508900	-5.48444500	-1.44773400	O	-2.02129900	1.20863400	0.68562600
Ru	-0.13198000	0.21976300	0.50972500	O	-2.05465900	0.74063500	2.89259800
P	-1.26011500	-1.47013200	-0.64666700	H	-5.16374900	0.56843700	1.44754600
P	2.13505600	-0.50403000	0.67892500				
H	-2.29713900	-4.03101500	4.49108900	<b>TS1'</b>			
H	-0.80576000	-0.22037800	2.16912700	C	-2.29973700	-0.77051000	-2.07369500
H	-0.26585600	-0.83287600	1.91171300	C	-2.39858300	0.59908600	-2.32943900
C	0.61860800	2.53700700	-0.24644700	H	-1.89145500	1.30506600	-1.68579200
C	0.96550800	3.91423300	-0.76762800	C	-3.14201900	1.07349100	-3.42416800
C	2.10978400	4.58379900	0.02111200	C	-3.78353600	0.15297600	-4.25221800
C	2.49313900	5.93105800	-0.55231600	H	-4.35886400	0.51407900	-5.10372200
C	3.43649300	6.02519000	-1.58575200	C	-3.70182700	-1.22961900	-4.02068000
C	3.77403700	7.26058400	-2.14046900	C	-2.95308900	-1.67657000	-2.93227600
C	3.17106800	8.42880000	-1.66894900	H	-2.87201600	-2.74510500	-2.75268600
C	2.23075100	8.35009300	-0.63974900	C	-3.24363000	2.56045200	-3.67915300
C	1.89713800	7.11167500	-0.08817600	H	-3.67515900	2.77106500	-4.66335100

H	-2.25949300	3.04011900	-3.62806500	H	4.18310500	0.47129600	5.92243700
H	-3.87774200	3.04980400	-2.92809800	C	4.43594900	-0.66776900	4.11092000
C	-4.40044100	-2.20438200	-4.94205900	C	3.91719100	-0.91398800	2.83848600
H	-4.27520000	-3.23670700	-4.60018800	H	4.40145500	-1.65474300	2.20875200
H	-4.00560400	-2.14236300	-5.96428900	C	1.97622000	1.98952700	5.37071300
H	-5.47669500	-1.99926600	-5.00185500	H	2.38008700	1.97756000	6.38843700
C	-0.46371300	-2.82859700	-1.50366800	H	0.89744100	1.80430900	5.42943300
C	-0.59945500	-4.16707500	-1.12502700	H	2.10447600	3.00393900	4.97189900
H	-1.20894000	-4.43010100	-0.26637200	C	5.65293800	-1.41143500	4.61401100
C	0.02070100	-5.19088000	-1.85655300	H	6.43073600	-0.72008500	4.96123100
C	0.76906700	-4.85095700	-2.98647400	H	6.08845100	-2.04049600	3.83110600
H	1.23306500	-5.64198400	-3.57376900	H	5.40189200	-2.06259000	5.46134400
C	0.92559000	-3.51809000	-3.38990900	C	3.32292600	0.21559800	-0.46775900
C	0.30397900	-2.51867400	-2.63754000	C	4.51950400	0.79990300	-0.02321000
H	0.38486200	-1.48488200	-2.96474200	H	4.76999300	0.78524400	1.03216300
C	-0.11234800	-6.63112900	-1.41834600	C	5.40029100	1.41360100	-0.92036000
H	0.62894800	-6.87322500	-0.64494500	C	5.06932700	1.42781300	-2.28269200
H	0.04760000	-7.32229900	-2.25286300	H	5.75071900	1.89853100	-2.98999200
H	-1.10239100	-6.83361800	-0.99492200	C	3.88348100	0.85901300	-2.75584300
C	1.75476700	-3.16776500	-4.60488500	C	3.01336700	0.26290400	-1.83265100
H	1.76617900	-3.98617900	-5.33290800	H	2.07292400	-0.15043300	-2.18133700
H	2.79809900	-2.96339600	-4.32793700	C	6.67540600	2.06474600	-0.43264200
H	1.37085300	-2.27329400	-5.10715000	H	6.59904300	3.15968800	-0.45753800
C	-2.56879600	-2.22162000	0.44730200	H	7.53216500	1.78748500	-1.05820700
C	-3.94363300	-2.12678600	0.20119900	H	6.90209900	1.77542400	0.59831600
H	-4.30230200	-1.59844000	-0.67558400	C	3.52941800	0.89069800	-4.22553400
C	-4.87746800	-2.70941400	1.07062400	H	3.50737200	-0.11928300	-4.65492800
C	-4.41070200	-3.39930800	2.19217500	H	4.25274600	1.47893300	-4.79937300
H	-5.12768800	-3.86280000	2.86785800	H	2.53640500	1.32824400	-4.38314700
C	-3.04235000	-3.50166500	2.47411900	C	2.46912700	-2.38552000	0.55440500
C	-2.13455300	-2.90323600	1.59566600	C	3.31243200	-2.93220100	-0.41615600
H	-1.07206200	-2.96679700	1.81368600	H	3.76708900	-2.28910900	-1.16363500
C	-6.35957200	-2.57371400	0.80210800	C	3.60596800	-4.30433500	-0.42898000
H	-6.74344100	-1.61086600	1.16518100	C	3.05095100	-5.11829300	0.56136800
H	-6.93132400	-3.36237300	1.30255700	H	3.29412000	-6.17972900	0.57475500
H	-6.57928100	-2.62267700	-0.27008000	C	2.19783700	-4.60000300	1.54577100
C	-2.56086900	-4.20876200	3.72067600	C	1.91354100	-3.23262900	1.52695700
H	-1.56699500	-4.64641700	3.57713400	H	1.27973200	-2.81434700	2.30564900
H	-3.24522300	-5.01118700	4.01714400	C	1.59374300	-5.50336400	2.59738700
C	2.77798900	-0.23153600	2.37068000	H	1.35831600	-4.95053300	3.51309900
C	2.16070100	0.70492200	3.20473300	H	2.27321300	-6.32108600	2.86231000
H	1.29051900	1.24582900	2.85393800	H	0.66039000	-5.96110600	2.24182800
C	2.65982100	0.96767100	4.49093300	C	4.49625000	-4.88479700	-1.50325100
C	3.79140200	0.27634300	4.92503400	H	5.29702200	-4.19043200	-1.78094800

H	3.91931600	-5.09791500	-2.41307700
H	4.95803300	-5.82393300	-1.18019700
Ru	-0.10498900	0.26218000	0.46391500
P	-1.30374400	-1.41245800	-0.64189500
P	2.09506700	-0.57238600	0.67476500
H	-2.48999100	-3.51101300	4.56554600
H	-0.94263100	-0.03948900	2.18728000
H	-0.31541600	-0.65708900	1.90638400
C	0.75331200	2.54594900	-0.31578500
C	1.17707100	3.91000000	-0.81738800
C	2.37547000	4.48953500	-0.03673200
C	2.81504400	5.83571200	-0.57035800
C	3.74998000	5.92189900	-1.61189100
C	4.13872600	7.15888600	-2.12843700
C	3.59625100	8.33669400	-1.60985100
C	2.66466300	8.26601500	-0.57208300
C	2.27991000	7.02604500	-0.05890900
H	1.40567300	3.82627600	-1.88443200
H	0.31649500	4.58747200	-0.72773500
H	2.09823200	4.56655000	1.01948400
H	4.17829700	5.00688100	-2.01688100
H	4.86835500	7.20355200	-2.93329300
H	3.89984200	9.30124300	-2.00828800
H	2.24042500	9.17716300	-0.15762400
H	1.55849000	6.97913600	0.75439500
O	0.78533800	2.26974500	0.92503300
O	0.35993600	1.65739700	-1.14110300
H	3.20733100	3.77740900	-0.09171500
C	-2.49069400	1.36349900	1.79614000
C	-3.73427100	2.22416900	1.97709900
C	-4.84975500	1.86128000	0.97175000
C	-6.06824500	2.74743100	1.11341000
C	-7.10885700	2.41005600	1.99013000
C	-8.21805100	3.24327900	2.14493300
C	-8.30607100	4.43456700	1.42185400
C	-7.27760200	4.78343200	0.54394100
C	-6.17131600	3.94591700	0.39318000
H	-4.08899500	2.11965500	3.00595000
H	-3.44346400	3.27207500	1.82871400
H	-4.43907800	1.93436100	-0.04047100
H	-7.04840600	1.48215600	2.55566400
H	-9.01507700	2.96032600	2.82807900
H	-9.16999100	5.08353700	1.53892500
H	-7.33857000	5.70618600	-0.02769100

H	-5.37563500	4.22202100	-0.29616200
O	-1.98421000	1.33039500	0.62373900
O	-2.03179300	0.73608900	2.78984900
H	-5.13176900	0.81159000	1.12323900

**Int2'**

C	-0.72070400	2.27819600	2.00061800
C	-1.71091700	1.39345400	2.43617300
H	-1.89399800	0.47558700	1.89182400
C	-2.45562500	1.65823700	3.59804200
C	-2.19231200	2.82644900	4.31383500
H	-2.75998900	3.03537800	5.21991600
C	-1.20610900	3.73597400	3.90046800
C	-0.47681300	3.44761900	2.74584900
H	0.29639700	4.14075500	2.42647100
C	-3.52716900	0.68857200	4.04341700
H	-3.21807400	-0.34708600	3.86603000
H	-4.46179300	0.84542700	3.48799400
H	-3.75688800	0.80247300	5.10833100
C	-0.93666200	4.99130100	4.70001000
H	-0.14623400	5.59385400	4.24138800
H	-0.62298300	4.75398900	5.72457800
H	-1.83357700	5.61898700	4.77785700
C	1.90991200	2.54573100	1.02857500
C	2.57992000	3.62426100	0.44452400
H	2.15907800	4.11933100	-0.42476900
C	3.78962300	4.09679700	0.97456400
C	4.30800200	3.48099300	2.11709200
H	5.23516400	3.85549300	2.54858500
C	3.66219100	2.39416900	2.72210400
C	2.46923600	1.93293300	2.16046000
H	1.95940700	1.09446400	2.62715000
C	4.52090500	5.23808600	0.30575000
H	5.21249300	5.73341100	0.99568700
H	3.82445400	5.99271900	-0.07678300
H	5.10937800	4.87750800	-0.54852600
C	4.21958100	1.75196200	3.97272300
H	5.29614500	1.92893500	4.06990000
H	4.05192900	0.66919000	3.97240600
H	3.73988100	2.15502300	4.87484900
C	-0.34389300	3.23623800	-0.71480200
C	-1.40632000	4.09253500	-0.40011000
H	-1.87257300	4.03907800	0.57794900
C	-1.88342200	5.03116000	-1.32702600

C	-1.26903400	5.10936000	-2.57929400	H	1.85226600	-2.95522500	5.42210100
H	-1.62446800	5.84212900	-3.30219600	H	0.52887900	-2.18693500	4.52143400
C	-0.20827700	4.26331300	-2.92912500	C	3.36273300	0.08342200	-0.92557700
C	0.23765600	3.32774500	-1.99034200	C	4.51331100	0.21559800	-0.14606500
H	1.04783300	2.65534400	-2.25615000	H	4.60668900	-0.34027200	0.78122900
C	-3.05228000	5.92556000	-0.97776200	C	5.57335100	1.04425400	-0.55035500
H	-3.03396000	6.85473100	-1.55745000	C	5.46051100	1.73479800	-1.75752600
H	-3.05191900	6.18863700	0.08561300	H	6.28586300	2.36324800	-2.08964200
H	-4.01090200	5.43145700	-1.18860800	C	4.31479500	1.62756800	-2.56085700
C	0.41207300	4.33703500	-4.30619000	C	3.27506200	0.80155800	-2.13129800
H	1.45016000	3.98923300	-4.29894600	H	2.39322800	0.68662300	-2.75589900
H	0.39937100	5.36037800	-4.69760400	C	4.22088000	2.38768700	-3.86485700
C	2.25830200	-2.34675300	-1.87381900	H	5.14030700	2.28810900	-4.45410100
C	1.21149100	-3.17677500	-2.28627500	H	4.06619900	3.46145700	-3.69295700
H	0.22930100	-3.05934900	-1.84281100	H	3.38926100	2.02697300	-4.47879800
C	1.40822400	-4.15275500	-3.27716500	C	6.80680800	1.17738500	0.31264400
C	2.67276900	-4.28597800	-3.85115200	H	7.12996500	0.20550300	0.70337300
H	2.83240500	-5.03909100	-4.62170700	H	6.61096700	1.82482500	1.17693100
C	3.74217800	-3.46643500	-3.46303100	H	7.64255800	1.61239800	-0.24563200
C	3.52119400	-2.50197000	-2.47723800	Ru	-0.16510400	-0.21176600	-0.39736600
H	4.34528900	-1.85853100	-2.18692200	P	0.25718000	1.91659800	0.45454300
C	0.25623500	-5.03210900	-3.70941500	P	1.98184500	-1.09092500	-0.51511000
H	-0.15025800	-5.60114700	-2.86424600	H	-0.13669800	3.70910800	-5.02087900
H	0.56386900	-5.74818800	-4.47874200	H	0.25490700	0.36807000	-1.85970300
H	-0.56837200	-4.43418200	-4.11689100	C	-1.49551200	-2.30647100	0.48222200
C	5.10030400	-3.61891100	-4.11128700	C	-2.37695500	-3.46833800	0.91227700
H	5.47685300	-4.64542800	-4.01877600	C	-2.06035200	-4.78365500	0.17108300
H	5.83752100	-2.94946400	-3.65644600	C	-2.96854100	-5.91970700	0.59059500
H	5.06032300	-3.38863800	-5.18385900	C	-2.66448600	-6.70807400	1.70962300
C	2.59556600	-1.99584600	0.98757900	C	-3.51620000	-7.73505900	2.11893400
C	3.67967400	-2.89035500	0.95027300	C	-4.69277900	-7.99357100	1.41234200
H	4.18694300	-3.08749800	0.01072100	C	-5.00778000	-7.21811200	0.29480300
C	4.11187000	-3.54929600	2.10340600	C	-4.15182500	-6.19216900	-0.10992300
C	3.43436400	-3.30710600	3.30859000	H	-2.27679000	-3.59355000	1.99484500
H	3.75715300	-3.82507700	4.21086500	H	-3.42198100	-3.18705800	0.71996600
C	2.34605900	-2.43546600	3.37594600	H	-2.14820900	-4.60395500	-0.90526200
C	1.93412200	-1.78551000	2.20135600	H	-1.74660500	-6.51678800	2.26205400
H	1.05846500	-1.14563700	2.22244900	H	-3.25866600	-8.33668400	2.98709900
C	5.27871200	-4.51062900	2.06101900	H	-5.35583200	-8.79507200	1.72732600
H	6.11244900	-4.15815100	2.68210200	H	-5.91810600	-7.41484300	-0.26610600
H	5.65421200	-4.63725300	1.04072000	H	-4.40072400	-5.59619700	-0.98581600
H	4.99537800	-5.50114300	2.43815300	O	-1.07021400	-1.48121500	1.34053100
C	1.61355000	-2.18985900	4.67605200	O	-1.20869600	-2.16012800	-0.75381100
H	1.87859700	-1.21536400	5.10767700	H	-1.01383600	-5.05360200	0.36159500

C	-2.77899700	0.69818900	-1.69373500
C	-4.21990000	1.10041000	-1.89722800
C	-5.07136300	1.01914600	-0.61946200
C	-6.49575900	1.47449600	-0.85855000
C	-7.46731500	0.57803100	-1.32504500
C	-8.77271100	1.00173200	-1.57834800
C	-9.12961600	2.33521900	-1.36710400
C	-8.17282800	3.23842000	-0.90005000
C	-6.86847700	2.80919700	-0.64840600
H	-4.21460500	2.12452600	-2.29402700
H	-4.63801900	0.47631500	-2.69601500
H	-5.06043300	-0.01312400	-0.25085900
H	-7.19852400	-0.46424600	-1.48530100
H	-9.51201600	0.28948200	-1.93562000
H	10.14643300	2.66656400	-1.56014100
H	-8.44283200	4.27690800	-0.72603600
H	-6.13003600	3.51675300	-0.27598400
O	-2.29493700	0.49363800	-0.57432400
H	-4.59989600	1.62945200	0.15785800
O	-2.08055900	0.60662800	-2.80695200
H	-1.13220200	0.39689000	-2.52295500

**TS2'**

C	1.90730800	2.86526900	-1.21972500
C	0.91551700	3.33646900	-2.08891600
H	0.18180300	2.64407600	-2.48926300
C	0.84610700	4.69344000	-2.43474700
C	1.77998700	5.57696900	-1.88719300
H	1.72679000	6.63432900	-2.14353300
C	2.78027800	5.13650700	-1.01147900
C	2.83561900	3.77670400	-0.68840500
H	3.60956500	3.43364400	-0.00960400
C	-0.21448100	5.17986000	-3.39676200
H	-1.15310800	4.63195200	-3.26269800
H	0.09771900	5.03400300	-4.43974300
H	-0.41827000	6.24788800	-3.26366800
C	3.76288300	6.11632000	-0.40959600
H	4.61628500	5.60045800	0.04251500
H	3.29139700	6.72186100	0.37585600
H	4.14926500	6.81276600	-1.16318000
C	3.08128600	1.03201400	0.65056700
C	4.36512700	0.47757700	0.65514700
H	4.75479100	0.00255400	-0.23924400
C	5.17163900	0.53445400	1.80016700

C	4.66929800	1.16585400	2.94193000
H	5.29508600	1.23240400	3.83061900
C	3.38494200	1.72511900	2.96954900
C	2.60018700	1.65060200	1.81440000
H	1.61341700	2.10420700	1.80961200
C	6.54943900	-0.08676000	1.79476900
H	7.15948800	0.28149600	2.62636200
H	7.08369000	0.12797400	0.86208100
H	6.48551400	-1.17891600	1.88649900
C	2.85206100	2.38610800	4.22026600
H	3.65150300	2.58019900	4.94295000
H	2.10455600	1.74990300	4.71146000
H	2.36294500	3.34017600	3.99220800
C	3.14752900	0.44329400	-2.18523800
C	4.14618400	1.27516600	-2.72504800
H	4.24552300	2.29631300	-2.37092900
C	5.01274000	0.81349200	-3.71764700
C	4.85603900	-0.50033300	-4.18716200
H	5.51172600	-0.86237800	-4.97764900
C	3.86760600	-1.34710900	-3.68411800
C	3.02882100	-0.86342700	-2.66657600
H	2.23998900	-1.50067600	-2.28276800
C	6.09047600	1.70684700	-4.28923200
H	7.09076500	1.29416100	-4.10597200
H	6.05578700	2.70700700	-3.84643000
H	5.98363900	1.81760000	-5.37546700
C	3.65241700	-2.73142800	-4.25061500
H	3.67231800	-3.49869100	-3.46780900
H	4.41775600	-2.98585600	-4.99079200
C	-0.97750300	-2.76950000	0.96267600
C	-2.36696700	-2.56134200	0.91500600
H	-2.75794000	-1.55076400	0.96885200
C	-3.25590500	-3.63252900	0.78620900
C	-2.73458700	-4.93115400	0.69650100
H	-3.41876900	-5.77346400	0.60454800
C	-1.35904200	-5.16986000	0.73393900
C	-0.48841700	-4.07814000	0.87796000
H	0.57731800	-4.26980500	0.93958100
C	-4.74770200	-3.39531900	0.72303800
H	-5.01434700	-2.42230200	1.14741900
H	-5.29981400	-4.16906400	1.26913800
H	-5.10313400	-3.41004000	-0.31521500
C	-0.80914600	-6.57409200	0.61677800
H	-1.55094500	-7.32152100	0.91782300



H	0.08118200	-6.70987400	1.24098800	C	-5.56799200	3.33041100	0.67314300
H	-0.51663100	-6.80320800	-0.41692900	C	-6.53179300	2.81128900	1.54868800
C	-0.46005200	-0.77662500	2.91450100	C	-7.51681200	3.63147200	2.10185400
C	-0.79347200	-1.75866500	3.86424900	C	-7.55494200	4.99112600	1.78670800
H	-0.72103500	-2.80981900	3.60082700	C	-6.60228400	5.52192200	0.91426600
C	-1.23041800	-1.41173200	5.14487400	C	-5.61988100	4.69716800	0.36435700
C	-1.34154900	-0.05185100	5.46848200	H	-3.42852800	2.15037800	1.98069400
H	-1.69615600	0.23017300	6.45913900	H	-2.79026300	3.49038300	1.02897800
C	-1.02194700	0.94887300	4.54813000	H	-4.23168300	2.76617300	-0.91629000
C	-0.57680500	0.57138700	3.27039600	H	-6.51216200	1.75131600	1.79398000
H	-0.36157900	1.33863600	2.53660700	H	-8.25771900	3.20702600	2.77480700
C	-1.59534600	-2.47357000	6.15809100	H	-8.32318100	5.63070000	2.21334700
H	-1.01267800	-2.36444400	7.08140700	H	-6.62676900	6.57807400	0.65760500
H	-1.41545200	-3.47899100	5.76497300	H	-4.88434900	5.11677400	-0.31916100
H	-2.65451700	-2.41054300	6.43821600	O	-0.88852800	1.94506400	0.46153100
C	-1.14533100	2.41066800	4.91852600	O	-2.38691400	0.41851600	-0.04239200
H	-0.23139200	2.77983700	5.40305200	H	-4.82449000	1.41058800	0.03238900
H	-1.97207000	2.57839800	5.61749700	C	-0.58192500	-0.34400600	-3.00436600
H	-1.31654000	3.03280500	4.03401500	C	-1.68174100	-1.29275000	-3.50056700
C	1.76779700	-2.03551800	1.54571700	C	-2.91570000	-1.40292600	-2.59898000
C	2.36614000	-2.01693100	2.81082800	C	-4.00792800	-2.22540300	-3.25085400
H	1.86715500	-1.52498000	3.63833300	C	-4.04572000	-3.62027800	-3.10345700
C	3.60458500	-2.63133200	3.03685900	C	-5.03446000	-4.38350900	-3.72802700
C	4.23503000	-3.28204800	1.97183400	C	-6.00667700	-3.76352900	-4.51586600
H	5.18701400	-3.78239800	2.14231300	C	-5.98221400	-2.37591300	-4.67086200
C	3.67046700	-3.30914800	0.69103000	C	-4.99224700	-1.61765200	-4.04332000
C	2.43953400	-2.67350900	0.49243300	H	-1.97159000	-0.89148700	-4.48095300
H	1.98602300	-2.69203700	-0.49448200	H	-1.23979000	-2.27818700	-3.68531800
C	4.37743800	-3.99663100	-0.45504300	H	-2.62921500	-1.85391600	-1.64440200
H	5.22198000	-4.59698600	-0.10151200	H	-3.29599200	-4.10888900	-2.48437000
H	4.76681900	-3.26536600	-1.17483400	H	-5.04690200	-5.46292500	-3.59690900
H	3.69998700	-4.66159900	-1.00420300	H	-6.77851200	-4.35559500	-5.00086000
C	4.24682400	-2.57246600	4.40365100	H	-6.73759100	-1.88207200	-5.27727600
H	3.50591700	-2.69761300	5.20124200	H	-4.98269300	-0.53627700	-4.16385800
H	4.73381900	-1.60154800	4.56430200	O	-0.89682600	0.84571200	-2.57196600
H	5.00939700	-3.34924400	4.52401400	H	-3.27604000	-0.39642400	-2.36951900
Ru	-0.17883600	0.20429700	-0.62458000	O	0.45788800	-0.43079600	-3.92342600
P	1.99326800	1.04086400	-0.85132900	H	1.03582800	0.33629000	-3.77244400
P	0.11009200	-1.26935400	1.20921800				
H	2.67265600	-2.79541300	-4.74005600	<b>Int3'</b>			
H	-0.07928400	-1.03757200	-1.89773600	C	1.90148200	2.78603800	-1.42966800
C	-2.10805400	1.56324300	0.42406000	C	0.89031000	3.20345400	-2.30258500
C	-3.19371200	2.47545600	0.95716800	H	0.13763200	2.49176800	-2.62768900
C	-4.47886600	2.44668200	0.10373200	C	0.83054700	4.53152500	-2.75164300

C	1.80049500	5.43545900	-2.31355400	H	4.32065300	-3.34512500	-4.77158600
H	1.76151000	6.46755300	-2.65974200	H	2.58197300	-3.09002800	-4.53208100
C	2.82175600	5.04818500	-1.43529200	C	-0.93313400	-2.74899600	1.09163200
C	2.86136900	3.72039100	-1.00066900	C	-2.32322300	-2.56713100	0.98973800
H	3.65018100	3.41835400	-0.31940200	H	-2.73186300	-1.56204000	0.97759500
C	-0.28624800	4.97109000	-3.67143700	C	-3.19165900	-3.65915500	0.89615900
H	-0.04820900	5.91711900	-4.16946700	C	-2.64819600	-4.95147300	0.89507100
H	-1.22120800	5.11646800	-3.11447400	H	-3.31623800	-5.80908500	0.83001600
H	-0.48848000	4.21954400	-4.44240600	C	-1.27089900	-5.16467100	0.98765700
C	3.85022900	6.05176900	-0.96343100	C	-0.42206700	-4.05241300	1.09720200
H	4.64174700	5.56968600	-0.38064600	H	0.64372500	-4.22267100	1.20390100
H	3.39426500	6.82236000	-0.32825300	C	-4.68447400	-3.45030200	0.77930300
H	4.32194400	6.57069600	-1.80701600	H	-4.98178800	-2.47377200	1.17435600
C	3.05019500	1.11284900	0.59069900	H	-5.24015400	-4.22276200	1.32333200
C	4.33221700	0.55967800	0.66025100	H	-5.00630600	-3.49178600	-0.26911700
H	4.73201000	0.00674000	-0.18348600	C	-0.69713700	-6.56396000	0.96387400
C	5.12638400	0.72003600	1.80482500	H	-1.42917300	-7.30346100	1.30575600
C	4.61147900	1.45021900	2.87946200	H	0.19005700	-6.64538700	1.60173100
H	5.22742800	1.59727100	3.76544500	H	-0.39272300	-6.85266600	-0.05133100
C	3.32678600	2.00965800	2.84195400	C	-0.47563300	-0.65134700	2.95496300
C	2.55607600	1.83409300	1.68910300	C	-0.84403000	-1.58952000	3.93518100
H	1.57244400	2.29082800	1.62974200	H	-0.78509700	-2.65118100	3.71459700
C	6.50524400	0.10451900	1.86915100	C	-1.29945100	-1.18524500	5.19249500
H	7.10498100	0.54604600	2.67204600	C	-1.39331200	0.18775000	5.46016100
H	7.04947700	0.23849700	0.92718200	H	-1.76294900	0.51475000	6.43129200
H	6.44169800	-0.97541700	2.05519600	C	-1.03685900	1.14624000	4.50869100
C	2.78197800	2.77553300	4.02587600	C	-0.57293800	0.71163500	3.25630200
H	3.58786100	3.16711500	4.65590100	H	-0.32405400	1.44476200	2.49897100
H	2.15398000	2.13083600	4.65491200	C	-1.70081900	-2.20075800	6.23883900
H	2.16034300	3.61877900	3.70567700	H	-1.54267500	-3.22361000	5.88315600
C	3.13778200	0.28427000	-2.18887200	H	-2.76049100	-2.10128500	6.50601100
C	4.17278300	1.04799200	-2.76082100	H	-1.12387000	-2.07376700	7.16350400
H	4.30068400	2.08618000	-2.47127100	C	-1.14325900	2.62280600	4.82136500
C	5.03900400	0.49757100	-3.70702400	H	-0.23944100	2.99263700	5.32381700
C	4.84543100	-0.83708900	-4.09807500	H	-1.98975500	2.83100300	5.48500200
H	5.50163300	-1.26899000	-4.85218900	H	-1.27281900	3.21534400	3.90987700
C	3.81889600	-1.61673900	-3.56459000	C	1.78999400	-1.93512500	1.68102500
C	2.97995000	-1.04306400	-2.59524100	C	2.37621400	-1.81900100	2.94657400
H	2.16181800	-1.62868300	-2.19121700	H	1.85982300	-1.28148100	3.73425800
C	6.15353200	1.31913000	-4.31462800	C	3.62391200	-2.39263100	3.22368800
H	6.16582500	2.33575900	-3.90971700	C	4.27769200	-3.09944000	2.20980400
H	6.04634200	1.39452400	-5.40395000	H	5.23788800	-3.56726200	2.42126600
H	7.13497500	0.86870200	-4.11944800	C	3.72602300	-3.22380000	0.92891400
C	3.56414000	-3.02558600	-4.04778400	C	2.48408200	-2.62943900	0.67861500

H	2.04140000	-2.73001300	-0.30826100
C	4.45654500	-3.97195900	-0.16315700
H	5.32256000	-4.51230600	0.23280800
H	4.81799800	-3.28554300	-0.93945900
H	3.80327000	-4.70187200	-0.65639900
C	4.24950400	-2.23180300	4.59006800
H	3.50854900	-2.35564900	5.38798200
H	4.68368200	-1.22991900	4.70514600
H	5.04975000	-2.96104700	4.75451100
Ru	-0.18355300	0.16049000	-0.63581300
P	1.98046400	0.99625100	-0.91846900
P	0.12351800	-1.21877400	1.28400800
H	3.56450800	-3.74534900	-3.22046700
H	-0.14389600	-1.14561100	-1.94727100
C	-2.09565500	1.55893100	0.37157200
C	-3.15677100	2.50862800	0.88583300
C	-4.45452700	2.46606600	0.05187800
C	-5.52985800	3.37219800	0.61217700
C	-6.48304600	2.88261500	1.51595200
C	-7.45638700	3.72276400	2.05963700
C	-7.49315200	5.07310100	1.70651400
C	-6.55090900	5.57448300	0.80585300
C	-5.58012500	4.72981900	0.26548800
H	-3.38093900	2.22472200	1.92378100
H	-2.73733200	3.51923300	0.91362000
H	-4.21995300	2.75467800	-0.98020400
H	-6.46456600	1.82988500	1.79073700
H	-8.18948800	3.32100700	2.75469200
H	-8.25251000	5.72808500	2.12558700
H	-6.57464800	6.62300400	0.51960000
H	-4.85309100	5.12639700	-0.44048700
O	-0.86801300	1.92612900	0.36980200
O	-2.39395800	0.40029200	-0.03981100
H	-4.80803300	1.43083800	0.01520200
C	-0.59707300	-0.51073800	-2.98370900
C	-1.72595000	-1.42023400	-3.49474100
C	-2.93222800	-1.54957300	-2.55829000
C	-4.04690800	-2.35511500	-3.19258800
C	-4.08997900	-3.75197800	-3.06683800
C	-5.09856700	-4.49953400	-3.67850300
C	-6.08616800	-3.86128500	-4.43175400
C	-6.05696200	-2.47142400	-4.56487300
C	-5.04715500	-1.72905600	-3.95020400
H	-2.03750700	-0.97675600	-4.44920600

H	-1.30456000	-2.40500600	-3.72748500
H	-2.61659700	-2.02405300	-1.62336500
H	-3.32681900	-4.25534800	-2.47640800
H	-5.11402400	-5.58088100	-3.56481400
H	-6.87321000	-4.44097900	-4.90715000
H	-6.82394800	-1.96350300	-5.14451100
H	-5.03321300	-0.64605200	-4.05420800
O	-0.90866400	0.70792100	-2.58240900
H	-3.28192500	-0.54787100	-2.29347700
O	0.43312000	-0.60722900	-3.92969500
H	1.01202600	0.16094200	-3.79236400

#### Int4-acid

C	-0.16259800	-1.71174500	2.80510700
C	1.23490100	-1.69481300	2.71037400
H	1.70616900	-1.51394400	1.75125100
C	2.03550900	-1.92643500	3.83896100
C	1.41606600	-2.16897700	5.06708800
H	2.03315700	-2.35024200	5.94600600
C	0.02228300	-2.18767400	5.19409200
C	-0.75522000	-1.96535000	4.05411000
H	-1.83378600	-2.00102700	4.15045600
C	3.54124200	-1.88645600	3.73178900
H	4.01855600	-2.36234200	4.59494800
H	3.89302400	-0.84995700	3.67839400
H	3.89243900	-2.39528500	2.82670700
C	-0.62561600	-2.43574500	6.53784500
H	-0.16511000	-3.28579200	7.05541000
H	-1.69547900	-2.64370900	6.43384300
H	-0.52190100	-1.56391400	7.19738500
C	-2.88539800	-1.44059300	1.99389400
C	-3.75314400	-2.54146200	1.96618900
H	-3.46979100	-3.43957100	1.42882500
C	-4.98130300	-2.51137600	2.63635900
C	-5.33469400	-1.35046300	3.33531700
H	-6.28550800	-1.31767700	3.86508300
C	-4.49077900	-0.23512900	3.38364300
C	-3.26576900	-0.29427400	2.70428700
H	-2.59359800	0.55678700	2.75112000
C	-5.88538100	-3.72387500	2.64271500
H	-6.94290500	-3.43804700	2.65664600
H	-5.70649100	-4.34658000	3.52961100
H	-5.71480400	-4.35377400	1.76362800
C	-4.88535000	1.00217600	4.15743400

H	-5.80959100	0.84007400	4.72173000	H	-1.67198700	2.51175800	1.61549900
H	-5.04180000	1.85688300	3.48923500	C	-6.66053900	4.16050900	0.32277500
H	-4.10334500	1.29000100	4.87070800	H	-6.95096900	3.83060100	-0.67967900
C	-1.13419800	-3.20604400	0.51733600	H	-6.74962900	5.25270000	0.35812200
C	-0.46262300	-4.27426600	1.12912200	H	-7.39679800	3.75514600	1.02930500
H	0.06123900	-4.11974200	2.06620500	C	-2.61847900	4.38658500	3.36066700
C	-0.45903200	-5.55154400	0.55424200	H	-2.89759900	5.43198800	3.53285900
C	-1.14250700	-5.74399500	-0.65238800	H	-1.52929300	4.33311300	3.26716800
H	-1.14949200	-6.73376900	-1.10714500	H	-2.89407300	3.82431200	4.26314300
C	-1.82196800	-4.69759900	-1.28678100	C	-3.63164500	0.00399600	-1.53564100
C	-1.80786100	-3.42961200	-0.69214200	C	-4.73385600	-0.39601200	-0.76014100
H	-2.32320000	-2.61058900	-1.18359700	H	-4.85120600	-0.02007000	0.25038100
C	0.23655200	-6.70531700	1.24193200	C	-5.70239700	-1.26394700	-1.27394500
H	0.72447800	-7.36943800	0.51965200	C	-5.54386800	-1.75478400	-2.57741400
H	-0.47526400	-7.31655100	1.81310600	H	-6.29588700	-2.42772100	-2.98694900
H	0.99855300	-6.35125600	1.94366300	C	-4.45122000	-1.39056100	-3.36730800
C	-2.53335500	-4.91812400	-2.60264900	C	-3.50177300	-0.50825500	-2.83240900
H	-3.45610700	-4.33110200	-2.65775600	H	-2.66293400	-0.21200700	-3.45171800
H	-2.78734500	-5.97346900	-2.74970600	C	-4.29500900	-1.90929800	-4.77934500
C	-1.95857600	2.21133300	-2.36086900	H	-4.33050900	-1.09137400	-5.50987100
C	-1.05407400	1.70932400	-3.30996300	H	-5.08876000	-2.61872300	-5.03515700
H	-0.57191600	0.75180700	-3.13963600	H	-3.33287700	-2.41799600	-4.91401500
C	-0.73717900	2.43520600	-4.46315200	C	-6.91489700	-1.64972000	-0.45737200
C	-1.33484300	3.68569000	-4.65442200	H	-7.83453800	-1.23910000	-0.89471600
H	-1.09160700	4.26056000	-5.54695000	H	-6.83710000	-1.28164700	0.56935900
C	-2.22770900	4.22042700	-3.72046600	H	-7.03892500	-2.73873500	-0.41589800
C	-2.52939000	3.47315900	-2.57463400	Ru	-0.34440400	0.16993800	-0.16943700
H	-3.21442800	3.89289200	-1.84639600	P	-1.18033100	-1.50325300	1.25998100
C	0.26843900	1.89619500	-5.45544000	P	-2.33753900	1.16316000	-0.86410900
H	1.28677800	2.21613100	-5.19725100	H	-1.90424100	-4.61079400	-3.44889600
H	0.06234600	2.25161100	-6.47113800	H	-0.44789100	3.12098700	-0.10497800
H	0.26817300	0.80110400	-5.47078100	C	1.03928800	-1.55371900	-1.49517300
C	-2.87664600	5.56647200	-3.95470600	C	1.82522700	-2.49197500	-2.38618300
H	-3.75767300	5.47753600	-4.60487400	C	2.71432000	-3.47250700	-1.59425500
H	-2.18664000	6.26544200	-4.44050600	C	3.50692700	-4.39093200	-2.49924100
H	-3.20981600	6.01903000	-3.01481100	C	2.98383800	-5.62680200	-2.90470300
C	-3.30319000	2.31862600	0.21675400	C	3.69938600	-6.46250400	-3.76395300
C	-4.60060800	2.74915900	-0.10771300	C	4.95556500	-6.07427300	-4.23452100
H	-5.10396500	2.34245700	-0.97999600	C	5.48920200	-4.84613900	-3.83831100
C	-5.25933700	3.70846300	0.66873700	C	4.76961200	-4.01486600	-2.97848800
C	-4.59140300	4.24255500	1.77969700	H	1.12088400	-3.02997900	-3.02803700
H	-5.08810900	5.00376100	2.38012800	H	2.45334100	-1.87818900	-3.04726500
C	-3.30543200	3.82417200	2.13638100	H	3.38769800	-2.89107300	-0.95622200
C	-2.67039600	2.85331400	1.34720400	H	2.00697400	-5.93524100	-2.53731000

H	3.27770900	-7.41903600	-4.06276500
H	5.51557800	-6.72492200	-4.90104500
H	6.46846000	-4.53684600	-4.19504300
H	5.19380800	-3.06121100	-2.67003400
O	-0.14280200	-1.20231700	-1.83181600
O	1.54086200	-1.09317100	-0.42330300
H	2.07719900	-4.06392500	-0.92613100
C	0.50735900	2.65838900	0.18061100
C	1.49437600	3.78266800	0.50740600
C	1.65708600	4.78609000	-0.65201800
C	2.67986200	5.86043900	-0.35048200
C	4.05034400	5.59216100	-0.48785700
C	5.00537600	6.56419500	-0.18904600
C	4.60614700	7.82770800	0.25426500
C	3.24618500	8.10809300	0.39555100
C	2.29414300	7.13140500	0.09470300
H	1.10920200	4.29766300	1.39695500
H	2.47039300	3.37525900	0.77830000
H	1.95393800	4.23442700	-1.55124700
H	4.36484700	4.60901300	-0.83312000
H	6.06223300	6.33765300	-0.30719700
H	5.34881000	8.58735500	0.48403200
H	2.92444300	9.08929600	0.73604800
H	1.23543600	7.35920000	0.20193100
O	0.87160500	1.90051100	-1.02530900
O	0.33895100	1.72079000	1.18592600
H	0.68533200	5.24509400	-0.87547400
H	1.81438500	1.61580400	-0.88490000
C	3.68132900	1.01095400	0.84366900
O	3.44696500	1.35422300	-0.31543100
O	2.79852700	0.97749700	1.82460500
H	1.83797300	1.23825100	1.54588100
C	5.07024800	0.58205200	1.28358100
H	5.25076200	0.95920800	2.29619900
H	5.06160100	-0.51284300	1.36865800
C	6.18113100	1.02678200	0.31684800
H	5.94429200	0.65314200	-0.68449900
H	6.17506000	2.12112100	0.24716500
C	7.54786400	0.54313500	0.75388500
C	8.03161600	-0.70760600	0.34502400
C	8.34955500	1.31959900	1.60205500
C	9.27655200	-1.17165500	0.77262200
H	7.42733900	-1.32150100	-0.32012800
C	9.59579300	0.86106700	2.03240800

H	7.99433700	2.29657100	1.92388000
C	10.06343100	-0.38798400	1.61922600
H	9.63413000	-2.14302000	0.44039700
H	10.20305000	1.48150400	2.68668100
H	11.03478500	-0.74581400	1.95023900

### TS3

C	0.30486700	-2.07038400	-2.71117800
C	-0.96415200	-1.54761800	-2.97248200
H	-1.46073000	-0.92814000	-2.23706500
C	-1.61267800	-1.80919100	-4.19264900
C	-0.96770900	-2.60829000	-5.13742700
H	-1.46127800	-2.80803900	-6.08760400
C	0.29959300	-3.15831000	-4.89727700
C	0.92510600	-2.88058600	-3.68140600
H	1.90743400	-3.30033600	-3.49251600
C	-2.98400300	-1.23667400	-4.46612300
H	-3.22335500	-1.26836300	-5.53448800
H	-3.04705400	-0.20234000	-4.11699700
H	-3.76258700	-1.80401300	-3.93830900
C	0.97424500	-4.01983800	-5.94118400
H	0.34115800	-4.86711500	-6.23309800
H	1.92381600	-4.42223600	-5.57394900
H	1.18615800	-3.44940000	-6.85473500
C	2.90829300	-1.93444700	-1.62293900
C	3.68134700	-3.06540600	-1.32594900
H	3.28670800	-3.83463800	-0.67127700
C	4.95547000	-3.23573500	-1.88040200
C	5.45425300	-2.24196600	-2.73165200
H	6.44233900	-2.36609000	-3.17216300
C	4.70856200	-1.09972200	-3.04466300
C	3.43267400	-0.96047400	-2.48237300
H	2.83373800	-0.09174700	-2.73863800
C	5.75558900	-4.48846800	-1.60101800
H	5.45591600	-4.95100100	-0.65507000
H	6.82959000	-4.27804000	-1.55182400
H	5.60847400	-5.23702400	-2.39117700
C	5.25721600	-0.04503500	-3.97857600
H	6.21481900	-0.35432200	-4.40995200
H	5.41241700	0.90649700	-3.45663700
H	4.56433900	0.15004000	-4.80624900
C	0.82765900	-3.32378600	-0.14529600
C	-0.02143100	-4.32204800	-0.63625000
H	-0.50257100	-4.19713500	-1.60081400

C	-0.26177700	-5.49282800	0.09796000	H	3.59091100	4.58602300	-4.04447700
C	0.36676400	-5.64543500	1.33680800	H	2.11939700	3.64377400	-3.73243700
H	0.19046900	-6.55193400	1.91394700	H	3.49713800	2.89427900	-4.54120800
C	1.21741800	-4.66008800	1.85772800	C	3.52906600	-0.14022900	1.72340900
C	1.43326400	-3.49875900	1.10988300	C	4.67382500	-0.66825800	1.10233300
H	2.07227100	-2.72011800	1.51556300	H	4.91057800	-0.39841300	0.07895600
C	-1.15624800	-6.57640200	-0.46166100	C	5.53689600	-1.52942900	1.78809900
H	-1.51623800	-7.24597900	0.32664500	C	5.22424600	-1.88748800	3.10612900
H	-0.62275000	-7.19359300	-1.19699800	H	5.89209100	-2.55499900	3.64858600
H	-2.02821600	-6.15225900	-0.97209400	C	4.08224600	-1.39783200	3.74448400
C	1.85898100	-4.83245900	3.21606600	C	3.24309300	-0.52338200	3.04000800
H	2.80510500	-4.28561300	3.28054700	H	2.36746000	-0.13018500	3.54322200
H	2.05599700	-5.88765400	3.43603300	C	3.76079000	-1.77191300	5.17431400
C	2.01468200	2.27270900	2.17682400	H	3.80122400	-0.89520900	5.83304000
C	1.02177100	1.95352800	3.11555200	H	4.46780100	-2.51211500	5.56274400
H	0.46889400	1.02333800	3.02274000	H	2.75184500	-2.19244600	5.26085200
C	0.70036800	2.83171000	4.15730100	C	6.80387100	-2.03827400	1.13873900
C	1.38236600	4.04919300	4.24302900	H	7.69105900	-1.55798500	1.57272400
H	1.13555200	4.74142200	5.04666700	H	6.80762000	-1.83843600	0.06370500
C	2.36505500	4.40496000	3.31249100	H	6.92240600	-3.11879200	1.28271700
C	2.67089300	3.50768800	2.28231100	Ru	0.35035700	0.13836600	0.08757000
H	3.42700000	3.78921000	1.55781700	P	1.14043200	-1.75268300	-1.08124800
C	-0.39802700	2.48423200	5.13667400	P	2.38731900	1.03309400	0.83496400
H	-1.38670500	2.70435100	4.71278400	H	1.20656300	-4.45041900	4.01286700
H	-0.30380700	3.05634200	6.06582800	H	0.75002800	3.06900400	-0.20503900
H	-0.38701800	1.41844300	5.39073300	C	-1.28381600	-1.32272000	1.39430900
C	3.09708700	5.72322900	3.43123400	C	-2.22968500	-2.11272700	2.27077300
H	3.85235900	5.69107700	4.22804100	C	-3.69196400	-2.06066200	1.79097300
H	2.41058600	6.54303600	3.67235800	C	-4.63076100	-2.82481300	2.70023200
H	3.61367900	5.97902000	2.50037600	C	-4.78096200	-4.21384000	2.57482700
C	3.51144400	1.96432200	-0.30549000	C	-5.62608900	-4.92529300	3.42718500
C	4.81362100	2.34658900	0.05879700	C	-6.34117100	-4.25695000	4.42386900
H	5.22120100	2.03736100	1.01685800	C	-6.20369300	-2.87444100	4.55908900
C	5.60103000	3.13182300	-0.78971400	C	-5.35559800	-2.16751000	3.70405300
C	5.05823900	3.54228300	-2.01547200	H	-1.86738500	-3.14957500	2.29512800
H	5.65637400	4.16913200	-2.67562100	H	-2.13642100	-1.73586900	3.29617200
C	3.76862600	3.17229700	-2.41019100	H	-4.00151900	-1.01185300	1.72161700
C	3.00363800	2.37557300	-1.54490900	H	-4.23261600	-4.74046700	1.79610900
H	1.99806500	2.08093700	-1.83710500	H	-5.73134300	-6.00098400	3.30965800
C	7.00803900	3.52591400	-0.39963700	H	-7.00334200	-4.80871500	5.08590300
H	7.18395900	3.37325300	0.66994100	H	-6.76028600	-2.34363100	5.32734000
H	7.20726200	4.57921200	-0.62839700	H	-5.25736000	-1.08928100	3.81215000
H	7.75399000	2.93166100	-0.94386000	O	-0.10860200	-1.04042000	1.82160400
C	3.21290300	3.60086800	-3.74979100	O	-1.62155700	-0.93383600	0.23518600

H	-3.73854500	-2.46385200	0.77352900
C	-0.24680900	2.70155600	-0.46844800
C	-1.10600400	3.89098700	-0.90140100
C	-1.22879800	4.95796300	0.20482000
C	-2.13118500	6.10570200	-0.19595500
C	-3.52462500	5.93888400	-0.20261500
C	-4.36886100	6.97987700	-0.58858500
C	-3.83384300	8.21149200	-0.97583500
C	-2.44989800	8.39053400	-0.97387800
C	-1.60848800	7.34471200	-0.58684900
H	-0.63280200	4.32592700	-1.79105900
H	-2.10056500	3.55701100	-1.20229800
H	-1.62052400	4.47763200	1.10867300
H	-3.94464800	4.98084600	0.09788200
H	-5.44594300	6.83179500	-0.58329500
H	-4.49094600	9.02438600	-1.27386600
H	-2.02312900	9.34551400	-1.27068300
H	-0.53041200	7.49300600	-0.58366200
O	-0.72389400	2.04880000	0.73431800
O	-0.13342000	1.68492800	-1.43429900
H	-0.23126800	5.33697400	0.46207500
H	-1.70237000	1.86541400	0.56951800
C	-3.37639500	1.20880300	-1.13569800
O	-3.23624400	1.65694400	0.01819300
O	-2.44945400	1.14725600	-2.04301700
H	-1.32612300	1.40810700	-1.74314700
C	-4.72820700	0.66123600	-1.57760700
H	-4.89157500	0.92372800	-2.62839200
H	-4.64592400	-0.43428700	-1.55046800
C	-5.90597400	1.11843700	-0.69962900
H	-5.66098700	0.91101800	0.34664500
H	-6.00994100	2.20756100	-0.78129400
C	-7.20713900	0.44334300	-1.07850000
C	-7.60674000	-0.74553800	-0.45151700
C	-8.03024900	0.97203000	-2.08292600
C	-8.78975400	-1.38944700	-0.81838600
H	-6.98760700	-1.16689600	0.33806900
C	-9.21440500	0.33265000	-2.45349200
H	-7.74114600	1.89838900	-2.57563100
C	-9.59823800	-0.85243900	-1.82227500
H	-9.08224000	-2.30754900	-0.31495600
H	-9.83963900	0.76272200	-3.23210700
H	-10.52177800	-1.34995700	-2.10678700

### Int5

C	-0.56294400	-2.02724400	2.75087600
C	0.72005600	-1.54976600	3.04035200
H	1.26936500	-0.96288700	2.31428000
C	1.32403200	-1.81998500	4.28089800
C	0.61965200	-2.57741100	5.21899700
H	1.07805200	-2.78253600	6.18563000
C	-0.66131600	-3.07967100	4.95159300
C	-1.24191400	-2.79663500	3.71408700
H	-2.23518200	-3.17917400	3.50366300
C	2.71434200	-1.30824600	4.57930600
H	2.86013100	-1.15670900	5.65482100
H	2.90068500	-0.36821700	4.05272200
H	3.47598500	-2.02713100	4.24647600
C	-1.39916900	-3.89657200	5.98877000
H	-0.80920100	-4.76368900	6.31101300
H	-2.35384600	-4.26652400	5.60119800
H	-1.61277000	-3.30348300	6.88735100
C	-3.13765400	-1.78096800	1.59250800
C	-3.95699100	-2.87639000	1.28700100
H	-3.57837700	-3.67921900	0.66369600
C	-5.25995000	-2.96657100	1.79192000
C	-5.73828100	-1.92916400	2.60144200
H	-6.74884300	-1.99071300	3.00209200
C	-4.94498400	-0.82175800	2.92386600
C	-3.64242900	-0.76245000	2.41149400
H	-3.00837600	0.07964300	2.67310100
C	-6.11354800	-4.18201600	1.50580900
H	-5.83531200	-4.65195200	0.55687400
H	-7.17748000	-3.92542900	1.45951900
H	-5.99729800	-4.94087900	2.29124500
C	-5.47461100	0.28046900	3.81255900
H	-6.45099100	0.01844900	4.23285100
H	-5.58629700	1.21953400	3.25780600
H	-4.79205200	0.47782700	4.64806000
C	-1.09130800	-3.27484300	0.17152500
C	-0.31884800	-4.32175100	0.68690900
H	0.13395900	-4.22798300	1.66865500
C	-0.11833800	-5.49990900	-0.04719600
C	-0.70827000	-5.60942000	-1.30955600
H	-0.56090200	-6.52086700	-1.88701600
C	-1.48230900	-4.57497600	-1.85439000
C	-1.66025400	-3.40770200	-1.10573400
H	-2.23800700	-2.59071200	-1.52720200

C	0.69435000	-6.63488700	0.53470000	C	-5.48423900	-1.29028900	-2.02500900
H	1.05654800	-7.31043700	-0.24746700	C	-5.13407600	-1.60561200	-3.34511700
H	0.09747700	-7.23489700	1.23469800	H	-5.79230300	-2.24544200	-3.93092600
H	1.56180400	-6.26197900	1.09049900	C	-3.96818000	-1.10737000	-3.93108100
C	-2.08026200	-4.70347600	-3.23726900	C	-3.14318100	-0.26560600	-3.17187800
H	-2.97636400	-4.08350400	-3.34169500	H	-2.25007700	0.13830000	-3.63429300
H	-2.35135400	-5.74102200	-3.46262000	C	-3.60022400	-1.44506900	-5.35852500
C	-1.81003000	2.42663700	-2.16449200	H	-2.64263900	-1.97783600	-5.40876000
C	-0.76611800	2.07841600	-3.03428400	H	-3.49544200	-0.53890700	-5.96769400
H	-0.27440900	1.11632400	-2.92922900	H	-4.35992200	-2.07794500	-5.82846100
C	-0.32082900	2.96544600	-4.02236700	C	-6.77610900	-1.80748000	-1.43409000
C	-0.93172100	4.21863700	-4.12255800	H	-7.64444300	-1.30645000	-1.88242300
H	-0.58707700	4.91812700	-4.88255600	H	-6.81434600	-1.64110300	-0.35407400
C	-1.96642600	4.60163600	-3.26096100	H	-6.89798000	-2.88195800	-1.61584400
C	-2.39511900	3.69640800	-2.28349500	Ru	-0.40943100	0.15760400	-0.01935700
H	-3.19021200	3.99651000	-1.60985300	P	-1.34919000	-1.69434800	1.10182000
C	0.82945600	2.58202700	-4.92544300	P	-2.33757000	1.18583000	-0.87777900
H	1.78415100	2.62988800	-4.38583100	H	-1.36767500	-4.37948800	-4.00784800
H	0.90299900	3.25114100	-5.78908000	H	-0.56085600	3.14341900	0.24280000
H	0.72249400	1.55691400	-5.29844600	C	1.15886600	-1.38956500	-1.28606800
C	-2.62145900	5.95795200	-3.39823100	C	2.08201800	-2.19984100	-2.16503100
H	-3.34034900	5.97235100	-4.22856000	C	3.53244300	-2.23140300	-1.64711000
H	-1.88233600	6.74181100	-3.59935900	C	4.46326100	-2.98492200	-2.57299200
H	-3.16635500	6.23299800	-2.48918200	C	4.56037600	-4.38301300	-2.51441400
C	-3.49541200	2.16037300	0.19031500	C	5.39908300	-5.08240700	-3.38294400
C	-4.76341100	2.57083200	-0.25591000	C	6.16113900	-4.39255100	-4.32889700
H	-5.12182800	2.25476500	-1.23100500	C	6.07703000	-3.00090100	-4.39726100
C	-5.57579600	3.39294100	0.53090800	C	5.23480900	-2.30586100	-3.52658600
C	-5.09341300	3.81275300	1.77923400	H	1.67025500	-3.21632700	-2.23092800
H	-5.71109400	4.46752200	2.39238700	H	2.03305600	-1.78591000	-3.17899200
C	-3.84030100	3.41636000	2.25498700	H	3.87767300	-1.20023400	-1.51464000
C	-3.04986100	2.58227800	1.44898000	H	3.97622000	-4.92655300	-1.77432000
H	-2.07507300	2.26579100	1.80939900	H	5.46301700	-6.16573300	-3.31717300
C	-6.94494700	3.82097200	0.05253000	H	6.81870700	-4.93507400	-5.00306300
H	-7.08562900	3.59718700	-1.00958300	H	6.67072600	-2.45381600	-5.12525600
H	-7.10064000	4.89680600	0.19499600	H	5.17760500	-1.22075400	-3.58241800
H	-7.73984800	3.30504600	0.60687000	O	0.02430300	-0.99486800	-1.74420400
C	-3.35046900	3.85380400	3.61703100	O	1.46658800	-1.07979600	-0.09810200
H	-3.79333700	4.81049400	3.91379600	H	3.53704700	-2.68827400	-0.65159100
H	-2.26101500	3.95993100	3.63525500	C	0.39012000	2.69948100	0.54452200
H	-3.61567800	3.11828900	4.38829300	C	1.34096000	3.78590000	1.03927900
C	-3.46452700	0.07085900	-1.85128800	C	1.71461700	4.78545300	-0.07449200
C	-4.63375400	-0.46435000	-1.28315800	C	2.79012500	5.75651700	0.36477800
H	-4.89970200	-0.22519400	-0.25921300	C	4.12509500	5.33090100	0.44650800



C	5.12778000	6.20349500	0.86871200	H	0.90109600	-2.67098300	6.29059100
C	4.81310600	7.52003500	1.21704900	C	-0.84328500	-2.92503200	5.05408300
C	3.48937500	7.95472300	1.13950700	C	-1.39764000	-2.66967000	3.79801500
C	2.48774100	7.07749800	0.71603600	H	-2.40863800	-3.00722900	3.59595000
H	0.84368500	4.31019800	1.86531200	C	2.63288400	-1.37396800	4.63123800
H	2.24287400	3.32828700	1.44854000	H	2.78986100	-1.20967600	5.70318200
H	2.06660000	4.21903200	-0.94356100	H	2.87041400	-0.45433400	4.08917600
H	4.36908000	4.30512500	0.17655200	H	3.35348300	-2.13938000	4.31096800
H	6.15702200	5.85745400	0.92254900	C	-1.63560700	-3.64622100	6.12169500
H	5.59458100	8.20119600	1.54385100	H	-1.08580500	-4.51042100	6.51455100
H	3.23478900	8.97775200	1.40562100	H	-2.59368500	-4.00649400	5.73350200
H	1.45793600	7.42391600	0.65362100	H	-1.84913400	-2.98828000	6.97408600
O	0.86602100	1.95316600	-0.56184800	C	-3.21579600	-1.73621800	1.57591600
O	0.07105900	1.72503900	1.56524900	C	-4.03317800	-2.83936700	1.28931200
H	0.81959700	5.33312600	-0.39715100	H	-3.63974400	-3.66996400	0.71355400
H	1.87163600	1.70552100	-0.36206000	C	-5.35269300	-2.90063900	1.75160300
C	3.42371700	0.96292600	1.18049400	C	-5.85055100	-1.82776600	2.50240200
O	3.27448900	1.40777500	-0.00021500	H	-6.87454300	-1.86652200	2.87078100
O	2.54681700	0.98233300	2.09613200	C	-5.06060700	-0.71375300	2.80583400
H	0.98993300	1.39934600	1.88227200	C	-3.74086400	-0.68223300	2.33398700
C	4.77363000	0.32924900	1.52808400	H	-3.11262000	0.16929300	2.57883100
H	4.96800400	0.47934500	2.59522900	C	-6.21063500	-4.11712800	1.48319500
H	4.65523000	-0.75484900	1.38895600	H	-5.79952500	-4.72436100	0.67056800
C	5.95529900	0.82938200	0.67718000	H	-7.23508600	-3.83692900	1.21246800
H	5.68926100	0.72986000	-0.37947600	H	-6.27677600	-4.75907900	2.37171300
H	6.09685400	1.90242200	0.86034200	C	-5.61030400	0.42524400	3.63394500
C	7.24024300	0.08463200	0.97130800	H	-6.61758800	0.20112200	3.99981200
C	7.59961700	-1.05084500	0.23072400	H	-5.66011600	1.35298900	3.05222600
C	8.08769600	0.49041400	2.01235100	H	-4.97450700	0.62401800	4.50552700
C	8.76571000	-1.76084600	0.52257500	C	-1.15299000	-3.28132700	0.24238300
H	6.96120100	-1.38010800	-0.58682700	C	-0.42575200	-4.33685100	0.80539400
C	9.25500200	-0.21524200	2.30842600	H	-0.00926400	-4.23507400	1.80237400
H	7.82963300	1.37290100	2.59474300	C	-0.22540000	-5.53209900	0.10073200
C	9.59830700	-1.34574100	1.56384200	C	-0.76869200	-5.65083600	-1.18237600
H	9.02559900	-2.63597100	-0.06798000	H	-0.62068900	-6.57557400	-1.73829200
H	9.89867800	0.12041900	3.11798200	C	-1.49613800	-4.60926200	-1.77413100
H	10.50853200	-1.89517900	1.79016000	C	-1.67536800	-3.42435300	-1.05274100
				H	-2.21677600	-2.60189700	-1.50993600
<b>TS4</b>				C	0.53318200	-6.67783000	0.73259200
C	-0.67037900	-1.98580400	2.80682400	H	1.00321400	-7.31414000	-0.02508200
C	0.63584100	-1.56840000	3.08888100	H	-0.13308400	-7.31787300	1.32679700
H	1.22118000	-1.05266600	2.33750600	H	1.31719100	-6.31536000	1.40608200
C	1.21564900	-1.81466600	4.34503800	C	-2.04313300	-4.74718200	-3.17712300
C	0.46219300	-2.48513300	5.31111400	H	-2.93627000	-4.12979500	-3.31735900

H	-2.30338700	-5.78653900	-3.40650000	C	-3.38898600	-1.47449400	-5.41640800
C	-1.68512900	2.42529700	-2.20220400	H	-2.57881000	-2.21521000	-5.41042900
C	-0.60439800	2.06179100	-3.01862300	H	-3.02027400	-0.59913500	-5.96301500
H	-0.12261500	1.10018800	-2.87596800	H	-4.22208500	-1.90173200	-5.98421800
C	-0.11437000	2.93255300	-3.99989600	C	-6.68941000	-1.79816400	-1.59371900
C	-0.71668700	4.18543400	-4.14591100	H	-7.54534100	-1.29714000	-2.06542400
H	-0.33651600	4.87248300	-4.90039200	H	-6.75639900	-1.63091100	-0.51514400
C	-1.78787700	4.58351900	-3.33717300	H	-6.80642400	-2.87276400	-1.77788700
C	-2.26154900	3.69382900	-2.36623000	Ru	-0.40056800	0.15298900	0.01320900
H	-3.08505100	4.00507400	-1.73296400	P	-1.41332900	-1.67658200	1.13066100
C	1.07322900	2.53297400	-4.84594500	P	-2.27197500	1.20296100	-0.92330500
H	2.00297100	2.58242700	-4.26452800	H	-1.30383400	-4.42487600	-3.92293200
H	1.18845500	3.19138400	-5.71330500	H	-0.50793400	3.12436700	0.20721300
H	0.97760300	1.50390800	-5.21117300	C	1.16368400	-1.45494600	-1.20000700
C	-2.43409000	5.93801400	-3.52508000	C	2.06983100	-2.31557200	-2.05005300
H	-3.13492700	5.93283400	-4.37092300	C	3.52137600	-2.35429700	-1.53588400
H	-1.68764700	6.71367900	-3.73073600	C	4.43503000	-3.16346800	-2.43128300
H	-2.99784200	6.23920400	-2.63594800	C	4.52253800	-4.55714500	-2.30014200
C	-3.46432800	2.20294700	0.08358900	C	5.34547200	-5.30791700	-3.14053900
C	-4.71653100	2.60251600	-0.41496100	C	6.10079800	-4.67521400	-4.13074100
H	-5.04268700	2.26002500	-1.39230500	C	6.02577000	-3.28847600	-4.27181600
C	-5.55306500	3.44592700	0.32205600	C	5.19941100	-2.54203000	-3.42898100
C	-5.11249200	3.89684800	1.57533600	H	1.64090600	-3.32691700	-2.07184000
H	-5.75015800	4.56585700	2.15169700	H	2.02467100	-1.94262900	-3.07966400
C	-3.87678500	3.51191800	2.10235300	H	3.88738100	-1.32522400	-1.44956100
C	-3.06074700	2.65700500	1.34483900	H	3.94298700	-5.05626800	-1.52599500
H	-2.09974600	2.34889000	1.74625000	H	5.40206900	-6.38675900	-3.01848800
C	-6.89988700	3.87271800	-0.21716100	H	6.74575800	-5.25790400	-4.78320200
H	-7.06531500	3.48923600	-1.22877200	H	6.61381400	-2.78532700	-5.03523700
H	-6.98815100	4.96551500	-0.25373700	H	5.14814000	-1.46107300	-3.54270400
H	-7.71792600	3.50598500	0.41579200	O	0.05649100	-1.02528500	-1.68871400
C	-3.43255800	3.98202200	3.46916400	O	1.45895700	-1.14512700	-0.00902500
H	-3.89312200	4.94016000	3.73254500	H	3.52039100	-2.76871700	-0.52196600
H	-2.34515200	4.09971000	3.51754400	C	0.42891100	2.65998300	0.53266700
H	-3.71351200	3.25980500	4.24745700	C	1.37582200	3.74612900	1.04212500
C	-3.37095300	0.08487200	-1.92456200	C	1.82002600	4.69365400	-0.09141500
C	-4.55564600	-0.44850600	-1.38856300	C	2.80556000	5.73917700	0.38503600
H	-4.85378800	-0.20076700	-0.37563500	C	4.16206100	5.41343600	0.53378200
C	-5.38160100	-1.28220900	-2.14982700	C	5.07899000	6.35641400	0.99848300
C	-4.99155100	-1.60522800	-3.45649200	C	4.65456200	7.64758300	1.32272400
H	-5.63181400	-2.24874000	-4.05815900	C	3.30812600	7.98544700	1.17745700
C	-3.80818900	-1.10957800	-4.01003800	C	2.39385700	7.03737300	0.71244800
C	-3.00895700	-0.26031000	-3.23269500	H	0.84757700	4.31344800	1.81923600
H	-2.10285200	0.14301200	-3.66959700	H	2.25035000	3.29554100	1.51681000

H	2.27366700	4.09191900	-0.88618900	H	2.90014900	-0.56516600	4.07572500
H	4.49511200	4.40929600	0.27824700	H	3.31593100	-2.27664100	4.21113100
H	6.12665100	6.08529300	1.10301300	C	-1.73157300	-3.48656500	6.18190300
H	5.36832800	8.38437200	1.68199800	H	-1.16642600	-4.26735100	6.70454200
H	2.96835200	8.98876600	1.42262800	H	-2.64510300	-3.94014700	5.78382400
H	1.34633000	7.30928600	0.59770400	H	-2.03302000	-2.74837400	6.93705600
O	0.92498400	1.86123800	-0.49351000	C	-3.25784900	-1.73128500	1.56387200
O	0.02549600	1.73206900	1.59888700	C	-4.06526200	-2.83966100	1.27415000
H	0.93813700	5.17902500	-0.52941800	H	-3.66008500	-3.67128400	0.70787300
H	2.08328900	1.56326900	-0.24371500	C	-5.39175000	-2.90470100	1.71847100
C	3.42983800	0.88164800	1.19869800	C	-5.90460000	-1.83103800	2.45610800
O	3.23517400	1.28383800	-0.01297600	H	-6.93368200	-1.87218800	2.80937200
O	2.58689400	0.93803200	2.12148000	C	-5.12371200	-0.71062000	2.76375300
H	0.90001300	1.39059800	1.95359200	C	-3.79934100	-0.67420000	2.30779500
C	4.80106300	0.27918400	1.48566400	H	-3.18032600	0.18452800	2.55100000
H	5.00807100	0.38735800	2.55487300	C	-6.23526100	-4.12978300	1.44341500
H	4.71255500	-0.79959900	1.29485700	H	-7.30042200	-3.88080500	1.38642400
C	5.95355400	0.85323300	0.63895500	H	-6.11902500	-4.87779500	2.23927200
H	5.68247900	0.77711100	-0.41840600	H	-5.94757900	-4.61066500	0.50265400
H	6.05875400	1.92374100	0.85745700	C	-5.69054700	0.42909300	3.57943200
C	7.26679700	0.14539600	0.89917100	H	-6.71276200	0.21359200	3.90720500
C	7.63485400	-0.98302900	0.15215100	H	-5.70881700	1.36155100	3.00374600
C	8.13073900	0.57860600	1.91474300	H	-5.08506000	0.61446900	4.47543800
C	8.82727300	-1.65994600	0.41372600	C	-1.18349200	-3.26820000	0.24747500
H	6.98265100	-1.33382700	-0.64532000	C	-0.48535500	-4.33502800	0.82596800
C	9.32471000	-0.09415200	2.18008200	H	-0.09364500	-4.24105100	1.83373400
H	7.86514600	1.45603000	2.50130300	C	-0.28354900	-5.53143200	0.12394700
C	9.67711900	-1.21782200	1.42979000	C	-0.79585500	-5.64016100	-1.17282500
H	9.09390600	-2.53044200	-0.18044800	H	-0.64639600	-6.56569300	-1.72711100
H	9.98138500	0.26195200	2.97008900	C	-1.49490800	-4.58798200	-1.77971500
H	10.60770100	-1.74171100	1.63228300	C	-1.67659500	-3.40211900	-1.06002900
<b>Int5-acid</b>				H	-2.19729000	-2.57215200	-1.52761100
C	-0.71692600	-1.97250200	2.81309200	C	0.44222900	-6.68934000	0.77203900
C	0.61280700	-1.61604200	3.07231300	H	0.93105500	-7.32502700	0.02571700
H	1.21272700	-1.15284900	2.29804300	H	-0.24967500	-7.32715600	1.33876400
C	1.19536200	-1.86471500	4.32609600	H	1.20690900	-6.33991300	1.47405000
C	0.42031900	-2.47208700	5.31705500	C	-2.00974800	-4.71599900	-3.19581100
H	0.86207700	-2.66004800	6.29474900	H	-2.89110800	-4.08671000	-3.35600100
C	-0.90947600	-2.84647100	5.08562000	H	-2.27776800	-5.75150600	-3.43367400
C	-1.46479500	-2.59443900	3.82858100	C	-1.68493300	2.47692300	-2.18004300
H	-2.49334600	-2.88675300	3.64632900	C	-0.59020100	2.13116600	-2.98383400
C	2.63836400	-1.49670800	4.58548800	H	-0.09446700	1.17799400	-2.83564600
H	2.83396900	-1.38343300	5.65747900	C	-0.10823100	3.00740000	-3.96554000
				C	-0.73121000	4.24785900	-4.12203800

H	-0.35941100	4.93705600	-4.87897700	H	-6.74203300	-1.63703000	-0.57279000
C	-1.81540000	4.63050900	-3.32178600	H	-6.78857700	-2.84821300	-1.86540800
C	-2.28302000	3.73480300	-2.35479500	Ru	-0.41961200	0.18363600	0.02859800
H	-3.11984700	4.03220300	-1.73270300	P	-1.45168200	-1.66136300	1.13132600
C	1.08843600	2.62133400	-4.80529400	P	-2.27300300	1.24172400	-0.91353900
H	2.01103600	2.65197700	-4.21140300	H	-1.24899300	-4.40176900	-3.92324700
H	1.21774400	3.29872100	-5.65591800	H	-0.50730900	3.14793400	0.25159900
H	0.99254100	1.60141300	-5.19580300	C	1.14379400	-1.42389800	-1.20347300
C	-2.46358600	5.98504500	-3.50321400	C	2.03366600	-2.28993200	-2.06757900
H	-2.84783000	6.11262600	-4.52321100	C	3.47951100	-2.38416600	-1.54552400
H	-1.74900800	6.79889200	-3.32632000	C	4.37469400	-3.20657200	-2.44752000
H	-3.30140500	6.12227300	-2.81203600	C	4.41660200	-4.60433300	-2.34000400
C	-3.47908500	2.22938300	0.09036600	C	5.22371300	-5.36633400	-3.18567500
C	-4.73163600	2.62204700	-0.41271200	C	6.00849600	-4.74114700	-4.15757300
H	-5.05065700	2.28081000	-1.39284900	C	5.97855600	-3.35052600	-4.27528400
C	-5.57766700	3.45723400	0.32298800	C	5.16800600	-2.59284300	-3.42713100
C	-5.14634400	3.90716300	1.57976100	H	1.57596100	-3.28741700	-2.11769400
H	-5.79118600	4.57019800	2.15507400	H	2.00792600	-1.89147100	-3.08837000
C	-3.91081400	3.52825800	2.11158400	H	3.87796400	-1.36898200	-1.44057500
C	-3.08514000	2.68167300	1.35530900	H	3.81325400	-5.09791200	-1.58064400
H	-2.12361200	2.37949800	1.75986200	H	5.24469100	-6.44838300	-3.08214800
C	-6.92591500	3.87419400	-0.22045400	H	6.64091600	-5.33282900	-4.81419700
H	-7.07290000	3.51523800	-1.24388100	H	6.58913500	-2.85336400	-5.02483100
H	-7.03439400	4.96568200	-0.22817000	H	5.15120100	-1.50904200	-3.52331300
H	-7.74425700	3.47499200	0.39234900	O	0.03998600	-0.98041800	-1.68447200
C	-3.47633700	3.99620100	3.48226700	O	1.45129700	-1.12874800	-0.01197500
H	-3.95397000	4.94412100	3.75222300	H	3.45800700	-2.81533000	-0.53868200
H	-2.39116500	4.13279300	3.53241700	C	0.43086100	2.65605800	0.54485100
H	-3.74487500	3.26332600	4.25500400	C	1.40440600	3.71627400	1.06165000
C	-3.35736900	0.12505900	-1.93300700	C	1.83475100	4.68196100	-0.06205100
C	-4.54735100	-0.41608800	-1.41610500	C	2.88762200	5.66946500	0.39334600
H	-4.86125800	-0.17295000	-0.40682200	C	4.24246200	5.30542700	0.40094600
C	-5.35621600	-1.25406200	-2.19048200	C	5.22198800	6.19415800	0.84508300
C	-4.94342400	-1.57439200	-3.49114900	C	4.86271600	7.46842300	1.29112800
H	-5.56889100	-2.22337100	-4.10240200	C	3.51829400	7.84416300	1.28804400
C	-3.75500900	-1.07088400	-4.02561100	C	2.54187900	6.95072800	0.84220800
C	-2.97291000	-0.21740800	-3.23510700	H	0.90986600	4.27445600	1.86719300
H	-2.06045300	0.18893200	-3.65590100	H	2.28509700	3.23940700	1.49956500
C	-3.31344100	-1.42442500	-5.42816100	H	2.21915700	4.08783000	-0.89813400
H	-3.09676200	-0.52499300	-6.01684600	H	4.52507400	4.31407500	0.05170500
H	-4.08281100	-1.99568400	-5.95779600	H	6.26704500	5.89422200	0.83830700
H	-2.39782700	-2.02910800	-5.41687400	H	5.62468400	8.16339100	1.63438500
C	-6.66892500	-1.77883900	-1.65463600	H	3.22872300	8.83520000	1.62889300
H	-7.52059900	-1.26374800	-2.11909700	H	1.49622800	7.25233300	0.83799900



H	-0.83895200	-2.73473800	-6.43690300	H	0.62907000	-3.61487800	-0.51831800
H	-1.15557200	-1.16551600	-5.67598900	C	-2.16028200	0.66838000	-1.13649700
C	3.70416200	-4.24366500	-4.88257900	C	-3.28439800	1.34859300	-1.89038100
H	3.93116500	-4.09528600	-5.94534800	C	-4.46107200	1.76105300	-0.98459100
H	3.40373800	-5.29296500	-4.76227400	C	-5.56624800	2.45088900	-1.75507400
H	4.63117600	-4.10051800	-4.31794600	C	-5.55447000	3.84118800	-1.93653700
C	3.46536300	-1.36929600	-0.47195200	C	-6.55379900	4.47848700	-2.67392500
C	4.74906000	-1.04382000	-0.93650400	C	-7.58728500	3.73270600	-3.24480500
H	4.86808500	-0.29661100	-1.71533400	C	-7.61289800	2.34741800	-3.07055500
C	5.88714500	-1.67902000	-0.42505900	C	-6.61111400	1.71545000	-2.33189800
C	5.71870600	-2.66114300	0.55977700	H	-2.87034700	2.21463400	-2.41707200
H	6.59572700	-3.17463500	0.95146700	H	-3.63674900	0.65263700	-2.66476000
C	4.45295200	-3.00043700	1.05106200	H	-4.84499000	0.86667400	-0.48333200
C	3.33088600	-2.34305400	0.52771300	H	-4.75431600	4.42729500	-1.48840900
H	2.34340400	-2.59470600	0.90308500	H	-6.52806400	5.55826200	-2.79889800
C	7.26768200	-1.30548000	-0.91653400	H	-8.36827200	4.22716800	-3.81653600
H	7.23188600	-0.87591800	-1.92301200	H	-8.41629200	1.75823600	-3.50574300
H	7.93347000	-2.17530100	-0.94220300	H	-6.64119300	0.63627700	-2.19509800
H	7.73493200	-0.55894000	-0.26033000	O	-0.96496100	0.75948700	-1.59196200
C	4.29769800	-4.03846200	2.13967000	O	-2.37385200	0.00605500	-0.08236000
H	5.07642700	-4.80632400	2.07560000	H	-4.08334100	2.42440000	-0.19773200
H	3.32353600	-4.53450700	2.08206900	C	-0.35073000	-3.20693600	-0.20629900
H	4.37205800	-3.58274200	3.13637900	C	-1.27575300	-4.34601600	0.23141900
C	2.48417400	0.98078000	-1.89888400	C	-2.64088300	-3.87150800	0.76766300
C	3.24733700	1.84783900	-1.09545900	C	-3.59148000	-5.01649600	1.04211900
H	3.55944300	1.53516000	-0.10458300	C	-3.62884800	-5.64273200	2.29597800
C	3.62676100	3.11196600	-1.55342900	C	-4.48598300	-6.71740000	2.53959500
C	3.21213800	3.51587300	-2.83164900	C	-5.32511500	-7.18723400	1.52742100
H	3.50393600	4.49867700	-3.19941800	C	-5.29961000	-6.57275700	0.27344900
C	2.44331800	2.68364300	-3.64735800	C	-4.44134000	-5.49813100	0.03604000
C	2.09015700	1.41253000	-3.16920600	H	-0.64202500	-2.32103100	1.66290800
H	1.50570000	0.75819000	-3.80662900	H	-1.43838300	-4.97397100	-0.65385600
C	1.99557000	3.12907000	-5.02142400	H	-0.75997900	-4.97138800	0.97259200
H	0.90506700	3.24276200	-5.06697600	H	-2.50179200	-3.29749300	1.69543200
H	2.27345800	2.39663300	-5.78886800	H	-2.97885100	-5.28191900	3.09119900
H	2.44278000	4.08999900	-5.29598500	H	-4.50059400	-7.18531400	3.52091100
C	4.47947600	4.02577300	-0.70236800	H	-5.99555400	-8.02183700	1.71505500
H	5.46210400	4.19563500	-1.16183100	H	-5.95301900	-6.92701200	-0.52001200
H	4.64213200	3.60506600	0.29417800	H	-4.43075000	-5.02006300	-0.94125800
H	4.00962400	5.00979300	-0.58031400	O	-0.88574700	-2.32220900	-1.04715900
Ru	-0.11051700	-0.56693500	-0.17358900	O	0.11201100	-2.39976700	1.05037100
P	0.19956100	1.11220800	1.48567700	H	-3.06742900	-3.17770200	0.03662900
P	1.93049700	-0.66773000	-1.24186100				
H	-1.37168600	5.12604600	-2.42700800				

**Int7**

C	1.66907400	2.12208200	2.48881100	H	0.41927000	7.02667900	-0.28330900
C	0.46451000	2.28390100	3.18772000	H	2.02324600	7.26235700	-0.98103800
H	-0.46678900	1.97840200	2.72618700	H	1.85541200	6.68941500	0.68821600
C	0.43988000	2.86815400	4.46203200	C	1.11149700	3.28864000	-4.12573200
C	1.64331900	3.29463300	5.02992700	H	1.66035400	2.38720600	-4.41775300
H	1.63266500	3.75399500	6.01743800	H	1.46563100	4.12266700	-4.74142300
C	2.86315400	3.14750200	4.35807000	C	-0.65389100	-3.06465900	-1.35616800
C	2.86190400	2.56117400	3.08802100	C	-1.82836200	-2.45252200	-1.82326000
H	3.80627300	2.45136000	2.56559300	H	-1.95712300	-1.38295200	-1.70892100
C	-0.86716200	3.01018800	5.20922500	C	-2.84266900	-3.21171400	-2.41814300
H	-1.11684500	2.08712600	5.74961800	C	-2.67081100	-4.59682900	-2.53126100
H	-1.69671800	3.21809500	4.52508500	H	-3.45606800	-5.19299100	-2.99406700
H	-0.82242900	3.81782200	5.94782800	C	-1.51875800	-5.23409500	-2.06161300
C	4.15566400	3.59668400	5.00224300	C	-0.51174800	-4.45297300	-1.47950100
H	4.96082200	3.68460800	4.26564100	H	0.38781400	-4.94493900	-1.12469000
H	4.48834900	2.88361300	5.76839100	C	-4.11715900	-2.55060900	-2.89335100
H	4.04128400	4.56857300	5.49638300	H	-3.94385100	-1.50786900	-3.17928600
C	3.43748300	0.86365900	0.65114900	H	-4.87809300	-2.54832600	-2.10127100
C	4.38680900	1.67315100	0.01189400	H	-4.54589900	-3.07513900	-3.75473400
H	4.07068600	2.58579500	-0.48351000	C	-1.36839500	-6.73593900	-2.15663600
C	5.74521600	1.33271400	0.01304400	H	-1.91072200	-7.13940700	-3.01882100
C	6.14186800	0.16255900	0.67301600	H	-1.76548000	-7.23351200	-1.26149200
H	7.19689700	-0.10646700	0.68866100	H	-0.31706000	-7.02940400	-2.25014600
C	5.21838900	-0.66713100	1.32004600	C	1.81251400	-3.25466100	0.13744400
C	3.86497500	-0.30526000	1.29482000	C	2.81829500	-3.93242800	-0.56558300
H	3.13896000	-0.94821100	1.78581800	H	3.00882600	-3.69242300	-1.60656100
C	6.76021600	2.20181300	-0.69458900	C	3.58400800	-4.93386200	0.04782300
H	7.71126100	2.23135600	-0.15118900	C	3.31489000	-5.26117100	1.38115400
H	6.39908200	3.22964800	-0.80345200	H	3.89534500	-6.04707500	1.86220400
H	6.97473100	1.82267300	-1.70267000	C	2.30743000	-4.61365200	2.10795900
C	5.66865900	-1.90938000	2.05479600	C	1.56492900	-3.61228400	1.47223400
H	6.68544500	-2.19659200	1.76691800	H	0.76612000	-3.12782100	2.02469800
H	5.00416200	-2.75670300	1.85440700	C	4.68676700	-5.63359700	-0.71460000
H	5.66870100	-1.74727200	3.14086200	H	4.47553200	-5.66195800	-1.78873900
C	1.51316900	2.78793700	-0.35695900	H	4.82283100	-6.66356800	-0.36759100
C	1.53684400	4.11655900	0.09126100	H	5.64778500	-5.11761100	-0.58610500
H	1.64441800	4.32752800	1.15060000	C	2.03431300	-4.98095400	3.54893400
C	1.43077900	5.18302700	-0.81005300	H	2.07875500	-6.06546100	3.70032500
C	1.30965200	4.89477300	-2.17550100	H	1.04745300	-4.63282500	3.86895400
H	1.24126900	5.71689800	-2.88677200	H	2.77651200	-4.53041000	4.22131500
C	1.27747500	3.57866000	-2.65104100	C	1.59370800	-1.45814800	-2.18624400
C	1.37611900	2.52976900	-1.72824300	C	2.96289900	-1.13589400	-2.15374600
H	1.33731100	1.50500100	-2.08437900	H	3.51977300	-1.22833900	-1.22815000
C	1.43616400	6.61409400	-0.32024700	C	3.63463600	-0.71244100	-3.30391900

C	2.91030200	-0.58399800	-4.49798200
H	3.42679100	-0.26003900	-5.40039600
C	1.54640100	-0.87439300	-4.55860600
C	0.90128000	-1.31897600	-3.39471000
H	-0.15200600	-1.56978900	-3.44916900
C	0.76958800	-0.72716000	-5.84762100
H	0.04198000	0.09183900	-5.78252700
H	0.20614500	-1.63841100	-6.08058200
H	1.43308300	-0.51567800	-6.69245900
C	5.11450500	-0.40479700	-3.27550100
H	5.65518100	-0.98370400	-4.03478400
H	5.55064400	-0.63228100	-2.29891700
H	5.30394300	0.65571000	-3.48591900
Ru	-0.17374500	-0.25121500	0.62426300
P	1.65093200	1.34522400	0.79180600
P	0.69479600	-1.99976700	-0.64980600
H	0.05591300	3.12010700	-4.37782300
H	-1.59102700	-3.11630600	1.38832700
C	-1.72694600	1.56564300	-0.29543600
C	-2.70189000	2.51337300	-0.95913900
C	-2.74380600	3.90086700	-0.28702600
C	-3.69584600	4.84871900	-0.98417500
C	-3.25821700	5.64778300	-2.05010600
C	-4.13930300	6.49855200	-2.71951000
C	-5.47934800	6.56537200	-2.33202600
C	-5.92849200	5.77686700	-1.27067100
C	-5.04293700	4.92790200	-0.60455200
H	-2.43329400	2.59690900	-2.01709300
H	-3.69833100	2.05191600	-0.92094300
H	-3.03071800	3.77154900	0.76155300
H	-2.21362500	5.60271200	-2.35259100
H	-3.77859200	7.11253900	-3.54114200
H	-6.16663300	7.22925000	-2.84989200
H	-6.96843200	5.82555000	-0.95757000
H	-5.39920200	4.32027700	0.22491900
O	-1.08232500	0.72595000	-1.01751200
O	-1.53017400	1.58537900	0.95381200
H	-1.73113000	4.32117600	-0.28635400
C	-2.21360000	-2.23054300	1.61463900
C	-3.69126300	-2.66888400	1.59918400
C	-4.67593200	-1.54502600	1.97535200
C	-6.12241500	-1.95636600	1.80974800
C	-6.80434900	-2.63658200	2.82912000
C	-8.12734300	-3.04839700	2.66147900

C	-8.79808600	-2.78544800	1.46495400
C	-8.13403800	-2.10627100	0.44153100
C	-6.81088800	-1.69633700	0.61580200
H	-3.91642800	-3.02643000	0.58726500
H	-3.81560200	-3.51991700	2.28101900
H	-4.49993000	-1.24678600	3.01794900
H	-6.29043100	-2.84269200	3.76595300
H	-8.63640800	-3.57151700	3.46746100
H	-9.82938200	-3.10269300	1.33343500
H	-8.64818700	-1.88970800	-0.49185300
H	-6.30214600	-1.15944700	-0.18253500
O	-2.02170200	-1.19717600	0.75349200
O	-1.79714100	-1.90595400	2.97661400
H	-4.45667100	-0.67433200	1.34865200
H	-0.08272300	-1.00483700	2.24755100
H	0.70970800	-0.86481300	2.03607300
H	-2.18256400	-1.02789500	3.14457200

**TS5**

C	0.87056300	2.26779400	2.55760500
C	-0.44684300	2.31459400	3.04118900
H	-1.25442400	1.94823600	2.41836000
C	-0.73727400	2.85669200	4.29863800
C	0.31286300	3.35948800	5.07560100
H	0.09519500	3.78758000	6.05327200
C	1.63454700	3.33045700	4.62177700
C	1.89935300	2.78572100	3.35801400
H	2.92395300	2.77599500	3.00258100
C	-2.15875900	2.88008600	4.81491300
H	-2.35677100	2.02381000	5.47412400
H	-2.88142800	2.83458700	3.99382600
H	-2.36096800	3.78669200	5.39666800
C	2.76189100	3.85462700	5.48304600
H	3.59135800	4.22955300	4.87382600
H	3.16707700	3.06652500	6.13225400
H	2.42459200	4.66848400	6.13438200
C	3.05049100	1.42130000	0.93246200
C	3.89754600	2.40069300	0.39443300
H	3.47592200	3.24103000	-0.14792700
C	5.28539500	2.32460200	0.55916900
C	5.81658700	1.24644100	1.27970900
H	6.89416300	1.18365500	1.42394200
C	4.99766200	0.25372400	1.82915900
C	3.61175100	0.35254100	1.64238300
H	2.96219500	-0.40986200	2.06361400



C	6.19463800	3.37893800	-0.03109000	C	4.46224100	-4.24467300	0.18522500
H	7.01600400	3.62675800	0.65097500	C	4.19959000	-4.57474900	1.52187100
H	5.64646800	4.30078300	-0.25065300	H	4.86702200	-5.26171700	2.04009400
H	6.64748200	3.03523400	-0.97047800	C	3.09708600	-4.05022300	2.20363700
C	5.58587200	-0.88792500	2.62700000	C	2.24226700	-3.17534500	1.51847700
H	6.67895900	-0.89756800	2.56274800	H	1.38025200	-2.76556700	2.03524000
H	5.21468700	-1.85578400	2.27265300	C	5.67132000	-4.81135100	-0.52463300
H	5.31807400	-0.80821700	3.68873300	H	5.56787600	-4.73761000	-1.61193000
C	0.93051700	2.99671400	-0.26310500	H	5.82853200	-5.86558900	-0.26956500
C	0.68197300	4.29366200	0.21123200	H	6.58617200	-4.27197400	-0.24512600
H	0.64632600	4.48061000	1.27990200	C	2.83877500	-4.39838000	3.65220800
C	0.48232900	5.35947900	-0.67389600	H	3.29607700	-5.35633800	3.92162900
C	0.54853100	5.10660800	-2.05054000	H	1.76594700	-4.46142100	3.86337100
H	0.40847500	5.93105200	-2.74850300	H	3.25571600	-3.63621900	4.32407200
C	0.79237600	3.82364900	-2.55244700	C	2.15316000	-1.03493200	-2.11070200
C	0.97635200	2.77192700	-1.64528400	C	3.45051900	-0.52285800	-1.92879400
H	1.14697700	1.76838200	-2.02251600	H	3.93001100	-0.59204700	-0.95853300
C	0.18965900	6.75107800	-0.15851400	C	4.15450400	0.06060600	-2.98625400
H	-0.88092700	6.98522200	-0.22816200	C	3.53333100	0.15268300	-4.23985700
H	0.72441400	7.51411200	-0.73607600	H	4.07711800	0.59864200	-5.07149500
H	0.47900300	6.85712300	0.89201600	C	2.23851400	-0.32598100	-4.44827200
C	0.83292400	3.56344500	-4.04133200	C	1.56147300	-0.92277900	-3.37449900
H	1.64623600	2.87738700	-4.30213300	H	0.56450800	-1.31305500	-3.54448900
H	0.97016700	4.49081100	-4.60768400	C	1.56884900	-0.21229300	-5.79948900
C	0.18856700	-3.08428100	-1.56212200	H	0.78350500	0.55457900	-5.79072800
C	-1.00553600	-2.68931600	-2.19274600	H	1.09268600	-1.15581100	-6.09019300
H	-1.33863000	-1.66015700	-2.11504900	H	2.28669800	0.05869200	-6.58070700
C	-1.78047900	-3.60766200	-2.90522700	C	5.56394300	0.57336600	-2.79602400
C	-1.35986700	-4.94411800	-2.96382800	H	6.26012800	0.09316500	-3.49539000
H	-1.96004600	-5.66755400	-3.51433900	H	5.92178200	0.38783200	-1.77937000
C	-0.19361700	-5.37103700	-2.32727300	H	5.62176200	1.65420900	-2.97795100
C	0.57776100	-4.42625900	-1.63260100	Ru	-0.19685700	-0.31027400	0.42458100
H	1.49007700	-4.75823600	-1.14860000	P	1.20133000	1.55157500	0.86327500
C	-3.06037300	-3.17530500	-3.58528700	P	1.20552900	-1.78552700	-0.69276200
H	-3.19560400	-2.09129000	-3.52279600	H	-0.10134700	3.10036300	-4.38576000
H	-3.93701000	-3.64677800	-3.12206700	H	-1.01790200	-3.31817600	1.37788200
H	-3.06809800	-3.45760800	-4.64565200	C	-2.04856000	1.15954800	-0.60596500
C	0.22876200	-6.82305100	-2.36363900	C	-3.16599700	1.94639000	-1.26083600
H	-0.24615000	-7.35730900	-3.19339700	C	-3.46219100	3.27838200	-0.53978400
H	-0.04961000	-7.34375000	-1.43743900	C	-4.53805300	4.08471800	-1.23478100
H	1.31453500	-6.92353500	-2.47458300	C	-4.20509300	5.01913700	-2.22564500
C	2.47201400	-2.82679300	0.18215900	C	-5.19486200	5.74266200	-2.89299100
C	3.58595400	-3.37540700	-0.47428700	C	-6.54088000	5.54300500	-2.57921300
H	3.77197300	-3.13492200	-1.51626900	C	-6.88712700	4.61662900	-1.59325600

C -5.89315600 3.89627700 -0.92874500  
H -2.89491900 2.11977400 -2.30683800  
H -4.06892000 1.32022400 -1.26381900  
H -3.75616600 3.05762200 0.49162100  
H -3.15715700 5.18135100 -2.47053700  
H -4.91475600 6.46544600 -3.65540300  
H -7.31307500 6.10732600 -3.09551900  
H -7.93178500 4.45775700 -1.33752000  
H -6.17026600 3.18019800 -0.15755000  
O -1.19673500 0.54876100 -1.32776300  
O -1.94857900 1.11022800 0.66176000  
H -2.53584000 3.86258300 -0.48498700  
C -1.85231200 -2.59413700 1.34457400  
C -3.19163000 -3.29759400 1.57084200  
C -4.39569000 -2.34288100 1.68137200  
C -5.71991900 -3.07572600 1.70718800  
C -6.28292300 -3.51105800 2.91494300  
C -7.49013400 -4.21173400 2.93517100  
C -8.15874400 -4.49028000 1.74141200  
C -7.61040700 -4.06197600 0.53060400  
C -6.40314700 -3.36157100 0.51658600  
H -3.33560700 -3.95743900 0.70535300  
H -3.12294100 -3.94051400 2.45626100  
H -4.30313400 -1.73887800 2.59472900  
H -5.77082500 -3.29342300 3.85026000  
H -7.91052200 -4.53620400 3.88385900  
H -9.10059900 -5.03249600 1.75479500  
H -8.12579600 -4.26840100 -0.40417300  
H -5.98432000 -3.02563000 -0.42993000  
O -1.83010400 -1.70854800 0.38741400  
O -1.48788300 -1.84075200 2.75184900  
H -4.35872800 -1.64937800 0.83546600  
H -0.48863400 -1.21669400 2.27277000  
H 0.40285800 -0.82703400 1.93453200  
H -2.13805400 -1.11132700 2.79285400

**TS5a**

C 1.25536300 -0.09943300 2.87555700  
C 2.25505300 0.82829800 2.55526600  
H 2.48053200 1.03499400 1.51601100  
C 2.98955000 1.47743000 3.55925600  
C 2.70899900 1.17919100 4.89488100  
H 3.27576300 1.67626100 5.68093100  
C 1.71899500 0.25274400 5.24782200

C 1.00099700 -0.38099800 4.22924300  
H 0.23719000 -1.10097200 4.50229800  
C 4.05067900 2.48939200 3.18991700  
H 3.60207800 3.42918800 2.84288700  
H 4.68717800 2.12069100 2.37749400  
H 4.69373400 2.72524000 4.04447000  
C 1.42486800 -0.04245900 6.70174200  
H 0.79188600 -0.92919400 6.80964500  
H 0.90228500 0.79556500 7.18175100  
H 2.34611400 -0.21397700 7.27123000  
C -1.13731100 -1.59524600 2.47137700  
C -1.19288100 -2.90808000 2.95935500  
H -0.40099700 -3.60976600 2.71665900  
C -2.25162800 -3.32982600 3.77310700  
C -3.25702900 -2.40884000 4.09482500  
H -4.07837800 -2.72344200 4.73672500  
C -3.22780800 -1.09056600 3.62428300  
C -2.16052600 -0.69837500 2.80534900  
H -2.12441400 0.32094800 2.43003500  
C -2.31263500 -4.75091000 4.28667900  
H -1.31546800 -5.20056300 4.33552100  
H -2.92471400 -5.38584700 3.63252200  
H -2.75527000 -4.79602800 5.28789800  
C -4.30202800 -0.10100300 4.01407100  
H -5.16406200 -0.60490400 4.46374300  
H -4.65315300 0.47070600 3.14854500  
H -3.92400100 0.62216600 4.74869300  
C 1.30986700 -2.46791400 1.16480500  
C 2.44676400 -2.80755100 1.91112800  
H 2.76057100 -2.17348800 2.73437100  
C 3.18569300 -3.96046400 1.61447500  
C 2.75658600 -4.77551200 0.56004200  
H 3.31453400 -5.68248000 0.33082400  
C 1.62685200 -4.45920700 -0.20510900  
C 0.91241500 -3.29617600 0.10525700  
H 0.04316900 -3.03150600 -0.48854300  
C 4.42771900 -4.30672800 2.40508600  
H 5.33044300 -3.91161300 1.92042700  
H 4.55659600 -5.39110900 2.49478700  
H 4.39066500 -3.88437600 3.41462400  
C 1.20087300 -5.33699100 -1.36020300  
H 0.11317800 -5.32848000 -1.48561300  
H 1.52307100 -6.37415000 -1.21654700  
C -2.36686500 0.70886400 -2.77042200

C	-1.24519300	0.79811600	-3.60461600	H	-0.98203100	-4.42392900	-4.16862200
H	-0.27668100	0.47735500	-3.23676300	H	-2.45329100	-3.76888200	-4.88697500
C	-1.34878900	1.31827100	-4.90238600	C	-3.94639500	-4.75684500	0.63678400
C	-2.60525300	1.72789400	-5.36057600	H	-4.89333300	-5.20029700	0.30332700
H	-2.69512000	2.14050100	-6.36423100	H	-4.14772000	-4.16456800	1.53387500
C	-3.74842200	1.62878700	-4.55775800	H	-3.28808100	-5.58679400	0.92344700
C	-3.61367500	1.12365100	-3.25969300	Ru	-0.00297100	0.50883900	-0.30021100
H	-4.49366000	1.06861300	-2.62687200	P	0.30933000	-0.95042700	1.51174500
C	-0.10772500	1.48756700	-5.74978300	P	-2.16538000	0.04619400	-1.04123400
H	0.52222300	2.28787800	-5.34036700	H	1.63891300	-4.98644400	-2.30443400
H	-0.35782500	1.74785000	-6.78344600	H	1.60122500	2.31952500	-2.33996200
H	0.49625000	0.57264100	-5.76585500	C	2.16847100	-0.32114100	-1.42098400
C	-5.10157400	2.04795200	-5.08731200	C	3.39409000	-0.83125400	-2.14750700
H	-5.79487300	2.28240700	-4.27286100	C	4.63829900	-0.92235200	-1.24004100
H	-5.55986300	1.25060600	-5.68815100	C	5.83864000	-1.48978100	-1.96664000
H	-5.02402700	2.93180300	-5.73044900	C	6.05743100	-2.87407000	-2.01352000
C	-3.65871100	0.75982300	-0.20544300	C	7.14413500	-3.40613300	-2.70932600
C	-4.90393000	0.11751300	-0.14637500	C	8.03426000	-2.55873900	-3.37271400
H	-5.01982000	-0.88232700	-0.55165700	C	7.82917200	-1.17812600	-3.33299300
C	-6.01966100	0.75319900	0.41450300	C	6.74102600	-0.65108000	-2.63516900
C	-5.87341100	2.05664400	0.90432000	H	3.15176000	-1.80622800	-2.58163700
H	-6.73820800	2.56394800	1.32925800	H	3.59836800	-0.15275700	-2.98774100
C	-4.64689600	2.72947400	0.84844900	H	4.86162100	0.07677900	-0.85216000
C	-3.54726100	2.06650600	0.29077400	H	5.36807900	-3.53796100	-1.49496100
H	-2.59851900	2.58854000	0.21587400	H	7.29846100	-4.48216000	-2.73014100
C	-7.35128200	0.04141100	0.49919400	H	8.88291100	-2.97053700	-3.91257700
H	-7.42554200	-0.75922600	-0.24400000	H	8.51945600	-0.50979000	-3.84156000
H	-8.18631400	0.73226200	0.33835000	H	6.59105100	0.42621400	-2.60325400
H	-7.49557400	-0.41593200	1.48725400	O	1.01359100	-0.76968200	-1.72896000
C	-4.50482900	4.13369000	1.39039000	O	2.26478100	0.55588000	-0.50622200
H	-3.74217700	4.69738500	0.84322500	H	4.39505700	-1.54950600	-0.37415200
H	-4.20544200	4.12298700	2.44699600	C	0.90732200	3.08674900	-1.95569900
H	-5.44856700	4.68565400	1.32528700	C	1.68672400	4.00872400	-1.01004400
C	-2.53513700	-1.75638700	-1.28369400	C	0.83306800	5.14254400	-0.41139800
C	-3.07462900	-2.55144700	-0.25621500	C	1.61095500	6.01171700	0.55156900
H	-3.31751100	-2.10884300	0.70338100	C	2.33659800	7.12240000	0.09730900
C	-3.32323000	-3.91318500	-0.45218200	C	3.08159600	7.90732200	0.97921100
C	-2.99515700	-4.48723300	-1.68890100	C	3.11443600	7.59638200	2.34016700
H	-3.18987000	-5.54639400	-1.85114900	C	2.39487400	6.49515800	2.80936400
C	-2.43560800	-3.73036900	-2.72037800	C	1.65205400	5.71331700	1.92195700
C	-2.21815400	-2.36148700	-2.50623500	H	-0.41164700	3.46939200	-3.28791500
H	-1.80485600	-1.76711200	-3.31410400	H	2.11571200	3.39041300	-0.21213800
C	-2.07083900	-4.35925900	-4.04625900	H	2.52948200	4.44010000	-1.56622500
H	-2.47523900	-5.37300700	-4.13349500	H	0.43653300	5.74490000	-1.23565000

H	2.31247700	7.37447900	-0.96090100
H	3.63316300	8.76582700	0.60353100
H	3.69066000	8.20884200	3.02890700
H	2.40483000	6.24830700	3.86837100
H	1.08822200	4.86089200	2.29677300
O	-0.20350700	2.47833300	-1.37200100
O	0.44450600	3.86915100	-3.06203500
H	-0.03071400	4.70483400	0.10347300
H	-0.33980400	2.24322800	0.04758200
H	-0.53190700	1.74640700	0.83180200

**Int8**

C	0.49363700	-2.40006300	1.89085400
C	1.53383400	-1.59910400	2.37110100
H	1.77292600	-0.66669800	1.87328700
C	2.24843600	-1.95794500	3.52596300
C	1.90344600	-3.13604300	4.19047400
H	2.44476200	-3.41737000	5.09325800
C	0.86425300	-3.96120200	3.73340500
C	0.16553700	-3.57871700	2.58637900
H	-0.65300500	-4.20183900	2.23643500
C	3.37217200	-1.07666200	4.02415000
H	3.20612500	-0.03300900	3.73853400
H	4.33787500	-1.38173000	3.59809500
H	3.47012700	-1.12571400	5.11441800
C	0.50751600	-5.22859800	4.47815100
H	-0.35899300	-5.72515100	4.02980900
H	0.26722000	-5.02145900	5.52849500
H	1.34004400	-5.94413500	4.47608200
C	-2.15217100	-2.38173500	0.92200200
C	-2.94035800	-3.33978600	0.27769800
H	-2.58206100	-3.82231000	-0.62615100
C	-4.19449500	-3.70500800	0.78801100
C	-4.63891500	-3.10670500	1.97067800
H	-5.60169500	-3.40120400	2.38601900
C	-3.87468000	-2.13852700	2.63551100
C	-2.63732600	-1.78126400	2.09402200
H	-2.03645700	-1.03486700	2.60669600
C	-5.05412000	-4.70907600	0.05489000
H	-5.78724300	-5.17549200	0.72186300
H	-4.44940200	-5.50492200	-0.39438400
H	-5.61006000	-4.22465200	-0.75909700
C	-4.35569500	-1.51318900	3.92571000
H	-5.44185500	-1.60260100	4.03501200

H	-4.09542200	-0.44987500	3.97320700
H	-3.89831200	-1.99871700	4.79831600
C	0.01178800	-3.22397600	-0.85694900
C	0.95350300	-4.22014100	-0.57587300
H	1.40649100	-4.27457900	0.40867100
C	1.33312100	-5.16230900	-1.54686600
C	0.74933200	-5.09241700	-2.81247700
H	1.03923000	-5.81522800	-3.57380800
C	-0.19963100	-4.10779300	-3.12829400
C	-0.54783600	-3.17598000	-2.14722800
H	-1.25496600	-2.38905600	-2.38984100
C	2.33771900	-6.24177800	-1.20933200
H	2.73200200	-6.71974800	-2.11213200
H	1.88391100	-7.02853700	-0.59223000
H	3.18489500	-5.84040400	-0.64083900
C	-0.82313000	-4.06241100	-4.50536100
H	-1.42114300	-3.15668700	-4.64396900
H	-1.48176900	-4.92462500	-4.67368100
C	-2.03205000	2.64280400	-1.73640000
C	-0.91404400	3.38848500	-2.12186400
H	0.05881100	3.14244000	-1.71144300
C	-1.02780700	4.43801900	-3.04861000
C	-2.28133600	4.73160000	-3.58573600
H	-2.37580600	5.54134900	-4.30828200
C	-3.42147400	4.00082100	-3.22265500
C	-3.28232900	2.96002100	-2.30193800
H	-4.16232600	2.38295900	-2.03674500
C	0.19789800	5.22752900	-3.45126600
H	0.61461300	5.78071300	-2.60008500
H	-0.03291900	5.95250500	-4.23900100
H	0.99205300	4.56774700	-3.82095100
C	-4.76909300	4.33196100	-3.82457300
H	-5.07835000	5.35617000	-3.57886100
H	-5.54667000	3.65280300	-3.46029400
H	-4.74859200	4.25859400	-4.91936500
C	-2.39634500	2.14254500	1.09646800
C	-3.44666500	3.07646300	1.13556500
H	-3.98169500	3.32696900	0.22468500
C	-3.80917800	3.70725100	2.32766600
C	-3.09447700	3.39663000	3.49519300
H	-3.36238900	3.89187300	4.42778000
C	-2.03667800	2.48586300	3.48668700
C	-1.69559600	1.86504400	2.27403300
H	-0.84331900	1.19453300	2.23659800

C	-4.93870800	4.71237100	2.36599000	H	6.59082600	8.02578000	1.47579500
H	-5.74710900	4.38368800	3.03186000	H	7.00255900	6.41275700	-0.37433800
H	-5.36861500	4.86721600	1.37130400	H	5.23559100	4.81323000	-1.04413500
H	-4.59549900	5.68661600	2.73616900	O	1.31813200	1.37365000	1.36369800
C	-1.26292600	2.16684500	4.74633600	O	1.43171600	2.04684400	-0.73985800
H	-1.56237100	1.19703900	5.16602800	H	1.74930800	4.93534500	0.15517100
H	-1.42654400	2.92399400	5.52062300	C	2.62659000	-1.18260900	-1.70536000
H	-0.18804800	2.10943500	4.54263500	C	4.03226300	-1.67703500	-1.88014500
C	-3.34052300	0.26340600	-0.95036000	C	4.93762200	-1.50076600	-0.65042700
C	-4.50860500	0.18215000	-0.18944500	C	6.33304100	-2.03885500	-0.88796500
H	-4.56307900	0.67731200	0.77448000	C	7.33519100	-1.22096800	-1.42794100
C	-5.63471900	-0.51355600	-0.65961700	C	8.61261700	-1.72326700	-1.68087300
C	-5.56921800	-1.12575800	-1.91241400	C	8.91010500	-3.05739500	-1.39545900
H	-6.44491500	-1.64812500	-2.29545600	C	7.92219600	-3.88248500	-0.85412300
C	-4.40732800	-1.07043700	-2.69667200	C	6.64629000	-3.37511400	-0.60318300
C	-3.30269200	-0.37399900	-2.20246500	H	3.96275700	-2.73575200	-2.17505300
H	-2.40475900	-0.29585500	-2.80977500	H	4.45318500	-1.16872500	-2.76173200
C	-4.35783000	-1.75157100	-4.04603600	H	4.97956600	-0.43666900	-0.39242600
H	-5.31491200	-1.66737200	-4.57357900	H	7.11360700	-0.17800900	-1.64557600
H	-4.13835100	-2.82327300	-3.94617700	H	9.37685500	-1.07091300	-2.09540000
H	-3.58242800	-1.31566100	-4.68501900	H	9.90520200	-3.44929900	-1.58797500
C	-6.88841700	-0.59015900	0.18111100	H	8.14607000	-4.92036800	-0.62121300
H	-7.12802000	0.37906800	0.63379100	H	5.88390400	-4.02209400	-0.17333600
H	-6.76527400	-1.30853100	1.00157300	O	2.22034000	-0.67546900	-0.66655400
H	-7.75165500	-0.90820900	-0.41322100	H	4.47291900	-2.00573000	0.20380200
Ru	0.18972300	0.20725000	-0.40822300	H	1.93927200	-1.29746000	-2.55796000
P	-0.44835700	-1.88809300	0.36370700				
P	-1.85961900	1.28072900	-0.46299100	<b>Int8a</b>			
H	-0.05976400	-4.08577600	-5.29260300	C	0.60851700	-2.03930800	2.39340900
H	-0.21677700	-0.27770100	-1.87635700	C	1.64609100	-1.20838700	2.82506000
C	1.78531600	2.14833800	0.48364900	H	1.89795300	-0.33117400	2.24295200
C	2.81693800	3.19957100	0.87419500	C	2.37568400	-1.50514200	3.98680700
C	2.74449700	4.48911500	0.03364500	C	2.05030000	-2.65322000	4.71062300
C	3.80881000	5.49441900	0.41885700	H	2.61294300	-2.89170800	5.61239800
C	3.59166500	6.41174000	1.45690000	C	1.01320900	-3.50630500	4.30588100
C	4.58395300	7.31633600	1.83765300	C	0.29983900	-3.18520200	3.14889700
C	5.81772400	7.32005900	1.18327200	H	-0.51083600	-3.83715000	2.83707100
C	6.04798400	6.41393900	0.14619500	C	3.48116400	-0.58034000	4.44539100
C	5.05134100	5.51187900	-0.23030000	H	3.07377800	0.33847600	4.88853800
H	2.69583100	3.41701700	1.94029700	H	4.12032100	-0.27899000	3.60717300
H	3.81246200	2.74644900	0.76122500	H	4.11540500	-1.05550700	5.20132500
H	2.83910200	4.21948900	-1.02309100	C	0.67779500	-4.74239700	5.11052400
H	2.63115400	6.41818500	1.96835300	H	-0.16087300	-5.28998900	4.66888200
H	4.39199100	8.02129700	2.64275900	H	0.40316300	-4.48735900	6.14194900

H	1.53234100	-5.42883500	5.16739300	H	1.38831200	4.07081800	-4.24841200
C	-2.02245100	-2.22789500	1.39473100	H	0.19314800	3.89577900	-5.53629800
C	-2.54773800	-3.47137500	1.01728300	H	0.82337000	2.45895100	-4.70681100
H	-2.01271100	-4.09013800	0.30365800	C	-3.16196000	6.17444800	-2.32273400
C	-3.75033900	-3.94132200	1.55928500	H	-3.36224000	6.42756600	-1.27570900
C	-4.42527600	-3.13890100	2.48872200	H	-4.13494300	6.06808700	-2.82097700
H	-5.35508900	-3.49982300	2.92622800	H	-2.64920500	7.02428300	-2.78518200
C	-3.92990400	-1.88910600	2.87856100	C	-3.38036200	1.85390100	0.65547000
C	-2.72379300	-1.44517000	2.32022700	C	-4.73039400	2.03506500	0.30591400
H	-2.32061100	-0.48044900	2.61538600	H	-5.08157500	1.72137600	-0.67252000
C	-4.31269200	-5.28332300	1.14705300	C	-5.63982900	2.61044800	1.19785600
H	-3.54192200	-5.91715900	0.69685100	C	-5.17588700	3.02150200	2.45674600
H	-5.11665100	-5.17039900	0.40781200	H	-5.87590500	3.47290900	3.15848200
H	-4.73563800	-5.82075400	2.00369400	C	-3.83883200	2.86738300	2.83114300
C	-4.65879400	-1.04475300	3.89965500	C	-2.95251300	2.27455800	1.91826000
H	-5.65354300	-1.44866100	4.11511000	H	-1.91187400	2.12499700	2.19318800
H	-4.77782900	-0.01236300	3.55201900	C	-7.09578200	2.77883000	0.82490600
H	-4.10599700	-1.00452400	4.84731300	H	-7.26654500	2.54777200	-0.23121800
C	0.19467000	-2.92567300	-0.36026300	H	-7.44075400	3.80401300	1.00616100
C	1.14921500	-3.90668500	-0.05728000	H	-7.73872500	2.11469100	1.41713200
H	1.58557600	-3.95003400	0.93538700	C	-3.34404500	3.34341300	4.17870000
C	1.55383700	-4.84407600	-1.01751100	H	-2.80942400	4.29850300	4.09030000
C	0.97239800	-4.79248200	-2.28937500	H	-2.64694700	2.62547600	4.62519300
H	1.26663400	-5.52643700	-3.03838500	H	-4.17132500	3.49461900	4.87993800
C	0.02211200	-3.82012900	-2.62383300	C	-3.14360000	0.03072900	-1.59247900
C	-0.35119500	-2.88566200	-1.65161300	C	-4.11194900	-0.80942800	-1.01511900
H	-1.07143900	-2.11397600	-1.90827400	H	-4.28472800	-0.78129700	0.05549700
C	2.61048300	-5.87583600	-0.68950100	C	-4.88348900	-1.67452600	-1.79772500
H	3.61628200	-5.50632400	-0.93118400	C	-4.65501700	-1.71808700	-3.17955600
H	2.45889900	-6.80006400	-1.25812100	H	-5.25122500	-2.38839900	-3.79685500
H	2.60689900	-6.12853500	0.37619400	C	-3.68737000	-0.91260000	-3.78305600
C	-0.57051500	-3.75827000	-4.01343100	C	-2.94215900	-0.03962800	-2.97691900
H	-1.62670300	-3.46977900	-3.98194700	H	-2.20943100	0.60085000	-3.45458400
H	-0.49370800	-4.72310800	-4.52658500	C	-3.44426200	-0.96296600	-5.27516100
C	-1.87551900	2.62859100	-1.68935100	H	-4.19743400	-1.57462400	-5.78248400
C	-0.87333400	2.53233600	-2.67305100	H	-2.45959500	-1.38923500	-5.50583400
H	-0.26822000	1.63223000	-2.73793000	H	-3.47092700	0.03969000	-5.71843400
C	-0.60070100	3.59745600	-3.53898200	C	-5.97272500	-2.51947100	-1.17699900
C	-1.34618800	4.78032800	-3.40609400	H	-6.96549400	-2.09029400	-1.36958300
H	-1.13910500	5.61774700	-4.07073900	H	-5.84787700	-2.59605200	-0.09327700
C	-2.34717600	4.90588600	-2.43881100	H	-5.97768300	-3.53393600	-1.59317600
C	-2.59970300	3.82026200	-1.58487800	Ru	-0.00499600	0.51457800	0.13826900
H	-3.36880100	3.92437400	-0.82681500	P	-0.35331900	-1.62691800	0.84636500
C	0.50711700	3.49675500	-4.56482700	P	-2.11589300	1.17626200	-0.53161900

H	-0.04905100	-3.01470800	-4.63107200
H	1.82984400	2.66903500	-1.66358000
C	2.19153000	-0.13782500	-1.19669400
C	3.48197500	-0.54965000	-1.88922400
C	4.27892300	-1.60800800	-1.09818200
C	5.52156200	-2.06517800	-1.83130400
C	5.45389200	-3.09896900	-2.77707700
C	6.58872000	-3.50571700	-3.48040800
C	7.81722100	-2.88254800	-3.24960500
C	7.89980200	-1.85264100	-2.31039200
C	6.76142500	-1.45028400	-1.60925400
H	3.23007000	-0.91627400	-2.88900300
H	4.10319500	0.34719200	-2.02562100
H	4.54117500	-1.18952500	-0.12127500
H	4.49897500	-3.58801600	-2.96041700
H	6.51477600	-4.31178500	-4.20636000
H	8.70291300	-3.19951200	-3.79408500
H	8.85227800	-1.36435900	-2.11950300
H	6.83475700	-0.65075500	-0.87471300
O	1.14234200	0.05864900	-1.87381300
O	2.18714400	0.01249300	0.07305600
H	3.62301100	-2.46509800	-0.90568500
C	1.78301200	3.30837600	-0.77713300
C	3.12124400	3.31384600	-0.04252800
C	3.13855700	4.17681900	1.23734800
C	4.51656700	4.24173900	1.86229700
C	5.40537600	5.27221100	1.52655700
C	6.68955900	5.31828600	2.07191100
C	7.10682900	4.33073500	2.96641300
C	6.23042700	3.29940600	3.31080600
C	4.94752200	3.25755800	2.76254300
H	0.62155700	4.59424800	-1.62293900
H	3.37781300	2.27673200	0.19463800
H	3.87685100	3.69621500	-0.73914100
H	2.78846100	5.18445000	0.99065700
H	5.08469500	6.04695800	0.83318600
H	7.36220600	6.12836900	1.80148600
H	8.10513300	4.36649500	3.39452800
H	6.54398100	2.52825200	4.00991000
H	4.26885400	2.45298600	3.03860700
O	0.72547800	2.70976900	-0.00460400
O	1.44759900	4.62649700	-1.10836200
H	2.43644600	3.76246800	1.97563000
H	0.74963000	3.04090000	0.90640500

H	-0.34805200	0.90446100	1.65943000
<b>TS6</b>			
C	-2.08196900	-2.11854900	-2.20731100
C	-1.11489000	-2.26129900	-3.20930700
H	-0.35890100	-1.49243700	-3.33096400
C	-1.11893500	-3.37640500	-4.05914600
C	-2.11110500	-4.34601700	-3.89326100
H	-2.12319000	-5.21328200	-4.55222500
C	-3.09309100	-4.22949800	-2.90078700
C	-3.06969300	-3.10820400	-2.06536700
H	-3.83568700	-3.00821800	-1.30347300
C	-0.04912600	-3.52835500	-5.11687300
H	-0.35256200	-4.23354300	-5.89818900
H	0.88618900	-3.90221500	-4.67984800
H	0.18132800	-2.56853000	-5.59194800
C	-4.14560300	-5.30210300	-2.72889100
H	-4.98322800	-4.94669600	-2.11979500
H	-3.73298200	-6.19070400	-2.23259300
H	-4.54582500	-5.63147800	-3.69506900
C	-3.16939300	-1.09154200	0.24101400
C	-4.40864300	-0.49212100	0.49014200
H	-4.74800000	0.32875400	-0.13346200
C	-5.23296900	-0.94382200	1.52905600
C	-4.79893800	-2.02151900	2.30837100
H	-5.44177700	-2.39473700	3.10421600
C	-3.56156100	-2.63884600	2.08650700
C	-2.75418500	-2.15955000	1.04967100
H	-1.80291000	-2.64500400	0.85194700
C	-6.55457400	-0.26520900	1.80652400
H	-7.22825900	-0.91368600	2.37675400
H	-7.06277600	0.01958000	0.87838600
H	-6.40621700	0.65315000	2.38991000
C	-3.10420600	-3.80238700	2.93716400
H	-3.84325000	-4.05147200	3.70558100
H	-2.15675500	-3.57411300	3.44057100
H	-2.93817500	-4.70080100	2.32951100
C	-3.16518700	0.56172300	-2.14353600
C	-3.99664400	0.08772500	-3.16398300
H	-4.00881000	-0.97080700	-3.40240300
C	-4.81648600	0.95830200	-3.89815600
C	-4.79030600	2.31981500	-3.59102000
H	-5.41652300	3.00486000	-4.16054600
C	-3.96889200	2.82937500	-2.57503100

C	-3.16218500	1.93841100	-1.86119300	C	-2.12577000	0.58733600	3.42034500
H	-2.51082500	2.31791600	-1.08044100	H	-1.68388500	-0.29421200	3.87195200
C	-5.69072800	0.42325000	-5.00980000	C	-3.29271100	1.12456700	3.98378400
H	-6.30616600	-0.41655500	-4.66571400	C	-3.84305600	2.27495400	3.41430600
H	-5.08610900	0.05475200	-5.84823200	H	-4.73527600	2.71404900	3.85830000
H	-6.36192400	1.19581700	-5.39847700	C	-3.26735800	2.88591300	2.29142400
C	-3.96097100	4.31100600	-2.27262900	C	-2.11050100	2.32176000	1.74674800
H	-4.89770100	4.62899300	-1.79623600	H	-1.63509600	2.80482900	0.89672500
H	-3.85065500	4.90384400	-3.18836200	C	-3.89295300	4.11981100	1.68170900
C	1.24110600	1.93369300	1.99905000	H	-4.40995600	4.72146900	2.43723200
C	2.57361800	1.83245500	1.56826900	H	-4.63285900	3.85317800	0.91527500
H	2.87642000	0.98952900	0.95671400	H	-3.14183900	4.75543100	1.20057600
C	3.52172800	2.80531500	1.90854500	C	-3.93497200	0.46090300	5.17990200
C	3.11865400	3.89378700	2.69180100	H	-3.18622200	0.15915900	5.92129700
H	3.85076600	4.65152100	2.96737700	H	-4.47455600	-0.44589600	4.87822600
C	1.80017900	4.02265600	3.13770100	H	-4.65101500	1.12664400	5.67307200
C	0.87219300	3.03035200	2.79177200	Ru	0.14747700	0.03996400	-0.74331800
H	-0.14377500	3.12300700	3.15898300	P	-2.06815100	-0.57970300	-1.16030200
C	4.94747400	2.69118800	1.41752300	P	0.06337400	0.54256000	1.57296500
H	5.24137700	1.64482800	1.28607500	H	-3.14090900	4.57891000	-1.59943000
H	5.65041900	3.15924400	2.11570500	H	-0.10280400	1.67969300	-1.06957000
H	5.06972200	3.18815800	0.44620100	C	2.16772100	-1.58685700	-0.65566700
C	1.37466900	5.21398900	3.96700300	C	3.31601800	-2.56979500	-0.78705700
H	1.02196000	6.03772300	3.33144100	C	4.62618700	-2.07865100	-0.14094100
H	2.20495400	5.60167100	4.56738600	C	5.76617900	-3.05722000	-0.32710700
H	0.55520000	4.95752700	4.64726100	C	5.98886000	-4.08759800	0.59708300
C	0.61515200	-0.73094900	2.81205900	C	7.01913800	-5.01077600	0.41113800
C	1.02776900	-0.36250900	4.10480900	C	7.84923500	-4.91834800	-0.70788100
H	1.03356000	0.68518500	4.39131000	C	7.64079200	-3.89591700	-1.63590500
C	1.44581000	-1.32118100	5.03032400	C	6.60895800	-2.97547300	-1.44458200
C	1.45294600	-2.66954800	4.64150500	H	3.00070800	-3.52965900	-0.36433300
H	1.78888700	-3.42349100	5.35244300	H	3.47672100	-2.74381200	-1.86028500
C	1.05757200	-3.06688700	3.36267400	H	4.88305700	-1.10728600	-0.57545600
C	0.63854100	-2.08192400	2.45272900	H	5.34991300	-4.16233600	1.47484100
H	0.37710200	-2.36429300	1.43939700	H	7.17666600	-5.79943200	1.14275100
C	1.90160200	-0.92123200	6.41579600	H	8.65447200	-5.63373400	-0.85309800
H	1.77833500	0.15358100	6.58154300	H	8.28519700	-3.81105900	-2.50738000
H	2.96088400	-1.16193500	6.57214600	H	6.45650600	-2.17756100	-2.16864600
H	1.33497800	-1.44872200	7.19332100	O	0.96904900	-2.01829300	-0.63273700
C	1.07223000	-4.52455700	2.95841800	O	2.38892000	-0.33796900	-0.59674000
H	0.08835100	-4.99064600	3.10384700	H	4.45142100	-1.90793300	0.92854400
H	1.79384700	-5.09782800	3.55036600	H	-0.83081700	1.71940200	-2.87112100
H	1.32793700	-4.64079200	1.89972800	C	0.20469200	1.48934900	-2.57894700
C	-1.52125400	1.17618300	2.30633900	C	1.13445500	2.68597800	-2.76941500



C	2.55921600	2.51182000	-2.22329000	H	1.69627600	-2.26031200	1.54887900
C	3.44386400	3.69471900	-2.55437900	C	6.75156700	-1.08507000	0.05724600
C	3.56878200	4.77212900	-1.66433300	H	7.43693700	-1.91642000	0.25342600
C	4.35928800	5.87928000	-1.98066600	H	7.13389200	-0.20052000	0.57941500
C	5.04084900	5.93023500	-3.19811000	H	6.79185700	-0.86887200	-1.01847000
C	4.92721700	4.86428500	-4.09354400	C	3.21187900	-4.50613000	1.25738300
C	4.13711100	3.75957700	-3.77190500	H	4.07915000	-5.17052100	1.33222000
H	1.17518200	2.84954900	-3.85757200	H	2.59796500	-4.85321000	0.41598100
H	0.66141100	3.57941800	-2.34163000	H	2.61144000	-4.62957600	2.16594400
H	2.50498500	2.37571800	-1.13915700	C	2.75686900	2.19760100	1.24485800
H	3.04564800	4.73685400	-0.71078700	C	3.58873300	2.64212300	2.28507200
H	4.44491800	6.70097400	-1.27363700	H	3.67155800	2.05794600	3.19635700
H	5.65856000	6.78982100	-3.44508600	C	4.30904200	3.83588600	2.17759500
H	5.45888200	4.89047200	-5.04164000	C	4.18868000	4.58916600	1.00213400
H	4.05934900	2.92995900	-4.47194200	H	4.74125500	5.52317600	0.91183500
O	0.63460200	0.28866100	-2.83649800	C	3.36896300	4.17777500	-0.05218100
H	2.97880600	1.58736200	-2.63142900	C	2.65710700	2.97734900	0.08668400
<b>Int9</b>				H	2.00269900	2.65579400	-0.71716000
C	1.58400200	0.44449900	3.21842100	C	5.17393700	4.32313200	3.31816300
C	0.49563500	1.08231300	3.82405800	H	5.42363300	3.50941100	4.00647900
H	-0.21791000	1.61734500	3.20279900	H	4.66059600	5.09916600	3.90127100
C	0.31470100	1.02661500	5.21443200	H	6.11092600	4.75988000	2.95400600
C	1.23973500	0.32267700	5.98771400	C	3.25660100	4.99868500	-1.31745800
H	1.10248800	0.27267900	7.06718300	H	3.92463300	4.61948300	-2.10222000
C	2.34030300	-0.32416200	5.40832600	H	3.52363000	6.04558400	-1.13960700
C	2.50256700	-0.25477200	4.02194700	C	-0.60596900	-0.10688000	-3.09247800
H	3.35331900	-0.75444100	3.57087200	C	-1.94810700	0.25949300	-2.91883400
C	-0.87136900	1.71728700	5.84942500	H	-2.42720800	0.10178300	-1.95829900
H	-0.87903200	1.58500100	6.93653500	C	-2.69074300	0.81287100	-3.97210600
H	-1.81614900	1.32450200	5.45446500	C	-2.06857800	0.99357600	-5.21034600
H	-0.86386200	2.79423000	5.64105700	H	-2.63783200	1.42182200	-6.03412700
C	3.32526000	-1.08322500	6.26948900	C	-0.73233900	0.62993700	-5.41857600
H	4.13966000	-1.50268300	5.67002800	C	-0.01381900	0.07549000	-4.35340600
H	2.83886200	-1.91386500	6.79681400	H	1.01768700	-0.21652000	-4.51869800
H	3.77190600	-0.43652000	7.03544500	C	-4.13353300	1.21166000	-3.75718600
C	3.08530700	-0.68913000	1.05149100	H	-4.70437500	0.40134100	-3.28867700
C	4.39978700	-0.39481500	0.67662400	H	-4.62297200	1.46766200	-4.70269800
H	4.70698900	0.63728200	0.53968000	H	-4.21414600	2.08346700	-3.09534400
C	5.34088700	-1.41628700	0.48683400	C	-0.07655400	0.84503200	-6.76454300
C	4.94233200	-2.74085200	0.69155200	H	-0.73269300	0.53308400	-7.58565100
H	5.67162200	-3.53970500	0.56558100	H	0.85924900	0.28277400	-6.84775700
C	3.63127500	-3.06677100	1.06282300	H	0.16080700	1.90472600	-6.92877100
C	2.71122000	-2.02862200	1.23772600	C	-0.23276100	-2.64361200	-1.78082300
				C	-0.58097800	-3.20755300	-3.01850800

H	-0.55880800	-2.59577200	-3.91532700
C	-0.96758000	-4.54754000	-3.12247700
C	-1.00094800	-5.32690900	-1.95887400
H	-1.30731800	-6.36989800	-2.02726300
C	-0.66177000	-4.79639800	-0.71066200
C	-0.27849100	-3.44883600	-0.63477200
H	-0.04989100	-3.01822600	0.33319900
C	-1.37357400	-5.13480100	-4.45564500
H	-0.98666600	-4.53949400	-5.28898100
H	-2.46639100	-5.16954600	-4.55842900
H	-1.00596100	-6.16083800	-4.57203300
C	-0.69479700	-5.65797300	0.53247900
H	0.26193400	-6.17499600	0.68708000
H	-1.47136700	-6.42776300	0.46599500
H	-0.88689500	-5.05779200	1.42791300
C	2.04104700	-0.92347600	-2.28916600
C	2.71812600	-2.12275500	-2.53562500
H	2.22664200	-3.07053100	-2.34115100
C	4.02378400	-2.12604400	-3.04425800
C	4.63999900	-0.90107300	-3.31886400
H	5.64677600	-0.89340900	-3.73362900
C	3.99297200	0.31691600	-3.07605500
C	2.69567100	0.28768900	-2.55487500
H	2.17504500	1.22480900	-2.37849300
C	4.67849200	1.63441000	-3.36065200
H	5.62719200	1.48644600	-3.88677900
H	4.89338300	2.17645100	-2.43067400
H	4.05117800	2.28889200	-3.97796400
C	4.74943200	-3.43163400	-3.27389300
H	4.08370600	-4.19241500	-3.69694800
H	5.13951800	-3.83210900	-2.32883200
H	5.59769000	-3.30638200	-3.95519400
Ru	-0.25143100	0.39139600	0.31073500
P	1.80400800	0.60584600	1.37727200
P	0.30082100	-0.86535700	-1.64487200
H	2.23841000	4.97371000	-1.72163300
H	-0.19332800	2.02646400	-0.51281600
C	-2.14234700	-1.16971400	1.05662500
C	-3.21223500	-2.07837500	1.62291900
C	-4.56808900	-1.36479600	1.80840200
C	-5.64780900	-2.29939900	2.31050900
C	-6.46684400	-2.99866700	1.41297400
C	-7.44295300	-3.88509500	1.87124500
C	-7.61764100	-4.08780400	3.24174400

C	-6.80977400	-3.39718900	4.14755600
C	-5.83525200	-2.51218700	3.68350000
H	-3.33468000	-2.91943400	0.92628400
H	-2.85268900	-2.49462100	2.56914800
H	-4.43585900	-0.53228200	2.51031200
H	-6.34037500	-2.84108100	0.34370000
H	-8.07070200	-4.41324500	1.15782700
H	-8.37974300	-4.77443000	3.60092600
H	-6.94130500	-3.54354300	5.21675900
H	-5.21333100	-1.97312300	4.39539600
O	-0.94642600	-1.24360800	1.50803900
O	-2.40164200	-0.34819800	0.12790600
H	-4.85992300	-0.92406000	0.84986400
H	-0.02560700	3.46493300	0.52044600
C	-0.80378000	2.70058600	0.33433500
C	-1.98259200	3.26727100	-0.46478100
C	-2.79649500	4.26662500	0.38227900
C	-3.99481600	4.81504900	-0.36178300
C	-5.17450100	4.06232400	-0.46884800
C	-6.27286300	4.54590200	-1.18126100
C	-6.21254700	5.79688000	-1.80061600
C	-5.04649300	6.55749300	-1.70024100
C	-3.94977700	6.06805400	-0.98751000
H	-1.61539000	3.75930700	-1.37617600
H	-2.62717700	2.43725500	-0.77109200
H	-3.11676600	3.74958700	1.29373700
H	-5.23097800	3.09132300	0.01890400
H	-7.17900700	3.94872300	-1.24690800
H	-7.06864100	6.17657100	-2.35224500
H	-4.99056700	7.53467500	-2.17369300
H	-3.04546000	6.66847600	-0.91022400
O	-1.12785300	1.96897200	1.41560200
H	-2.14480600	5.09339900	0.69590000

**Int10**

C	-0.35373900	-0.66107300	-2.96526300
C	0.77639000	-1.47734900	-2.78992700
H	1.43932800	-1.30013400	-1.95042400
C	1.07345500	-2.50094000	-3.69480000
C	0.20896400	-2.71360600	-4.77808900
H	0.43111600	-3.51001000	-5.48741300
C	-0.92423000	-1.92065100	-4.97677100
C	-1.18901900	-0.88704700	-4.06607700
H	-2.05684600	-0.25731200	-4.23191200

C	2.31347500	-3.35029000	-3.52282300	C	-1.34661900	-0.75639200	5.42762000
H	2.08081000	-4.42061900	-3.57969700	C	-1.20411600	0.39901200	6.21214500
H	2.79479200	-3.16024600	-2.55859300	H	-1.03481100	0.29609000	7.28298500
H	3.05136800	-3.14065800	-4.30840100	C	-1.27902500	1.67459600	5.65299800
C	-1.85915600	-2.17869500	-6.13739700	C	-1.50339300	1.79312100	4.27081000
H	-2.35797200	-1.25916400	-6.46230900	H	-1.57875600	2.78599000	3.84018700
H	-2.64568100	-2.89525300	-5.86430100	C	-1.29573700	-2.12936400	6.05986100
H	-1.32518000	-2.59681400	-6.99780100	H	-2.26267100	-2.39884400	6.50601500
C	-2.30570400	1.35650300	-2.22145900	H	-0.54818400	-2.17500200	6.86013400
C	-2.53261600	2.65247200	-2.69950400	H	-1.05008200	-2.89937500	5.32150800
H	-1.70171100	3.33786800	-2.82499600	C	-1.11096800	2.91298800	6.50499400
C	-3.82199300	3.08814200	-3.03156800	H	-0.13261600	3.38338300	6.33906000
C	-4.88754100	2.19343400	-2.89562900	H	-1.18530600	2.67766600	7.57179700
H	-5.89100000	2.51503900	-3.16973900	H	-1.87242200	3.66678800	6.27222800
C	-4.69458500	0.88753100	-2.42666700	C	-3.55080300	-0.21787800	1.61291500
C	-3.39805200	0.48625000	-2.08478300	C	-4.58763700	0.15766600	2.48881600
H	-3.23515700	-0.52620400	-1.73026400	H	-4.45890600	1.02002000	3.13695400
C	-4.04382300	4.50186500	-3.51928100	C	-5.77784300	-0.56618200	2.55306800
H	-5.04805500	4.63007300	-3.93646600	C	-5.91422700	-1.70212700	1.73790600
H	-3.31839300	4.77728600	-4.29368200	H	-6.83324500	-2.28402400	1.79124900
H	-3.92916600	5.22292300	-2.69951500	C	-4.89603300	-2.11500200	0.87842300
C	-5.85534900	-0.07347000	-2.30327300	C	-3.71274900	-1.35545000	0.82042400
H	-6.79858100	0.40220800	-2.59103700	H	-2.89753500	-1.67135600	0.17850900
H	-5.96022600	-0.44149800	-1.27609900	C	-6.89825200	-0.14746400	3.47801600
H	-5.71633400	-0.95116800	-2.94735100	H	-7.76552700	0.22180000	2.91489300
C	0.48631200	2.05800600	-2.49234200	H	-6.57921100	0.65064000	4.15582800
C	1.13694500	1.88582800	-3.72491900	H	-7.24757900	-0.98800500	4.08965700
H	1.02154000	0.95715100	-4.27258100	C	-5.04267000	-3.36296900	0.03671900
C	1.93771600	2.89412500	-4.27010400	H	-4.30418900	-4.12318400	0.31971600
C	2.07282800	4.09711200	-3.56397700	H	-4.88738100	-3.15129300	-1.02816300
H	2.68460300	4.89426400	-3.98404400	H	-6.03716500	-3.80695400	0.14887300
C	1.43522400	4.30236600	-2.33717000	C	-2.43187000	2.47851900	1.31669700
C	0.64745600	3.26909900	-1.80649300	C	-3.72095500	2.86038400	0.93518200
H	0.15620500	3.41375400	-0.84997300	H	-4.48867400	2.10898900	0.78635900
C	2.65004800	2.69097500	-5.58859400	C	-4.04831300	4.21001500	0.72920000
H	2.50477800	3.54647500	-6.25908600	C	-3.05936900	5.17547900	0.92121100
H	2.28871900	1.79451000	-6.10194600	H	-3.30724200	6.22640300	0.77897100
H	3.73208700	2.57533700	-5.44381900	C	-1.75263800	4.82498900	1.29318000
C	1.58255500	5.61208900	-1.59566200	C	-1.44474500	3.47261800	1.46562700
H	0.62079200	6.13300400	-1.50975000	H	-0.42696100	3.18729200	1.71566000
H	2.27995400	6.28378900	-2.10666900	C	-0.71203000	5.89525500	1.53505000
C	-1.64028200	0.66234600	3.46269600	H	0.29754200	5.47362000	1.55854100
C	-1.55969300	-0.60922400	4.05703400	H	-0.88008500	6.39968300	2.49606300
H	-1.65881300	-1.49931000	3.44268900	H	-0.74038000	6.66901100	0.75898000



H	1.36361600	-4.96900700	3.91989000	H	-3.39590300	5.90421800	-3.10170000
C	0.86639800	-0.44891600	2.39937700	H	-3.76042200	4.42961300	-2.18528000
C	0.70995900	0.09560300	3.67568900	H	-3.16369600	4.31386100	-3.84023000
H	-0.27557000	0.38367800	4.02715300	C	1.37752300	7.17067000	-2.10836300
C	1.81231100	0.26824300	4.52737800	H	2.36984000	6.99413900	-1.68152100
C	3.06842700	-0.14658800	4.08373300	H	0.93090100	8.02009000	-1.57641000
H	3.92569600	-0.04507100	4.74814000	H	1.51331400	7.48179400	-3.15201300
C	3.25504900	-0.69949700	2.80721500	C	2.47568600	1.85901400	-1.45409800
C	2.14928200	-0.82743200	1.96242400	C	2.55007600	2.22466400	-2.80663400
H	2.26201300	-1.24169700	0.96387800	H	1.69979400	2.69949400	-3.28695200
C	1.63530700	0.90383400	5.88684800	C	3.71037800	2.00423400	-3.56003500
H	0.69468800	0.59467700	6.35639300	C	4.80941500	1.40909100	-2.93210900
H	1.61278400	1.99855100	5.80329600	H	5.72205800	1.24406800	-3.50238400
H	2.45524200	0.64127800	6.56385100	C	4.76351900	1.01524500	-1.58954300
C	4.62606600	-1.17566300	2.38267900	C	3.58303300	1.22951500	-0.86576800
H	4.98261600	-1.98500800	3.03284600	H	3.53027900	0.89809800	0.16639100
H	5.36968100	-0.37077300	2.44256700	C	3.78272800	2.44303600	-5.00517600
H	4.62166000	-1.55462800	1.35665300	H	4.08049500	3.49723600	-5.08510000
C	-2.04349800	-0.47028100	2.35638500	H	2.81280200	2.34169200	-5.50372300
C	-2.43485700	-1.38220400	3.35204900	H	4.51542000	1.85352400	-5.56618900
H	-1.88289300	-2.30759300	3.48385900	C	5.95872400	0.34190100	-0.95380200
C	-3.53453600	-1.12635000	4.17479100	H	6.89733700	0.71920400	-1.37441800
C	-4.24758000	0.06732200	3.98952800	H	5.94062200	-0.74288800	-1.12259400
H	-5.11030500	0.27288500	4.62178400	H	5.98307000	0.50391700	0.12828200
C	-3.88819000	0.99136100	3.00619700	C	1.27742300	2.81864600	1.09133200
C	-2.78066100	0.70768700	2.19126000	C	2.55157900	3.25488900	1.47534200
H	-2.52497100	1.38876400	1.38822800	H	3.40576400	3.08559400	0.82892600
C	-3.96578700	-2.12113700	5.22895100	C	2.74916200	3.92655400	2.68890500
H	-3.22956700	-2.92226600	5.34775100	C	1.64233400	4.18142900	3.50563700
H	-4.92366700	-2.58890200	4.96674100	H	1.78507100	4.71914800	4.44174400
H	-4.10055000	-1.63923700	6.20494200	C	0.35451400	3.77138700	3.14231400
C	-4.66499800	2.27510700	2.81605700	C	0.19105500	3.08289400	1.93601800
H	-5.67026300	2.20332600	3.24453800	H	-0.80535500	2.76449500	1.64371500
H	-4.76269400	2.52470800	1.75380400	C	-0.84131800	4.08519400	4.01303900
C	0.18642300	3.60606700	-1.36024300	H	-1.41220000	4.93288800	3.61128500
C	-1.12941400	3.66315400	-1.82465700	H	-0.53865500	4.34820900	5.03205600
H	-1.77789600	2.79856000	-1.72962100	H	-1.52631700	3.23171000	4.07102800
C	-1.64417400	4.84404700	-2.38971000	C	4.13731400	4.34965300	3.11320200
C	-0.81759400	5.96325800	-2.47465900	H	4.77352800	4.56447000	2.24779200
H	-1.20944000	6.88250900	-2.90791400	H	4.63234000	3.55795100	3.69167500
C	0.50704600	5.93832100	-2.00817000	H	4.10951600	5.24448500	3.74448900
C	0.99296700	4.75612600	-1.45155800	Ru	-0.54389600	0.21035900	-0.86332100
H	2.01406700	4.73132800	-1.08107600	P	-0.56569400	-0.78683000	1.28037000
C	-3.06573000	4.87908700	-2.90397400	P	0.86709500	2.06377200	-0.55616000

H	-4.16222000	3.12281600	3.30072300
H	0.01687800	-2.23529100	-2.38606300
C	-3.10609700	-0.04261300	-1.30782300
C	-4.58067800	-0.12721800	-1.65268000
C	-5.11680700	-1.56450100	-1.78595000
C	-6.57815900	-1.59630400	-2.18140000
C	-7.58812800	-1.56156000	-1.20974200
C	-8.93576000	-1.55510400	-1.57333500
C	-9.29762100	-1.58353200	-2.92175300
C	-8.30235000	-1.62037500	-3.90049000
C	-6.95629300	-1.62727400	-3.53103000
H	-5.13932900	0.43406300	-0.89532500
H	-4.72736500	0.41488900	-2.59776900
H	-4.51023000	-2.09716900	-2.52546500
H	-7.31340300	-1.54466400	-0.15683600
H	-9.70305600	-1.53266500	-0.80349900
H	10.34625500	-1.58203400	-3.20735800
H	-8.57366100	-1.64938500	-4.95282100
H	-6.18625800	-1.66295400	-4.29909800
O	-2.63241800	1.04236200	-0.83740400
O	-2.32863200	-1.02626400	-1.51266300
H	-4.97455500	-2.08615400	-0.83181600
C	1.02314200	-1.80623600	-2.24455300
C	2.03688500	-2.96607200	-2.20686500
C	3.50251800	-2.50834900	-2.10414000
C	4.48153800	-3.65556200	-1.97896300
C	5.22233800	-4.10322200	-3.08154900
C	6.11093800	-5.17471000	-2.96780800
C	6.27660500	-5.82103700	-1.74184000
C	5.54549400	-5.38706100	-0.63315800
C	4.65873700	-4.31665800	-0.75325800
H	1.96056600	-0.43432100	-3.26269000
H	1.78450600	-3.59653500	-1.34544400
H	1.90252500	-3.57570700	-3.10932000
H	3.75486200	-1.91135400	-2.98928600
H	5.10009000	-3.60384500	-4.04050600
H	6.67541400	-5.50249900	-3.83741300
H	6.96930700	-6.65359300	-1.64985200
H	5.66838300	-5.88176600	0.32738800
H	4.08974800	-3.98791700	0.11427800
O	1.12294100	-1.03717700	-1.11820500
O	1.20210800	-1.01444300	-3.45284000
H	3.59205300	-1.84200300	-1.23938600
H	-0.68867200	0.95361000	-2.61683000

H	-0.19387300	0.36378700	-2.78540900
<b>TS5'</b>			
C	0.65821700	2.56361600	1.57807400
C	1.34163500	3.31415700	0.61160100
H	1.83569700	2.80585100	-0.20895200
C	1.39212300	4.71269200	0.68390200
C	0.73878400	5.35699400	1.73924600
H	0.76644600	6.44432600	1.79914800
C	0.04827600	4.63604500	2.71969400
C	0.01867100	3.23925200	2.62954000
H	-0.51938000	2.68035300	3.38804500
C	2.16055400	5.50540400	-0.34996700
H	2.21576500	4.96849000	-1.30244600
H	3.19210100	5.69174500	-0.02155500
H	1.69832200	6.48182000	-0.53389600
C	-0.67502000	5.35314700	3.83816900
H	-1.63962400	5.75345900	3.49782800
H	-0.09106900	6.20039300	4.21600700
H	-0.87894000	4.68125700	4.67845300
C	-0.67926500	0.26860200	2.63695900
C	-0.46420200	-0.39369600	3.84691500
H	0.53712400	-0.70796200	4.12298000
C	-1.52552900	-0.65644100	4.72804400
C	-2.80318300	-0.21281300	4.38527800
H	-3.62881300	-0.38671100	5.07422700
C	-3.04877300	0.46053000	3.17854400
C	-1.98376100	0.67456800	2.30001500
H	-2.15046100	1.17906100	1.35178700
C	-1.28051300	-1.41632200	6.01111400
H	-0.33900000	-1.11403600	6.48375900
H	-1.21451300	-2.49523600	5.81790600
H	-2.08869400	-1.25840500	6.73326800
C	-4.43456700	0.97920500	2.86666500
H	-4.70077200	1.81715600	3.52464600
H	-5.19951000	0.20641700	3.01196900
H	-4.50591100	1.33654700	1.83492700
C	2.22374700	0.29147600	2.40986700
C	2.60936400	1.01924300	3.54921600
H	2.00733300	1.85981800	3.88171600
C	3.76504300	0.68983700	4.26065200
C	4.54383400	-0.38832600	3.81235500
H	5.45125700	-0.64872300	4.35588400
C	4.19377900	-1.12531000	2.67951800

C	3.02713600	-0.77069600	1.98135900	C	-2.31903200	-3.37956300	1.43871800
H	2.76917400	-1.29727300	1.06870500	H	-3.23445300	-3.19057300	0.88793100
C	4.18009400	1.47936100	5.48191400	C	-2.38604300	-4.13743300	2.61634200
H	3.46147100	2.27402000	5.70517200	C	-1.20136000	-4.41553000	3.30487500
H	5.16220700	1.94804000	5.34047100	H	-1.24228600	-5.01965600	4.21000900
H	4.25640200	0.83718900	6.36851200	C	0.03721800	-3.94269300	2.85364000
C	5.04025000	-2.28697100	2.20851200	C	0.06984700	-3.16783200	1.69037700
H	6.05497000	-2.23642800	2.61724200	H	1.02471900	-2.79146600	1.33369300
H	5.11205200	-2.30928700	1.11549400	C	1.31534800	-4.27985200	3.58790400
C	-0.22711600	-3.41197600	-1.64539100	H	1.83958100	-5.11686100	3.10738100
C	0.92854400	-3.30419600	-2.42057000	H	1.11768800	-4.57108700	4.62507000
H	1.48530900	-2.37483200	-2.42379400	H	2.00443500	-3.42807600	3.59850000
C	1.39754900	-4.39632400	-3.17221700	C	-3.71943300	-4.62262700	3.13818400
C	0.68396800	-5.59348400	-3.13413300	H	-4.39756100	-4.89286300	2.32102300
H	1.04165000	-6.44496000	-3.71158800	H	-4.21871300	-3.84248800	3.72855000
C	-0.48149400	-5.73220100	-2.36260400	H	-3.60337700	-5.49841900	3.78559100
C	-0.92090800	-4.63650800	-1.62097600	Ru	0.44394700	-0.06653300	-0.83862100
H	-1.81463200	-4.73961600	-1.01183500	P	0.68276500	0.70112100	1.45768800
C	2.65338100	-4.25759800	-4.00283900	P	-0.85723600	-1.97345900	-0.63516200
H	2.94333400	-5.21207300	-4.45442400	H	4.60871600	-3.24761500	2.52015200
H	3.49372300	-3.90104300	-3.39526900	H	-0.21806300	2.42598700	-2.15303300
H	2.51631300	-3.53227300	-4.81519600	C	2.93252600	0.23474400	-1.51067700
C	-1.23786300	-7.04164300	-2.34428000	C	4.36453700	0.31478500	-2.00404400
H	-2.04343300	-7.02618300	-1.60332400	C	4.99724900	1.71080000	-1.84683500
H	-0.57659700	-7.88306200	-2.10337000	C	6.39968900	1.77598200	-2.41353200
H	-1.68911400	-7.25857100	-3.32144000	C	7.51548100	1.49190700	-1.61399500
C	-2.55583700	-1.75373000	-1.35691200	C	8.80643900	1.52027800	-2.14454600
C	-2.75849000	-2.03400600	-2.71812300	C	9.00410900	1.83490200	-3.49048000
H	-1.95024800	-2.45910200	-3.30577000	C	7.90201600	2.12202000	-4.29865000
C	-3.99253300	-1.79764800	-3.33803600	C	6.61371700	2.09274600	-3.76258400
C	-5.03680500	-1.27481700	-2.56627900	H	4.95330900	-0.44780500	-1.48330700
H	-6.00630100	-1.10052900	-3.03021200	H	4.36212400	0.02912300	-3.06585000
C	-4.86507700	-0.97023700	-1.21123600	H	4.35136600	2.44155300	-2.34422200
C	-3.61236600	-1.19520500	-0.62272000	H	7.36963700	1.25184500	-0.56266000
H	-3.46335000	-0.93023000	0.41953400	H	9.65806400	1.30093900	-1.50534500
C	-4.20528200	-2.14996300	-4.79343000	H	10.00847600	1.86080000	-3.90496900
H	-4.61903200	-3.16184000	-4.89839400	H	8.04552100	2.37448900	-5.34629700
H	-3.26514100	-2.12430600	-5.35413500	H	5.76026700	2.32445200	-4.39675000
H	-4.90810100	-1.46132900	-5.27511000	O	2.47194200	-0.88071400	-1.09758100
C	-6.00784300	-0.38025100	-0.41566400	O	2.17468200	1.25272700	-1.53623300
H	-6.97407800	-0.74998400	-0.77600400	H	5.01051200	1.97694000	-0.78287700
H	-6.02998000	0.71452700	-0.49937500	C	-1.20689000	1.99294300	-1.93616300
H	-5.92641200	-0.62547300	0.64766600	C	-2.30776400	3.03978900	-2.08912800
C	-1.09822100	-2.88039700	0.96991000	C	-3.73848100	2.50116900	-1.91187900

C	-4.78231200	3.59759900	-1.93008400	H	2.67316700	0.20220600	5.68904200
C	-5.37768100	4.00915000	-3.13088500	C	2.67684900	-0.06979600	3.55613200
C	-6.32017400	5.03851600	-3.15095300	C	1.87396400	-0.30701000	2.43091600
C	-6.68606800	5.67733600	-1.96431400	H	2.33984800	-0.37577800	1.45248200
C	-6.10230500	5.27779500	-0.76038900	C	0.02737100	-0.00602600	6.32089900
C	-5.16019200	4.24783200	-0.74631200	H	-0.21675600	1.03896600	6.55470500
H	-2.09243300	0.50944100	-3.14440300	H	0.69062600	-0.36889200	7.11383400
H	-2.10979900	3.79908000	-1.32107700	H	-0.90606800	-0.57613300	6.37123300
H	-2.19795700	3.53382900	-3.06134200	C	4.17601700	0.07058000	3.41988000
H	-3.96142000	1.77702500	-2.70609000	H	4.64346300	0.28379700	4.38676600
H	-5.10081600	3.51369800	-4.05937600	H	4.44213900	0.87623000	2.72712900
H	-6.77137000	5.33930800	-4.09321500	H	4.62838800	-0.84991200	3.02920800
H	-7.42178500	6.47714800	-1.97736300	C	-2.23184500	-0.90299200	1.69846700
H	-6.38286300	5.76581500	0.16970000	C	-2.88849900	-2.08956900	2.05722200
H	-4.70983300	3.94140600	0.19584100	H	-2.39016900	-3.04428200	1.92771900
O	-1.28258700	1.21336200	-0.88598600	C	-4.18193200	-2.06830900	2.59301900
O	-1.28586400	1.04977300	-3.27468100	C	-4.80626300	-0.82942500	2.78239000
H	-3.78256500	1.95119100	-0.96695600	H	-5.80476500	-0.79873800	3.21640400
H	0.26882800	-0.42121600	-2.54247300	C	-4.17540900	0.37174600	2.43885800
H	-0.42189700	0.25559800	-2.89544200	C	-2.88661600	0.32205600	1.89091800

**TS5a'**

C	-0.13282100	-2.69200600	0.80842700	C	-4.89024000	-3.35588200	2.95049800
C	-0.78613600	-3.37539600	-0.23034400	H	-4.17673600	-4.15909500	3.16188000
H	-1.47166500	-2.83701000	-0.87673800	H	-5.53218900	-3.69875500	2.12810500
C	-0.57205400	-4.74294100	-0.44071800	H	-5.53116500	-3.23064500	3.83041400
C	0.31697200	-5.42138000	0.40051500	C	-4.87352300	1.69790500	2.63830500
H	0.49023400	-6.48502400	0.24418900	H	-4.17444500	2.46427900	2.98894900
C	0.99087000	-4.76589500	1.43627400	H	-5.68826500	1.61619000	3.36570200
C	0.74927600	-3.40004700	1.63683300	C	0.98851100	3.45350000	-1.87686300
H	1.25247200	-2.89548600	2.45463800	C	1.53029300	3.02849800	-3.09620600
C	-1.26440300	-5.46067500	-1.57735900	H	1.80841800	1.98747800	-3.22978200
H	-1.42406900	-6.51966200	-1.34643800	C	1.73857100	3.92243100	-4.15290900
H	-0.66438600	-5.41367100	-2.49595300	C	1.38920600	5.26417900	-3.97161800
H	-2.23564500	-5.00874600	-1.80340000	H	1.53982900	5.96757800	-4.78898200
C	1.97552600	-5.51199500	2.30775100	C	0.85744600	5.72447000	-2.76198500
H	2.12833800	-5.00425100	3.26605300	C	0.67244900	4.81029500	-1.71779100
H	2.95327100	-5.58950600	1.81395600	H	0.27509000	5.17124400	-0.77519000
H	1.63491100	-6.53275600	2.51522200	C	2.34020600	3.43905700	-5.45321600
C	0.48744900	-0.47012500	2.55083600	H	2.28292000	4.20775500	-6.23065900
C	-0.09918600	-0.38041100	3.82160900	H	1.82432500	2.54537900	-5.82341800
H	-1.16927200	-0.51524800	3.93473800	H	3.39799600	3.17301400	-5.32806100
C	0.67468100	-0.12683600	4.95945700	C	0.46818500	7.17603200	-2.59299500
C	2.05907000	0.02118500	4.80831600	H	0.44393800	7.46396100	-1.53662400
				H	-0.52975100	7.37239300	-3.00787200



H	1.16846300	7.84220200	-3.10944500	C	-7.26817900	-1.23238900	-0.95373600
C	2.66341100	2.28003800	0.01237100	C	-8.64155600	-1.20574500	-1.20115300
C	3.20597600	3.43438200	0.60308700	C	-9.12402100	-1.39217300	-2.49845200
H	2.55688600	4.26280800	0.87089500	C	-8.22282500	-1.60595900	-3.54335300
C	4.57689500	3.54646800	0.83996900	C	-6.85015600	-1.63195100	-3.29040700
C	5.41001700	2.48708800	0.44867700	H	-4.75261400	0.65912300	-1.11170900
H	6.48343100	2.57041900	0.61209800	H	-4.41606000	0.38808300	-2.81669300
C	4.90328000	1.33664200	-0.15967300	H	-4.34245400	-2.08446300	-2.43994100
C	3.51567500	1.23833200	-0.36825300	H	-6.89705800	-1.09149700	0.05973400
H	3.09436300	0.36467700	-0.86168300	H	-9.33571400	-1.04409900	-0.38007900
C	5.15604300	4.77613900	1.50231700	H	10.19325500	-1.37525000	-2.69263600
H	6.06669600	5.11312300	0.99365500	H	-8.58829400	-1.75760800	-4.55591600
H	5.42620200	4.57759400	2.54809800	H	-6.15390700	-1.80514000	-4.10855700
H	4.44144200	5.60544200	1.49922100	O	-2.25168000	1.04770500	-0.99269200
C	5.83179200	0.22758700	-0.60007600	O	-2.01905400	-0.97115600	-1.81721900
H	5.79686500	0.08709700	-1.68743500	H	-4.66151100	-1.84657100	-0.72684300
H	5.56295200	-0.73414400	-0.14758300	C	1.37606300	-1.88676400	-2.77302800
H	6.86947000	0.44532800	-0.32719200	C	2.27513200	-2.98661800	-2.18508500
C	-0.05561400	3.08948200	0.83129000	C	3.78322600	-2.71720800	-2.34021400
C	0.39209600	3.15283900	2.15833900	C	4.64312400	-3.78240200	-1.69353600
H	1.33907900	2.70093600	2.43445000	C	5.26609100	-4.77637200	-2.45938300
C	-0.36923700	3.78716900	3.14844100	C	6.04402700	-5.76925300	-1.85911000
C	-1.59467900	4.35952000	2.78912200	C	6.21602700	-5.78398600	-0.47434800
H	-2.18967500	4.86161700	3.55054900	C	5.60147800	-4.79931300	0.30388900
C	-2.07777100	4.29753600	1.47596000	C	4.82193800	-3.81238100	-0.30152100
C	-1.30572100	3.64278200	0.50953300	H	2.46973100	-1.22827700	-4.22310100
H	-1.68838200	3.55436300	-0.50198900	H	2.02590400	-3.10589200	-1.12607900
C	-3.39187900	4.94155000	1.09506200	H	2.02479600	-3.93193300	-2.68345200
H	-3.94012600	4.32903100	0.37110900	H	4.03118900	-2.65569800	-3.40757600
H	-3.23155100	5.92424000	0.63167700	H	5.14119700	-4.77011500	-3.54017200
H	-4.03384200	5.09378700	1.96900500	H	6.51878000	-6.52873700	-2.47536500
C	0.14195800	3.87529000	4.56871200	H	6.82533600	-6.55204600	-0.00526800
H	0.77368700	4.76281100	4.71064800	H	5.73498600	-4.79602200	1.38309000
H	0.74617400	2.99961600	4.82729500	H	4.33948900	-3.05469100	0.31274600
H	-0.68251900	3.94726500	5.28654800	O	1.55582900	-0.67360700	-2.09219500
Ru	-0.25428600	0.25869700	-1.10389200	O	1.62266200	-1.70051700	-4.16653400
P	-0.49824400	-0.88286500	1.03337700	H	4.01272500	-1.74063600	-1.89939200
P	0.87687000	2.20146300	-0.49314100	H	-0.09674800	0.76083700	-2.80937000
H	-5.30716600	2.06400500	1.69830400	H	0.67038700	0.17582900	-2.70029400
H	0.33074600	-2.21710200	-2.73140100				
C	-2.77158700	0.00991800	-1.52546700	<b>Int8'</b>			
C	-4.25730700	-0.02323600	-1.80980800	C	-1.68775900	0.46629200	-2.59784200
C	-4.86223700	-1.43888900	-1.72454500	C	-2.79895500	1.04417000	-1.96655000
C	-6.35187300	-1.44465300	-1.99373700	H	-2.96156800	0.87748100	-0.90598800

C	-3.71238600	1.82567000	-2.68593100	C	-1.19983700	-5.38858300	0.64999300
C	-3.48507700	2.03924800	-4.04977500	H	-0.12458800	-5.53368100	0.49987300
H	-4.19089500	2.64346900	-4.61814100	H	-1.70038000	-6.35115700	0.50081200
C	-2.37634200	1.48846400	-4.70286900	C	2.97029400	0.53935800	2.76428300
C	-1.48963300	0.69342900	-3.96682700	C	2.56122700	1.70815100	3.41245400
H	-0.64166800	0.24747400	-4.47564000	H	1.81465800	2.34415200	2.94807500
C	-4.91134400	2.43135000	-1.99025400	C	3.08101700	2.07307100	4.66313900
H	-5.66131300	2.77338400	-2.71163400	C	4.02252300	1.23650700	5.26474400
H	-4.62371900	3.29443600	-1.37627300	H	4.42786500	1.50462900	6.23922000
H	-5.39060900	1.70871700	-1.32012200	C	4.45487000	0.05612100	4.64488600
C	-2.13531800	1.75521100	-6.17193200	C	3.92646900	-0.27604500	3.39485100
H	-1.48589200	0.99343200	-6.61589600	H	4.25641300	-1.19423400	2.92011200
H	-1.64933000	2.72825600	-6.32544000	C	2.62296200	3.34808600	5.33453300
H	-3.07430800	1.77141700	-6.73707500	H	2.92930100	4.23310000	4.76210700
C	0.71816700	-1.12506000	-2.82022700	H	3.04224400	3.44309000	6.34135900
C	0.68902100	-2.37522400	-3.45409000	H	1.53016800	3.38308400	5.42064000
H	-0.09357400	-3.08695200	-3.21202300	C	5.46329100	-0.84156000	5.32624600
C	1.65321400	-2.72490300	-4.40664200	H	5.04900700	-1.28845100	6.23934400
C	2.64600700	-1.79110300	-4.72860400	H	6.36067700	-0.28400500	5.62145800
H	3.39223000	-2.04711500	-5.47918700	H	5.77787600	-1.66017200	4.67103700
C	2.69859500	-0.53251300	-4.11847600	C	3.75116500	0.91401700	0.06945000
C	1.73165200	-0.21486000	-3.15411400	C	5.07011900	0.45114300	0.22523200
H	1.75954200	0.75758300	-2.67007600	H	5.27381200	-0.40449500	0.86147300
C	1.62896600	-4.08670300	-5.06413700	C	6.13584400	1.07345900	-0.42593200
H	2.00964900	-4.04357000	-6.09061800	C	5.86802700	2.19334900	-1.22941300
H	0.61420800	-4.49725300	-5.09512100	H	6.69467400	2.69419300	-1.73158400
H	2.25335000	-4.80526500	-4.51615100	C	4.57147900	2.68230200	-1.39628000
C	3.76302800	0.47077900	-4.50121700	C	3.51246500	2.02319300	-0.74769200
H	4.49277700	0.03358000	-5.19073700	H	2.49147600	2.36507900	-0.89202300
H	4.30265000	0.83758000	-3.62118300	C	7.54892600	0.55564200	-0.27879300
H	3.32317100	1.34629900	-4.99620500	H	7.61837200	-0.19566900	0.51424700
C	-1.55079300	-2.14283500	-1.34280000	H	8.24891200	1.36464400	-0.03796800
C	-2.76202600	-2.37408300	-2.01416500	H	7.90352400	0.08999200	-1.20782800
H	-3.15199300	-1.62403000	-2.69414400	C	4.30125300	3.91021700	-2.23673200
C	-3.47683400	-3.56252400	-1.83008100	H	4.14801200	4.79548800	-1.60539000
C	-2.94901000	-4.53248200	-0.96751700	H	3.39607300	3.78923300	-2.84194000
H	-3.48622500	-5.47006700	-0.83073500	H	5.13648800	4.12877000	-2.91052200
C	-1.74446200	-4.33257400	-0.28486900	C	2.60807700	-1.65201700	0.90339100
C	-1.05509500	-3.12624900	-0.47478500	C	3.21304900	-2.23159800	-0.21944900
H	-0.12393800	-2.95996300	0.05885300	H	3.57294600	-1.60246000	-1.02758900
C	-4.79315100	-3.79269800	-2.53817400	C	3.36250700	-3.62150300	-0.32239700
H	-5.64315000	-3.59309300	-1.87217300	C	2.89363200	-4.42463400	0.72253600
H	-4.88870500	-4.82928600	-2.88140000	H	3.01392500	-5.50497600	0.65594000
H	-4.89882700	-3.13634000	-3.40794900	C	2.27207900	-3.87511400	1.85213000

C	2.11972300	-2.48656500	1.92217300	H	-1.88169700	3.02313100	0.29314300
H	1.61592400	-2.05158100	2.77931500	H	-1.15599800	3.69595400	1.75889100
C	1.80571000	-4.75612800	2.98937100	H	-0.09066600	5.52469900	0.39912000
H	0.92509700	-4.33458100	3.48533400	H	-3.05887400	5.34515300	-1.70285200
H	2.58784500	-4.86378800	3.75308100	H	-5.13995200	6.63574700	-1.32717900
H	1.55178000	-5.76310600	2.64136200	H	-5.49076000	7.84040200	0.82288800
C	4.04471300	-4.22951400	-1.52694200	H	-3.73569500	7.74401500	2.58495100
H	5.13803700	-4.19431300	-1.42582000	H	-1.66071000	6.45276800	2.20313000
H	3.78488100	-3.68908700	-2.44321300	O	0.42472000	2.24875200	-0.76454300
H	3.76414600	-5.28036900	-1.65670900	H	-0.78997400	4.84046800	-1.06758500
Ru	0.12112100	0.67332100	0.65813500	H	1.14848500	3.20995000	0.89411400
P	-0.55505400	-0.59799500	-1.58202900				
P	2.34790800	0.17423300	1.03996100				
H	-1.34077400	-5.10152100	1.70011800	<b>TS6'</b>			
H	0.22408500	1.33845900	2.10343300	C	1.00798600	-0.67641700	2.87137300
C	-1.87639900	-0.52629700	1.76086900	C	2.15015700	0.13190600	2.75815500
C	-2.94564800	-1.32190500	2.47943800	H	2.49463800	0.43551800	1.77534800
C	-4.33034100	-1.22847200	1.80957700	C	2.86009200	0.53500400	3.89303300
C	-5.38250200	-2.02774500	2.54835700	C	2.40680100	0.12480900	5.15357100
C	-5.57726100	-3.38813300	2.26887800	H	2.95554800	0.43299700	6.04262600
C	-6.52515900	-4.13628200	2.96898300	C	1.27025700	-0.67479600	5.29783200
C	-7.29798700	-3.53444600	3.96448400	C	0.58256900	-1.07744600	4.14401100
C	-7.11569300	-2.18029600	4.25192600	H	-0.28811000	-1.71599000	4.25151400
C	-6.16647700	-1.43645600	3.54857300	C	4.08398600	1.41389000	3.76659000
H	-2.60990100	-2.36157400	2.54796600	H	3.84985300	2.45797600	4.01519400
H	-3.00417400	-0.94597900	3.51078600	H	4.48079700	1.39819000	2.74647900
H	-4.62147300	-0.17442200	1.75478500	H	4.88244100	1.09387900	4.44650700
H	-4.98019800	-3.86040100	1.49104300	C	0.77847500	-1.08662700	6.66753000
H	-6.66375300	-5.18881100	2.73403600	H	0.30463700	-2.07420600	6.64457300
H	-8.03889100	-4.11465800	4.50829200	H	0.03174900	-0.37864800	7.05204500
H	-7.71625200	-1.70066800	5.02083500	H	1.59751200	-1.12046800	7.39423600
H	-6.03431500	-0.38000700	3.77355200	C	-1.37241200	-2.02342400	1.95892100
O	-0.65519300	-0.90865400	1.84430000	C	-1.61406800	-3.39929700	1.88930200
O	-2.15292100	0.51178500	1.09449600	H	-0.88301600	-4.05491900	1.42680600
H	-4.24512900	-1.58614800	0.77685100	C	-2.78976400	-3.95373700	2.41379400
C	0.24988200	2.81261900	0.39308100	C	-3.71294400	-3.10525500	3.03296700
C	-1.02416500	3.58238500	0.67624600	H	-4.61949800	-3.52898000	3.46273300
C	-0.96050300	4.97989600	0.00627900	C	-3.49975100	-1.72263300	3.11732000
C	-2.21528500	5.79687500	0.22591300	C	-2.32932100	-1.19393800	2.56388700
C	-3.21050500	5.86469400	-0.75910000	H	-2.15432600	-0.12318400	2.62045600
C	-4.38330300	6.59329900	-0.54769000	C	-3.05392500	-5.43720000	2.29219600
C	-4.58030800	7.27054800	0.65701500	H	-3.80595300	-5.77267100	3.01423400
C	-3.59508600	7.21497500	1.64561700	H	-2.14176300	-6.02200800	2.45600100
C	-2.42520900	6.48577800	1.42924600	H	-3.42321100	-5.68963500	1.28922300
				C	-4.49747900	-0.82106400	3.80915900

H	-5.47438200	-1.30613000	3.90823200	H	-2.13893600	2.04179500	1.56909600
H	-4.63663200	0.11528600	3.25749200	C	-7.04802500	2.75769900	-0.58480000
H	-4.15990000	-0.55589600	4.82014000	H	-7.11703400	2.32016600	-1.58566400
C	1.22088500	-2.69825200	0.83149000	H	-7.28022600	3.82655400	-0.67048000
C	2.14377800	-3.27155400	1.71913100	H	-7.83624400	2.30731500	0.03214400
H	2.25716300	-2.86349700	2.71792600	C	-3.77860100	3.48319700	3.21283800
C	2.93269700	-4.36395200	1.34046400	H	-2.78736700	3.94990400	3.21382000
C	2.77778400	-4.88536400	0.05064400	H	-3.76634200	2.70920800	3.99151600
H	3.38468000	-5.73700800	-0.25407400	H	-4.51302600	4.23871000	3.51110100
C	1.86222300	-4.34080400	-0.85720700	C	-2.82219900	-1.03185500	-1.22394300
C	1.09034300	-3.24195100	-0.45507200	C	-4.01274100	-1.44861200	-0.62554500
H	0.39480600	-2.79333700	-1.15532500	H	-4.54972500	-0.78044200	0.03933300
C	3.94982800	-4.94811000	2.29499300	C	-4.54247500	-2.72465000	-0.87892000
H	4.93687700	-4.48764200	2.15436400	C	-3.85870400	-3.57019200	-1.75288600
H	4.07042400	-6.02646900	2.14295800	H	-4.27313200	-4.55278200	-1.97458900
H	3.66052900	-4.78214500	3.33796200	C	-2.65554300	-3.18267000	-2.36333000
C	1.70128500	-4.93747000	-2.23760000	C	-2.14116100	-1.91515500	-2.08298500
H	0.92571500	-5.71517000	-2.24938100	H	-1.21523300	-1.59589700	-2.55479300
H	2.63072700	-5.40254800	-2.58356900	C	-1.94588800	-4.12227100	-3.31138900
C	-2.30571500	1.35266000	-2.72493700	H	-1.13529600	-3.61537800	-3.84401600
C	-1.64553700	2.53390800	-3.08414400	H	-2.63604300	-4.53107300	-4.05944200
H	-0.97344900	3.01061400	-2.37908600	H	-1.50976000	-4.97593800	-2.77677800
C	-1.82091800	3.11927900	-4.34404700	C	-5.83013800	-3.15867400	-0.21720800
C	-2.68131200	2.50022200	-5.25539300	H	-6.60875800	-2.39239300	-0.31274400
H	-2.82710000	2.94704600	-6.23761600	H	-5.67828300	-3.33253600	0.85529200
C	-3.35795300	1.31879200	-4.93295500	H	-6.21402800	-4.08545000	-0.65632200
C	-3.16535500	0.75985600	-3.66405200	Ru	0.09476200	0.68657100	-0.25712100
H	-3.69397900	-0.15366400	-3.41396300	P	0.17475700	-1.23801400	1.30885600
C	-1.07110500	4.37948000	-4.71303700	P	-2.10418200	0.65937200	-0.99543900
H	-1.02727600	5.08127100	-3.87249300	H	1.40939100	-4.17793900	-2.97008700
H	-1.54134200	4.89322800	-5.55815400	H	0.29058700	2.10689000	-1.11838600
H	-0.03539100	4.15454800	-5.00034500	C	2.16188600	-0.22222300	-1.49823400
C	-4.25994300	0.64570200	-5.94313900	C	3.32302400	-0.76215800	-2.30773300
H	-3.68168400	0.02520400	-6.64096900	C	4.57997200	-1.03839600	-1.45918400
H	-4.80882700	1.38005900	-6.54357500	C	5.72592400	-1.58355300	-2.28446400
H	-4.99058900	-0.00824600	-5.45566600	C	5.91140500	-2.96539300	-2.43064200
C	-3.42666100	1.60592900	-0.09751300	C	6.94902800	-3.47257000	-3.21489300
C	-4.69903500	1.81392200	-0.66091900	C	7.82292500	-2.60195300	-3.86914600
H	-4.92667700	1.41633600	-1.64576900	C	7.65142900	-1.22285500	-3.73076900
C	-5.67924900	2.53773000	0.01937400	C	6.61273800	-0.72134000	-2.94490700
C	-5.36495300	3.07027000	1.28017400	H	2.98856500	-1.66745500	-2.82447400
H	-6.11951600	3.64687000	1.81366500	H	3.55704400	-0.02721000	-3.09114100
C	-4.10666800	2.89593500	1.85801600	H	4.87550300	-0.10824700	-0.96285000
C	-3.13876400	2.15550700	1.15618300	H	5.23687600	-3.64701900	-1.91616100

H	7.07819000	-4.54787600	-3.31106900	H	-3.01696300	5.65239800	1.53249000
H	8.63359500	-2.99433800	-4.47755100	H	-1.74311600	6.64651700	2.24796100
H	8.33044200	-0.53656800	-4.23069200	C	-0.85993500	0.50052200	2.30969600
H	6.48989700	0.35448500	-2.83601200	C	-0.48748400	0.36591100	3.65251700
O	0.96500400	-0.45904000	-1.87710600	H	0.55432700	0.46742400	3.93893900
O	2.35881500	0.47450700	-0.45426100	C	-1.44562400	0.11043400	4.64303700
H	4.31992200	-1.74873900	-0.66601100	C	-2.78684700	-0.00153100	4.26206600
C	0.13070700	2.88580100	0.27030700	H	-3.54024100	-0.18901700	5.02521200
C	1.42733000	3.67900800	0.16189700	C	-3.19118700	0.13404100	2.92680300
C	1.50719600	4.73718300	1.28704200	C	-2.21279000	0.38164700	1.95596300
C	2.74685200	5.59994500	1.18591700	H	-2.50387500	0.49049800	0.91484500
C	3.98513500	5.13218700	1.64990100	C	-1.02943000	-0.02436900	6.09108000
C	5.13693200	5.91091000	1.53323200	H	-1.89749200	-0.14824200	6.74661400
C	5.07135700	7.17768300	0.94805200	H	-0.47609500	0.85942900	6.43116200
C	3.84568600	7.65653300	0.48254000	H	-0.37242700	-0.89030500	6.24020700
C	2.69621100	6.87264900	0.60152900	C	-4.64821300	0.01039000	2.54340900
H	2.27492700	2.99079600	0.22802000	H	-5.29424000	0.02377100	3.42747100
H	1.47493200	4.17319600	-0.81723600	H	-4.83816200	-0.92251800	1.99990600
H	0.61312100	5.37415600	1.25026500	H	-4.96000200	0.83114900	1.88664600
H	4.04373500	4.14776100	2.10902800	C	1.98848200	0.90136000	1.88355000
H	6.08566700	5.53014900	1.90320700	C	2.59609300	2.07971600	2.34626800
H	5.96699400	7.78692500	0.85913600	H	2.11703000	3.03829900	2.17798600
H	3.78209800	8.64286700	0.02963900	C	3.81479000	2.04354600	3.03310400
H	1.74362800	7.25552600	0.24064200	C	4.41552700	0.79913900	3.26134400
O	-0.04773900	2.12286100	1.31833800	H	5.35831300	0.75665400	3.80496400
H	1.48344200	4.21263900	2.24923700	C	3.83331800	-0.39181900	2.81513900
H	-0.76085200	3.43280500	-0.08365100	C	2.61749800	-0.32799200	2.12074100
<b>Int9'</b>				H	2.16583400	-1.24504100	1.75826200
C	0.07533500	2.73858700	0.72714200	C	4.47521800	3.31900400	3.50682300
C	0.81659500	3.39922900	-0.26521500	H	5.26214400	3.64232700	2.81239100
H	1.51589900	2.83733800	-0.87630100	H	4.94556800	3.18698100	4.48796300
C	0.65675800	4.77204300	-0.48754400	H	3.75304400	4.13812600	3.58489100
C	-0.27175300	5.47525500	0.28834300	C	4.50711600	-1.72327000	3.05786200
H	-0.41313700	6.54044300	0.11203100	H	3.78804200	-2.47523900	3.40034200
C	-1.02986400	4.84258000	1.27930100	H	5.30061400	-1.63974300	3.80804500
C	-0.83865200	3.47191300	1.49740100	C	-0.57400200	-3.16954000	-1.99814900
H	-1.41741500	2.98087200	2.27255000	C	-0.67366100	-2.50818600	-3.22939100
C	1.48462400	5.47896700	-1.53722300	H	-0.90347000	-1.44411800	-3.24917300
H	0.96344900	6.35687900	-1.93398200	C	-0.52801900	-3.20652800	-4.43798700
H	1.71725500	4.81250600	-2.37426200	C	-0.29105900	-4.58172600	-4.39034800
H	2.44063800	5.82665800	-1.12270900	H	-0.17959300	-5.13397100	-5.32227400
C	-2.06126900	5.61289700	2.07189900	C	-0.20539200	-5.27333600	-3.17303100
H	-2.25116100	5.14563700	3.04420300	C	-0.35250400	-4.55582900	-1.98327400
				H	-0.29685500	-5.08822700	-1.03857000

C	-0.62268500	-2.47248000	-5.75626600	P	-0.84151500	-2.15253700	-0.46315500
H	-1.51971500	-1.84358900	-5.79854800	H	4.96096600	-2.11082200	2.13650800
H	-0.65665600	-3.16813700	-6.60104100	H	-0.24605800	2.06867400	-2.70696300
H	0.23997100	-1.81025500	-5.90469100	C	2.77804800	0.04403300	-1.49868000
C	0.04931700	-6.76387400	-3.15463000	C	4.26154500	0.10770600	-1.79746600
H	1.07927000	-6.99678700	-3.45569900	C	4.86611200	1.49356600	-1.47828000
H	-0.61513800	-7.29278800	-3.84827200	C	6.36148200	1.53602300	-1.70721600
H	-0.10511200	-7.18322900	-2.15525600	C	7.25230900	1.21383800	-0.67364900
C	-2.66181100	-2.43893800	-0.24181300	C	8.63174900	1.21907600	-0.88644300
C	-3.18121900	-3.60339300	0.34827500	C	9.14569600	1.54839900	-2.14247200
H	-2.51263700	-4.33308500	0.79428200	C	8.26994600	1.87294800	-3.18066800
C	-4.55608700	-3.84878200	0.36320800	C	6.89127900	1.86650600	-2.96229500
C	-5.40939700	-2.91331400	-0.24144300	H	4.76293500	-0.67636400	-1.22270700
H	-6.48226900	-3.10111900	-0.24554700	H	4.41269700	-0.11862100	-2.86161900
C	-4.91935500	-1.75552200	-0.85057900	H	4.36132800	2.24295200	-2.09689000
C	-3.53359200	-1.52234800	-0.84125600	H	6.85634300	0.96180000	0.30830400
H	-3.11616400	-0.63947000	-1.32267300	H	9.30557600	0.97022400	-0.07030300
C	-5.11831000	-5.10076400	0.99862600	H	10.21956200	1.55613800	-2.30978400
H	-4.32572000	-5.71944400	1.43144400	H	8.66039200	2.13625800	-4.16052300
H	-5.65705000	-5.71391500	0.26514600	H	6.21499300	2.12612800	-3.77432700
H	-5.82954900	-4.86054700	1.79901400	O	2.30418500	-0.93230100	-0.83476300
C	-5.85919700	-0.76801500	-1.50526400	O	1.99483600	0.96798000	-1.89748100
H	-5.52792300	-0.51571300	-2.51890000	H	4.64448500	1.74243000	-0.43319700
H	-5.91014500	0.17406200	-0.94444800	C	-1.28357500	1.69553900	-2.71466500
H	-6.87616800	-1.16854700	-1.57158100	C	-2.21361000	2.83029400	-2.25927000
C	-0.02577300	-3.09986900	0.89315200	C	-3.70809200	2.47464600	-2.36495000
C	-0.57500000	-3.14278800	2.18444400	C	-4.62111800	3.56361400	-1.84483800
H	-1.52720700	-2.66152200	2.38488500	C	-4.84264500	3.71393300	-0.46662600
C	0.08593100	-3.79796400	3.22982400	C	-5.66231200	4.73056400	0.02630900
C	1.31891100	-4.40780000	2.96665300	C	-6.27864300	5.62400200	-0.85394200
H	1.83750100	-4.92583500	3.77212000	C	-6.06784400	5.48790200	-2.22685900
C	1.90340900	-4.36342600	1.69592700	C	-5.24820500	4.46701900	-2.71361900
C	1.22704700	-3.69120600	0.67009700	H	-1.97520300	3.09175200	-1.22270800
H	1.68916000	-3.62287600	-0.30918800	H	-2.00690600	3.72368000	-2.86698700
C	3.22507700	-5.04440500	1.42013800	H	-3.95476200	2.25413100	-3.41283300
H	3.84559600	-4.45044300	0.74039100	H	-4.36131600	3.02570600	0.22572700
H	3.07485900	-6.02437600	0.94768400	H	-5.82690700	4.82067900	1.09754500
H	3.79217200	-5.21011500	2.34213500	H	-6.91982700	6.41466000	-0.47297600
C	-0.53417800	-3.86998500	4.60687900	H	-6.54508400	6.17453400	-2.92189700
H	-1.10666900	-4.79830300	4.73834000	H	-5.09370600	4.36589500	-3.78599200
H	-1.22099300	-3.03483300	4.77658900	O	-1.41738600	0.52864200	-1.94139600
H	0.23031800	-3.84999300	5.39181400	H	-3.87746200	1.55109100	-1.80108400
Ru	0.24248600	-0.17059000	-0.99238800	H	-1.51832300	1.45209500	-3.76915100
P	0.36104000	0.92353700	0.98717300				

**Int11**

C	-1.88989500	2.37574100	-1.13887900	C	0.70205100	6.85050300	-0.23746800
C	-1.18898300	2.38479300	-2.35319100	H	-0.24488500	6.94519700	-0.77885100
H	-0.15677200	2.04941400	-2.37551400	H	1.51028700	6.93131700	-0.97646100
C	-1.79385400	2.83113400	-3.53660100	H	0.79468400	7.70914300	0.43722800
C	-3.11967900	3.27397000	-3.48504800	C	2.69635400	4.04408000	3.47413000
H	-3.59606100	3.63089000	-4.39721300	H	2.28180200	3.38790200	4.24631700
C	-3.84653900	3.27889400	-2.28674200	H	2.91934200	5.01485100	3.93001100
C	-3.21723500	2.83169800	-1.11856200	C	0.78071500	-3.18649000	1.68682600
H	-3.77185300	2.84652100	-0.18658000	C	0.57801900	-4.06553000	0.61005600
C	-1.02251500	2.80638100	-4.83616700	H	-0.06245600	-3.76570300	-0.21351700
H	-0.79695500	1.77419900	-5.13168100	C	1.17279900	-5.32628800	0.58097700
H	-0.06399200	3.33047200	-4.74229900	C	1.99779000	-5.70316200	1.65257100
H	-1.58654400	3.27623900	-5.64853200	H	2.46814600	-6.68528900	1.64113100
C	-5.28732400	3.73838900	-2.26075400	C	2.22016300	-4.85350300	2.73508600
H	-5.60184000	4.01166800	-1.24831200	C	1.59400800	-3.59529700	2.74536100
H	-5.96277800	2.94617000	-2.61103500	H	1.74690000	-2.94788700	3.60218500
H	-5.44338200	4.60720600	-2.91042900	C	0.95080100	-6.26801100	-0.58127200
C	-2.33033100	1.88772300	1.67171700	H	0.69722500	-7.27757900	-0.23588300
C	-2.36506200	2.91224400	2.62869700	H	1.85174700	-6.35629000	-1.20226000
H	-1.57900400	3.65859700	2.65444200	H	0.13957900	-5.91936000	-1.22847900
C	-3.40886000	3.00241600	3.55717000	C	3.11902500	-5.26422900	3.88006300
C	-4.43591500	2.05274400	3.50573100	H	4.08161900	-4.73712300	3.84157200
H	-5.26135900	2.12346000	4.21223200	H	3.33180900	-6.33808400	3.85604200
C	-4.43673200	1.02229300	2.55877700	H	2.66525600	-5.03220100	4.85098400
C	-3.37037500	0.94740300	1.65190900	C	-1.84314400	-2.38040100	2.04386100
H	-3.36339400	0.15353300	0.91143000	C	-2.06923400	-3.01908600	3.27674000
C	-3.41980400	4.10101800	4.59655000	H	-1.31710100	-2.96664700	4.05830900
H	-4.44207500	4.38018700	4.87445700	C	-3.24007200	-3.73959200	3.51368400
H	-2.90904700	4.99906300	4.23328400	C	-4.18773900	-3.83633900	2.48148500
H	-2.90728500	3.78546300	5.51517800	H	-5.09897300	-4.40827500	2.65073000
C	-5.56652100	0.01903800	2.50598900	C	-3.98382500	-3.23080700	1.24117400
H	-6.33531500	0.24742800	3.25132300	C	-2.80295600	-2.49534000	1.03575900
H	-5.20595100	-0.99911900	2.69101000	H	-2.62168300	-2.02149100	0.07637900
H	-6.04928300	0.01453700	1.52062900	C	-3.48493700	-4.41695100	4.84318300
C	0.07091300	3.22451800	0.81514200	H	-3.63940700	-5.49605800	4.71927300
C	-0.00903700	4.44884800	0.13596100	H	-4.38090200	-4.01910100	5.33659800
H	-0.69634700	4.56366500	-0.69543200	H	-2.63953000	-4.27695600	5.52391800
C	0.77817300	5.54227700	0.51757100	C	-5.00179200	-3.36649200	0.13085600
C	1.64192000	5.39573000	1.60979300	H	-5.88746100	-3.91675100	0.46460500
H	2.24272900	6.24610600	1.92973700	H	-4.58346200	-3.90357800	-0.73009000
C	1.74413500	4.18695200	2.30830600	H	-5.33536500	-2.38683300	-0.23302900
C	0.95666800	3.10401600	1.89579300	C	0.28405100	-0.73319800	3.22679600
H	1.03438100	2.16114900	2.42687500	C	-0.66486000	-0.25218300	4.14099200
				H	-1.72283600	-0.41486900	3.96263600

C	-0.27320300	0.44682400	5.28941000	C	6.96165400	-4.09294100	-4.12330800
C	1.09193800	0.66434200	5.51020000	C	7.43742400	-4.96103600	-3.13890600
H	1.40666200	1.20064200	6.40424600	C	6.83443500	-4.96599000	-1.87876100
C	2.06223000	0.21565900	4.60624800	C	5.76603900	-4.10987000	-1.60889900
C	1.64327700	-0.46762200	3.45814100	H	1.74491400	-0.26799900	-2.65748900
H	2.38393400	-0.78135100	2.73046400	H	2.71144100	-3.93653300	-1.85442300
C	3.53525600	0.44087600	4.86392900	H	2.63669500	-3.37551300	-3.53017000
H	4.06471500	0.70397900	3.94169800	H	4.13160200	-1.45423200	-2.95535000
H	4.01165200	-0.46492500	5.26206200	H	5.52856600	-2.56316400	-4.61929400
H	3.69853200	1.24255100	5.59183000	H	7.42563400	-4.07726600	-5.10662800
C	-1.30511400	0.92821900	6.28440900	H	8.27212900	-5.62462500	-3.34986800
H	-1.49728100	0.17159900	7.05746300	H	7.20030300	-5.63435800	-1.10289100
H	-2.25952300	1.14381700	5.79333800	H	5.30286400	-4.11670200	-0.62414100
H	-0.97136300	1.83650500	6.79850900	O	1.62323100	-1.68226300	-0.87681100
Ru	0.27082300	-0.23768500	-0.16070100	O	1.43421900	-1.06808800	-3.14053200
P	-0.99744000	1.76787000	0.37984100	H	4.14131100	-1.96750200	-1.26536500
P	-0.19603300	-1.59911500	1.66557700	C	-1.80268000	-0.84022800	-2.57557700
H	3.65138200	3.60483800	3.15620400	C	-3.28187100	-0.85269300	-2.91776200
H	0.60906100	-2.75369900	-2.32332700	C	-3.62654600	-1.01847900	-4.40815300
C	2.42635600	1.13106200	-0.47402200	C	-5.12243600	-0.97489100	-4.64354400
C	3.77827200	1.79992900	-0.57135300	C	-5.88364500	-2.15067200	-4.68075300
C	3.76790100	3.06066700	-1.46076100	C	-7.26755400	-2.10570900	-4.86249600
C	5.12155800	3.73601900	-1.51553700	C	-7.91511500	-0.87798300	-5.01075800
C	5.44774100	4.76003700	-0.61555400	C	-7.16841500	0.30213800	-4.97855100
C	6.70562900	5.36503500	-0.64121500	C	-5.78557300	0.25152100	-4.79663000
C	7.66204300	4.95338500	-1.57155000	H	0.04560500	-0.84182300	-3.34731200
C	7.34996700	3.93515000	-2.47501300	H	-3.75247200	-1.64288800	-2.32075700
C	6.09056100	3.33435400	-2.44573800	H	-3.69323300	0.09157400	-2.53736900
H	4.11781100	2.03528600	0.44207700	H	-3.13171300	-0.22415100	-4.97595700
H	4.48574300	1.06373800	-0.97796400	H	-5.38529100	-3.11205800	-4.57313500
H	3.44207900	2.77513100	-2.46652400	H	-7.83831900	-3.03035900	-4.89370600
H	4.70280300	5.08691100	0.10734400	H	-8.99142300	-0.84087300	-5.15648500
H	6.93733400	6.16072000	0.06254400	H	-7.66246800	1.26263300	-5.10248400
H	8.64110400	5.42465800	-1.59527300	H	-5.20746700	1.17317800	-4.77724900
H	8.08599500	3.61113700	-3.20643900	O	-1.47293400	-0.88713100	-1.37443800
H	5.85283300	2.54552600	-3.15665200	O	-0.99329300	-0.76642600	-3.58836500
O	2.06821600	0.57878700	0.61253300	H	-3.21388000	-1.96563400	-4.77370000
O	1.62635000	1.11107400	-1.47176100				
H	3.01782100	3.75950100	-1.07286800	<b>TS7</b>			
C	1.53312800	-2.17493200	-2.11728400	C	1.87319300	-2.35626000	-1.23541200
C	2.74457800	-3.04289500	-2.48995200	C	1.17669400	-2.29405800	-2.45029800
C	4.09587500	-2.33154400	-2.29742100	H	0.15165400	-1.93815900	-2.46083000
C	5.27589500	-3.23275500	-2.58825100	C	1.77743700	-2.69292200	-3.65225400
C	5.89191300	-3.23892800	-3.84749700	C	3.09449800	-3.16209300	-3.61847000



H	3.56846500	-3.48119500	-4.54574500	H	-2.96962800	-5.16502200	3.70986000
C	3.81647500	-3.23917400	-2.41975300	C	-0.69971200	3.10299700	1.82481700
C	3.19155400	-2.83772100	-1.23297400	C	-0.45777400	4.02688800	0.79374200
H	3.74293400	-2.90621700	-0.30154300	H	0.20226500	3.75595600	-0.02498400
C	1.01133700	-2.58623500	-4.95060200	C	-1.03522600	5.29551500	0.80570800
H	0.79202700	-1.53637400	-5.18073200	C	-1.88239900	5.63636200	1.87276500
H	0.05021100	-3.11118800	-4.89234300	H	-2.34029000	6.62420100	1.89307400
H	1.57623700	-3.00840700	-5.78819100	C	-2.14115900	4.74359400	2.91120100
C	5.24936600	-3.72321600	-2.41247600	C	-1.53279000	3.47648200	2.88013900
H	5.55080600	-4.06711500	-1.41765000	H	-1.71572700	2.79352700	3.70276700
H	5.94037900	-2.92083100	-2.70447200	C	-0.76394900	6.28917200	-0.30170400
H	5.39782700	-4.54998700	-3.11646700	H	-0.39255300	7.24119400	0.09750400
C	2.31302400	-1.99919400	1.59586500	H	-1.67484200	6.51327100	-0.87151800
C	2.32785600	-3.06223600	2.51016800	H	-0.01825700	5.90798000	-1.00668900
H	1.52778800	-3.79383800	2.50644000	C	-3.05886200	5.11675100	4.05406800
C	3.37080400	-3.21136300	3.43188900	H	-4.00984700	4.57076600	3.99806400
C	4.41668700	-2.28129800	3.41668400	H	-3.29245100	6.18642800	4.04638700
H	5.24202000	-2.39754800	4.11729000	H	-2.60904300	4.87747100	5.02521900
C	4.43753800	-1.21365700	2.51198100	C	1.90721200	2.23327600	2.14419400
C	3.37158400	-1.07986100	1.61143900	C	2.15264800	2.82146300	3.39842000
H	3.37936500	-0.25874800	0.90158100	H	1.40577100	2.75308500	4.18391900
C	3.36087700	-4.35166700	4.42535900	C	3.33741000	3.51312900	3.65173100
H	4.37761700	-4.65549800	4.69745200	C	4.27807800	3.63274600	2.61550400
H	2.84096700	-5.22730100	4.02249400	H	5.20009800	4.18294200	2.79813100
H	2.84647900	-4.06750300	5.35314100	C	4.05438200	3.07784800	1.35498500
C	5.58943400	-0.23464000	2.49569000	C	2.86001100	2.36956100	1.13181800
H	6.34868700	-0.50348600	3.23728900	H	2.65999400	1.93502600	0.15704400
H	5.25058900	0.78510500	2.71007400	C	3.60449200	4.13604000	5.00340600
H	6.07756400	-0.21085500	1.51326700	H	3.78257100	5.21521600	4.91782200
C	-0.10403800	-3.26667700	0.67534900	H	4.49389500	3.70079600	5.47681500
C	-0.05397600	-4.45331700	-0.06984800	H	2.75980700	3.99021000	5.68388700
H	0.62477300	-4.53583400	-0.91203600	C	5.06529300	3.23911800	0.24168300
C	-0.86185500	-5.54966200	0.25752100	H	5.96573100	3.75547900	0.58985600
C	-1.71512900	-5.44533000	1.36258400	H	4.65095000	3.82103100	-0.59152900
H	-2.33164600	-6.29928300	1.64028700	H	5.37265700	2.26928300	-0.16797000
C	-1.78746500	-4.27448700	2.12670900	C	-0.25136300	0.58216000	3.27247700
C	-0.98003700	-3.18761400	1.76780100	C	0.68722800	0.05808800	4.17334400
H	-1.03411600	-2.27366500	2.34962700	H	1.74762900	0.21732400	4.00697800
C	-0.81969800	-6.81461300	-0.57042000	C	0.28190400	-0.68109300	5.29153100
H	0.13379500	-6.91511500	-1.09918800	C	-1.08641800	-0.89433000	5.49547400
H	-1.61497900	-6.82094700	-1.32772700	H	-1.41175900	-1.46211500	6.36592900
H	-0.95891400	-7.70607500	0.05146800	C	-2.04693300	-0.40226700	4.60356900
C	-2.72947200	-4.17571400	3.30543300	C	-1.61451400	0.32022200	3.48498100
H	-2.29735600	-3.57086300	4.10928700	H	-2.34748900	0.66540000	2.76367000

C	-3.52341200	-0.62461700	4.84334300	H	-2.59525800	3.53557900	-3.35946200
H	-4.04964000	-0.84303400	3.90771300	H	-4.16033600	1.66082300	-2.83963800
H	-3.99388400	0.26757000	5.27767600	H	-5.55061400	2.89211200	-4.42410100
H	-3.69806200	-1.45523200	5.53531700	H	-7.40083100	4.49269700	-4.80268300
C	1.30372600	-1.21016200	6.27264300	H	-8.15711000	5.98621800	-2.96076000
H	1.50848700	-0.48004500	7.06758600	H	-7.04235700	5.85641100	-0.73857800
H	2.25481400	-1.42782100	5.77596700	H	-5.19132700	4.25344300	-0.36848200
H	0.95335400	-2.12710700	6.75947400	O	-1.61865000	1.71608100	-0.78403100
Ru	-0.26076900	0.22305100	-0.13499900	O	-1.46273000	1.17529700	-3.09979900
P	0.98597800	-1.80760600	0.30677200	H	-4.12361400	2.09638100	-1.12847700
P	0.24540600	1.49759500	1.74558300	C	1.73109500	0.93407000	-2.53562600
H	-3.67708800	-3.70063600	3.01839600	C	3.21043400	0.99940600	-2.89807100
H	-0.57643000	2.81081300	-2.18435400	C	3.51691100	1.16739000	-4.39577900
C	-2.44416800	-1.09658400	-0.51654700	C	5.00674700	1.18554600	-4.66789200
C	-3.80150600	-1.74638900	-0.65944600	C	5.71474800	2.39265300	-4.74150400
C	-3.78826000	-2.97752100	-1.59012500	C	7.09433300	2.40599400	-4.95755200
C	-5.14787400	-3.63542400	-1.68981500	C	7.79214500	1.20593300	-5.10500800
C	-5.50555300	-4.67478600	-0.81980600	C	7.09927600	-0.00509900	-5.03662400
C	-6.76965200	-5.26343700	-0.88552200	C	5.72054000	-0.01241300	-4.82017100
C	-7.70094600	-4.82001800	-1.82673200	H	-0.30731900	0.98636400	-3.27037000
C	-7.35725400	-3.78663200	-2.70093800	H	3.66249800	1.81350800	-2.31822000
C	-6.09169900	-3.20217400	-2.63159800	H	3.66736700	0.07610200	-2.51929300
H	-4.16120700	-2.01186400	0.33930100	H	3.04203200	0.34848800	-4.94565600
H	-4.49464100	-0.99055200	-1.05472100	H	5.17681000	3.33260100	-4.63469800
H	-3.44185900	-2.66281000	-2.58017600	H	7.62261300	3.35436500	-5.01635000
H	-4.78038500	-5.02704700	-0.08876200	H	8.86514200	1.21399000	-5.27767100
H	-7.02577700	-6.07126300	-0.20445200	H	7.63228300	-0.94491300	-5.15845100
H	-8.68478700	-5.27853300	-1.88155300	H	5.18444100	-0.95825800	-4.77212800
H	-8.07326500	-3.43799100	-3.44086800	O	1.45948000	0.92894900	-1.30384600
H	-5.82954900	-2.40162700	-3.32058200	O	0.89951600	0.88249300	-3.50343900
O	-2.08212200	-0.61444900	0.59887800	H	3.05448000	2.09232700	-4.75830900
O	-1.64172900	-1.02549600	-1.51358300				
H	-3.05226200	-3.69650100	-1.21219700	<b>Int12</b>			
C	-1.52490900	2.28537300	-1.96667800	C	1.87717000	-2.36619300	-1.36923700
C	-2.71214000	3.18136200	-2.32808600	C	1.28409700	-2.11386200	-2.61196900
C	-4.08247300	2.50539500	-2.14364500	H	0.30788600	-1.64643500	-2.65893300
C	-5.23510600	3.45966800	-2.37066000	C	1.93634300	-2.45000300	-3.80717100
C	-5.87404600	3.54433800	-3.61527000	C	3.19349600	-3.05613300	-3.73605300
C	-6.91767400	4.44702200	-3.82968100	H	3.70773700	-3.32226100	-4.65857500
C	-7.34272200	5.28512000	-2.79734200	C	3.80685600	-3.33481000	-2.50637800
C	-6.71575000	5.21181600	-1.55110500	C	3.13670400	-2.98732500	-1.32903500
C	-5.67370000	4.30753500	-1.34250100	H	3.60638300	-3.20592700	-0.37602100
H	-1.76779800	0.35639600	-2.63266700	C	1.28044900	-2.13622000	-5.13180800
H	-2.65076000	4.05901400	-1.67207800	H	1.00992700	-1.07522200	-5.18002100

H	0.35585800	-2.71182000	-5.26608500	H	-2.51519100	6.29516600	2.16557200
H	1.94217100	-2.36519500	-5.97374100	C	-2.40849600	4.31507200	2.99210300
C	5.17496800	-3.97793500	-2.45674000	C	-1.75462600	3.07210500	2.92328600
H	5.39081300	-4.38206700	-1.46236300	H	-2.03464400	2.30136700	3.63243100
H	5.96552400	-3.25387500	-2.69519900	C	-0.59351000	6.24450800	0.23713200
H	5.26028400	-4.79696400	-3.18050700	H	-0.21411600	7.10574400	0.80147200
C	2.23099500	-2.12962700	1.48150700	H	-1.43907900	6.60349600	-0.36317500
C	2.21107600	-3.19361900	2.39242200	H	0.19605200	5.92629800	-0.45121900
H	1.39350300	-3.90589200	2.37850600	C	-3.50433000	4.53868800	4.01010300
C	3.24749300	-3.37177500	3.31750400	H	-4.41164800	3.97834400	3.74947800
C	4.31400700	-2.46618900	3.30968100	H	-3.77795500	5.59656600	4.07816600
H	5.13533500	-2.60713900	4.01042300	H	-3.19699200	4.20541200	5.00855100
C	4.36558200	-1.39529100	2.40841500	C	1.86147300	2.00201200	2.34608700
C	3.31076500	-1.23493800	1.50086200	C	2.03319000	2.54209700	3.63445800
H	3.34107500	-0.42304700	0.78082500	H	1.25279600	2.42423500	4.38057900
C	3.21065200	-4.52260200	4.29827900	C	3.18694900	3.24966200	3.97189500
H	4.21702600	-4.79442000	4.63440600	C	4.16906600	3.43816900	2.98567600
H	2.75018700	-5.41129900	3.85312700	H	5.06644900	4.00345300	3.23339400
H	2.62494700	-4.26855100	5.19167400	C	4.01649800	2.93547600	1.69306600
C	5.53787600	-0.44123300	2.40773800	C	2.85307500	2.20747800	1.38374100
H	6.35423300	-0.81445000	3.03482000	H	2.70203700	1.81499600	0.38236600
H	5.24733700	0.54669400	2.78398800	C	3.38023900	3.80874200	5.36344600
H	5.93185800	-0.29565400	1.39488700	H	3.67454800	4.86466400	5.33316200
C	-0.15478100	-3.38683500	0.42651700	H	4.16961500	3.27094400	5.90497600
C	-0.08436700	-4.51491500	-0.40387200	H	2.46250000	3.73230000	5.95507200
H	0.61135500	-4.53087700	-1.23576000	C	5.06895700	3.17527200	0.63393200
C	-0.89474100	-5.63378100	-0.17604600	H	5.93831300	3.69927000	1.04417600
C	-1.77257400	-5.61204300	0.91457900	H	4.67382100	3.78192300	-0.19063800
H	-2.39254200	-6.48489100	1.11477300	H	5.42010000	2.23388000	0.19484700
C	-1.86673200	-4.50104600	1.76041700	C	-0.28829800	0.24196000	3.30989300
C	-1.05562200	-3.38816300	1.50120100	C	0.63227000	-0.26453100	4.23853100
H	-1.12707300	-2.51921200	2.14689300	H	1.69068900	-0.05519300	4.12451700
C	-0.83097900	-6.83371100	-1.09418400	C	0.21267500	-1.05123600	5.31884200
H	0.12779000	-6.88418500	-1.62033100	C	-1.15138300	-1.32995400	5.45730400
H	-1.62010500	-6.79261700	-1.85669100	H	-1.48796500	-1.93276000	6.29941600
H	-0.96488800	-7.77000700	-0.54069700	C	-2.09295500	-0.86096900	4.53319700
C	-2.83404400	-4.49283900	2.92266100	C	-1.64542100	-0.09447700	3.45035800
H	-2.40734200	-3.97980600	3.79082500	H	-2.36026600	0.22052000	2.69803000
H	-3.10539200	-5.51016800	3.22459200	C	-3.56741500	-1.14995400	4.70531500
C	-0.75053200	2.83449900	1.98400900	H	-4.05912100	-1.30034400	3.73833600
C	-0.38585200	3.87544400	1.10961200	H	-4.07890900	-0.31473300	5.20238600
H	0.41390400	3.71757800	0.39036900	H	-3.73457000	-2.04303100	5.31666600
C	-1.00775500	5.12215000	1.16243600	C	1.21586400	-1.55882800	6.32992500
C	-2.02571000	5.32395700	2.10955500	H	1.37524700	-0.82823900	7.13469400

H	2.18838600	-1.74628100	5.86326300
H	0.87575100	-2.48798000	6.80032900
Ru	-0.24128200	0.12425100	-0.15080200
P	0.94004900	-1.91016700	0.16883000
P	0.23420600	1.24935600	1.84893200
H	-3.76349500	-3.96877600	2.66320900
H	-0.53557700	2.56106500	-2.31243700
C	-2.43198900	-1.14355500	-0.69266500
C	-3.77998200	-1.78236600	-0.94291100
C	-3.71584000	-2.96900900	-1.92784900
C	-5.06868600	-3.61642500	-2.13229900
C	-5.48402100	-4.67947000	-1.31799900
C	-6.74344100	-5.25920200	-1.48022900
C	-7.61231200	-4.78346000	-2.46438700
C	-7.21043200	-3.72696600	-3.28447500
C	-5.94977100	-3.15112500	-3.11850000
H	-4.19567300	-2.09272800	0.02059400
H	-4.45070500	-1.00820900	-1.34181400
H	-3.31534500	-2.61089400	-2.88189500
H	-4.80742500	-5.05879400	-0.55452800
H	-7.04438100	-6.08574900	-0.84118100
H	-8.59220000	-5.23523700	-2.59456200
H	-7.87672800	-3.35362800	-4.05806200
H	-5.64130100	-2.33321400	-3.76666200
O	-2.13420000	-0.70884400	0.46405400
O	-1.57777300	-1.02278300	-1.63284000
H	-3.00246700	-3.70663900	-1.54289900
C	-1.48253000	2.49023400	-1.76675500
C	-2.57931700	3.43951300	-2.15352200
C	-3.94376100	3.13112200	-1.51735900
C	-4.96620500	4.21137400	-1.79813600
C	-5.73326400	4.19448100	-2.97134200
C	-6.65280800	5.20929400	-3.24180200
C	-6.82135700	6.26201100	-2.33967300
C	-6.06454600	6.29047100	-1.16658400
C	-5.14642400	5.27311200	-0.90018400
H	-1.98125700	0.14714000	-3.08413000
H	-2.23507500	4.44228400	-1.85094500
H	-2.63831900	3.45095700	-3.24669500
H	-4.29201300	2.16672900	-1.90597800
H	-5.60965500	3.37529400	-3.67669800
H	-7.24061800	5.17552100	-4.15566300
H	-7.53934200	7.05108800	-2.54736200
H	-6.19313600	7.10263000	-0.45517100

H	-4.56282700	5.29607700	0.01836900
O	-1.57555900	1.74453300	-0.78834200
O	-1.84237000	0.89433300	-3.69695100
H	-3.81138700	3.00835700	-0.43772600
C	1.76015600	1.04040200	-2.35199500
C	3.24194300	1.24210400	-2.69669100
C	3.50396000	1.60035500	-4.16855800
C	4.97978000	1.74549600	-4.47302000
C	5.59377900	3.00471900	-4.51089300
C	6.96090600	3.13333000	-4.76569500
C	7.74183000	1.99808600	-4.98863000
C	7.14406300	0.73573600	-4.95503600
C	5.77777400	0.61379700	-4.69997200
H	-0.86304000	0.92391200	-3.72782700
H	3.65610800	2.01281700	-2.03437200
H	3.76415000	0.31245700	-2.43479500
H	3.06188300	0.82258400	-4.80007400
H	4.99046400	3.89521500	-4.34562100
H	7.41430300	4.12114900	-4.79559400
H	8.80516100	2.09554300	-5.19171600
H	7.74228000	-0.15450700	-5.13383100
H	5.31707100	-0.37209000	-4.67869900
O	1.54882000	0.87178800	-1.09031500
O	0.91079400	1.04498900	-3.26081300
H	2.97477500	2.52842500	-4.41293200

**TS4-6**

C	1.07997700	0.13079800	3.04128400
C	0.74307400	1.48363300	3.14829500
H	0.50019700	2.05089500	2.25910500
C	0.72896700	2.12978000	4.39452900
C	1.06464000	1.39694100	5.53340300
H	1.05496400	1.89017000	6.50440600
C	1.41442000	0.04032000	5.45912400
C	1.41655700	-0.58008800	4.20849500
H	1.68389000	-1.63012400	4.14573700
C	0.34689200	3.58972500	4.48386600
H	0.97301700	4.20612000	3.82768000
H	0.45121900	3.96992400	5.50528800
H	-0.69325500	3.74615500	4.17170900
C	1.77139500	-0.72967200	6.71089800
H	2.08526500	-1.75147300	6.47496100
H	0.91776900	-0.79438400	7.39784900
H	2.58854400	-0.24598700	7.26051900

C	0.80678700	-2.45607400	1.88963700	H	-1.70275200	2.53731200	-6.23288900
C	1.81116800	-3.43437600	1.87331700	H	-0.18561200	2.02806600	-5.47028700
H	2.79615700	-3.19397600	1.48817800	C	-5.19626900	-0.86504800	-4.99232100
C	1.57219100	-4.72396300	2.36337600	H	-5.61666500	-1.65917300	-4.36712900
C	0.29907100	-5.02629300	2.86189000	H	-5.08961500	-1.26218000	-6.00990200
H	0.10242100	-6.02577500	3.24656500	H	-5.93289200	-0.05330400	-5.04076400
C	-0.72417300	-4.07213300	2.89216400	C	-2.66179100	-2.20216500	-0.49680500
C	-0.45433800	-2.78707200	2.40274400	C	-3.13975200	-3.40123700	-1.05609900
H	-1.23602200	-2.03405200	2.43808500	H	-2.65173400	-3.82217600	-1.93029700
C	2.67898700	-5.75444900	2.39412300	C	-4.23917000	-4.06619700	-0.50724400
H	3.17248400	-5.77633000	3.37511700	C	-4.86893600	-3.50479400	0.61467200
H	3.44932400	-5.53683400	1.64726600	H	-5.73667500	-4.00643000	1.04055900
H	2.29619400	-6.76324900	2.20359800	C	-4.41276600	-2.32072500	1.19827400
C	-2.08893300	-4.41397800	3.44500500	C	-3.29663900	-1.68004600	0.63549500
H	-2.10089500	-5.41643900	3.88513800	H	-2.92425800	-0.76260600	1.08510800
H	-2.85492200	-4.37888200	2.66149300	C	-4.74233000	-5.36282400	-1.10083100
H	-2.39170200	-3.70267500	4.22316500	H	-4.26112300	-5.57722800	-2.06037200
C	2.90618900	-0.71144100	0.92329800	H	-5.82601700	-5.33393900	-1.26608200
C	3.89742900	-0.17167600	1.75230800	H	-4.54202600	-6.21130800	-0.43359500
H	3.62333500	0.27566200	2.70239500	C	-5.09378100	-1.73199100	2.41316300
C	5.24840900	-0.20596700	1.37878100	H	-5.36034800	-0.68142000	2.24930500
C	5.58999300	-0.80418900	0.16093400	H	-4.43617300	-1.75942300	3.29129200
H	6.63856300	-0.85421200	-0.12969200	H	-6.00869600	-2.27829300	2.66463000
C	4.61932200	-1.34461500	-0.69298000	C	-0.16364000	-2.50913200	-1.98456400
C	3.27705500	-1.28432500	-0.30320100	C	0.06105500	-3.73226000	-1.33054100
H	2.51453600	-1.68659400	-0.96327500	H	-0.45008400	-3.95200100	-0.39895700
C	6.30897300	0.40394800	2.26822000	C	0.92399900	-4.69146000	-1.87098000
H	6.48118900	1.45882500	2.01591500	C	1.58880500	-4.39907000	-3.06971200
H	7.26786800	-0.11536500	2.16282500	H	2.25857600	-5.14205100	-3.50029800
H	6.01683400	0.36714000	3.32303200	C	1.40307500	-3.18245600	-3.73218100
C	5.00950500	-1.95724800	-2.01929300	C	0.51869400	-2.24647400	-3.17896400
H	4.29115600	-2.72271600	-2.33005500	H	0.35969500	-1.30773200	-3.69834200
H	6.00333700	-2.41644300	-1.97241700	C	2.13645500	-2.87087700	-5.01746400
C	-2.08699300	-0.49528000	-2.78866100	H	2.94294000	-2.14533200	-4.84934400
C	-1.42258500	0.54951700	-3.44520300	H	1.46389200	-2.43567200	-5.76543900
H	-0.48407400	0.92629100	-3.05138900	H	2.58635700	-3.77055800	-5.45008200
C	-1.95924400	1.13368100	-4.60150000	C	1.10876200	-6.03407700	-1.20091700
C	-3.17853100	0.65831900	-5.08835100	H	0.56164600	-6.82207500	-1.73589500
H	-3.60522500	1.10980000	-5.98293200	H	0.74436400	-6.01698100	-0.16996600
C	-3.87208200	-0.37762500	-4.44799500	H	2.16377500	-6.33193400	-1.18408300
C	-3.31544500	-0.94578500	-3.29859900	Ru	-0.21564500	0.49508100	-0.14413000
H	-3.85583000	-1.74041400	-2.79593700	P	1.11009100	-0.69635800	1.37548000
C	-1.23617600	2.27631300	-5.27732300	P	-1.29188900	-1.21994700	-1.26651700
H	-1.24295100	3.17220600	-4.64380800	H	5.03945200	-1.19768300	-2.81224500

H	-3.09239100	0.78619900	-0.64062900	C	0.24816400	-2.87137600	0.61842300
C	1.80775600	1.82604600	-0.96527400	C	-0.38276200	-3.53500200	-0.44687200
C	2.92822000	2.61623800	-1.60373100	H	-1.14142100	-3.01904100	-1.02513100
C	3.86666600	3.27287400	-0.57037500	C	-0.03651900	-4.84712300	-0.79185000
C	4.99533800	4.03983200	-1.22527600	C	0.96876900	-5.49474400	-0.06341900
C	6.19060500	3.39524500	-1.57480300	H	1.24676900	-6.51440700	-0.32756500
C	7.22308100	4.08971200	-2.20709200	C	1.61975400	-4.86144800	1.00005600
C	7.07714700	5.44708900	-2.50158400	C	1.24466300	-3.55247900	1.33457500
C	5.89292000	6.10208800	-2.15761600	H	1.74596400	-3.06951500	2.16582000
C	4.86349700	5.40273300	-1.52509100	C	-0.75574400	-5.55638100	-1.91786600
H	3.48235800	1.94979100	-2.27199600	H	-0.09686500	-6.26371400	-2.43416100
H	2.47320000	3.39247700	-2.23490900	H	-1.13888300	-4.84360300	-2.65512100
H	3.27335000	3.93500800	0.06827600	H	-1.61428000	-6.12942100	-1.54196500
H	6.31076200	2.33858900	-1.34308800	C	2.72464400	-5.56118500	1.76121700
H	8.14351700	3.57215000	-2.46603700	H	2.57056000	-6.64569400	1.78492200
H	7.88108100	5.99059600	-2.99102400	H	2.78590900	-5.20491200	2.79514700
H	5.77162200	7.15985900	-2.37730600	H	3.70494100	-5.38200800	1.29873200
H	3.94583100	5.92105500	-1.25424900	C	0.95445800	-0.75523300	2.38341200
O	1.39444000	0.74959700	-1.52459200	C	0.65590400	-0.97635100	3.73382700
O	1.25589500	2.21109300	0.10925600	H	-0.33860300	-1.30619900	4.01932600
H	4.27442100	2.48956500	0.07917900	C	1.62532600	-0.79072500	4.72806500
C	-2.69660000	1.66136800	-0.11364500	C	2.90946600	-0.38359100	4.34445700
C	-3.83097500	2.64307600	0.17771600	H	3.67318900	-0.24725600	5.10871200
C	-3.40068200	3.92621400	0.91404400	C	3.23827400	-0.15405600	3.00251200
C	-4.55655300	4.87444700	1.14848800	C	2.24637300	-0.33791600	2.03009900
C	-5.31419900	4.81206000	2.32658400	H	2.48612700	-0.16730900	0.98421000
C	-6.39918400	5.66620900	2.53186300	C	1.28622600	-1.00877100	6.18549900
C	-6.74757400	6.60364500	1.55743500	H	0.49240200	-1.75388500	6.30369800
C	-6.00122100	6.67890800	0.37937300	H	0.93318200	-0.08096200	6.65545400
C	-4.91733800	5.82249600	0.18007700	H	2.15891900	-1.34844800	6.75412400
H	-4.29416300	2.90465500	-0.78313700	C	4.63791600	0.25425200	2.60107000
H	-4.59660200	2.11567900	0.76347000	H	5.20096400	0.64783800	3.45424400
H	-2.94796500	3.64793300	1.87293200	H	4.61877800	1.02080600	1.81857900
H	-5.04515900	4.08789500	3.09312600	H	5.20177800	-0.60027800	2.20363500
H	-6.96952200	5.60259100	3.45544000	C	-1.85890400	-1.30680500	1.89831200
H	-7.58963800	7.27229200	1.71643200	C	-2.33709900	-2.54019500	2.37023100
H	-6.25978700	7.40920300	-0.38355100	H	-1.74807300	-3.44026000	2.22094500
H	-4.33655100	5.89134500	-0.73757400	C	-3.56626300	-2.63031000	3.03115000
O	-1.58275100	2.23643000	-0.77862700	C	-4.31140200	-1.45718600	3.22229800
O	-1.95092800	1.28647700	1.07170200	H	-5.26707400	-1.51550500	3.74173200
H	-2.62317300	4.42297700	0.32265600	C	-3.86091800	-0.21616700	2.76348900
H	-1.31354700	2.20220200	0.49194300	C	-2.63097200	-0.15563700	2.09309000
				H	-2.27879800	0.79625200	1.70745100
				C	-4.08607400	-3.96021200	3.53010600

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H	-5.00596400	-4.25199000	3.00734800	C	-1.25662100	3.99258200	3.72087400
H	-4.32380000	-3.92294300	4.60057700	H	-1.63486800	4.37941200	4.66614700
H	-3.35183000	-4.75748500	3.37719600	C	-1.90075700	4.34152900	2.53323100
C	-4.68034400	1.03909900	2.96167800	C	-1.38455500	3.85723000	1.32237600
H	-4.06984500	1.84835900	3.37929100	H	-1.87258200	4.14733100	0.39888800
H	-5.52494800	0.86564600	3.63685900	C	-3.13121700	5.22090200	2.53859800
C	-0.34511500	3.63625300	-1.50916100	H	-4.04264200	4.63103900	2.37415000
C	-1.61507400	3.45195800	-2.07762700	H	-3.08845400	5.97371700	1.74333000
H	-2.17453500	2.54842000	-1.85354700	H	-3.24566600	5.74347800	3.49406800
C	-2.18038800	4.42513000	-2.91404200	C	0.54926200	2.81055500	5.02986200
C	-1.45722300	5.59434500	-3.17033000	H	-0.12529900	2.24958100	5.68953800
H	-1.89081600	6.35821500	-3.81418700	H	0.85054700	3.71452100	5.57429300
C	-0.19024800	5.80720900	-2.61513800	H	1.43995300	2.19771200	4.86726500
C	0.35196600	4.82142300	-1.78226600	Ru	-0.22841700	0.23140400	-1.00541500
H	1.33059200	4.98893700	-1.34384300	P	-0.24770500	-1.10849300	1.01186400
C	-3.53629300	4.19661700	-3.54371300	P	0.35334400	2.35597200	-0.33917500
H	-3.44915600	3.61046500	-4.46838500	H	-5.08433200	1.40229000	2.00785600
H	-4.02416200	5.14271700	-3.80217300	H	1.37799400	-0.78014600	-3.27724800
H	-4.20085400	3.64172300	-2.87275500	C	-2.66856300	-0.45940600	-1.61111000
C	0.58853600	7.06547100	-2.92651400	C	-4.14083900	-0.67776800	-1.90456500
H	1.17734700	6.95068800	-3.84663600	C	-4.58138700	-2.13165800	-1.62989500
H	1.28924700	7.31254000	-2.12193200	C	-6.05261000	-2.35593000	-1.90354500
H	-0.07697700	7.92348200	-3.07310900	C	-7.00593200	-2.17638100	-0.89129300
C	2.15642700	2.76596700	-0.43584600	C	-8.36682900	-2.35474500	-1.14557700
C	2.89462800	3.43137300	0.54712600	C	-8.79955500	-2.71764600	-2.42273200
H	2.41633300	3.75180000	1.46721800	C	-7.86103200	-2.90096200	-3.44047300
C	4.25611400	3.71972300	0.35342700	C	-6.50139900	-2.72147300	-3.18049900
C	4.85556900	3.34138100	-0.85033400	H	-4.72658600	0.02689700	-1.30621400
H	5.90695100	3.57395100	-1.01446100	H	-4.32028300	-0.43512700	-2.96096500
C	4.13277800	2.68877800	-1.86100200	H	-3.97131300	-2.79839100	-2.24805800
C	2.78344500	2.40323300	-1.64202400	H	-6.67337500	-1.89943900	0.10726200
H	2.18492500	1.92271800	-2.41489900	H	-9.08908100	-2.21474300	-0.34501600
C	5.04963900	4.42341000	1.43216200	H	-9.85838200	-2.86059300	-2.62221500
H	5.38893200	3.71881600	2.20330700	H	-8.18699800	-3.18909900	-4.43684000
H	4.44819200	5.18740600	1.93733500	H	-5.77528000	-2.87200500	-3.97694300
H	5.94002100	4.91083200	1.02108400	O	-2.31877200	0.60139600	-0.97715400
C	4.80655500	2.30344800	-3.15938100	O	-1.79754000	-1.29861500	-1.96363700
H	5.42275000	3.12153700	-3.55089700	H	-4.35724700	-2.37563100	-0.58414000
H	4.07052300	2.03991500	-3.92549600	C	2.05141900	-1.00369500	-2.43804600
H	5.47209300	1.43937400	-3.02573900	C	3.29225700	-1.80972000	-2.67911200
C	-0.25855300	3.02391300	1.28744000	C	4.16101100	-2.04492900	-1.43249700
C	0.34919700	2.66890300	2.50582800	C	5.33233000	-2.96288500	-1.71000200
H	1.20735400	2.00689800	2.51200400	C	6.59069300	-2.44975100	-2.05089800
C	-0.12913100	3.15950500	3.72478200	C	7.66120500	-3.30089300	-2.33248900

C	7.48872700	-4.68504700	-2.27652300	H	-3.53590700	-4.87127600	4.74697100
C	6.23990500	-5.21023300	-1.93623700	H	-1.95360500	-5.25965000	4.04763200
C	5.17301200	-4.35552500	-1.65525300	H	-3.40947000	-5.36651100	3.05591900
H	2.96742300	-2.76711600	-3.11664800	C	-4.62862300	-0.01535600	3.73868600
H	3.86359300	-1.31808000	-3.48156800	H	-5.43568300	-0.46609200	4.32543100
H	4.51564300	-1.07662300	-1.06095500	H	-5.07188200	0.43855900	2.84493800
H	6.73493300	-1.37164900	-2.08930400	H	-4.19847900	0.79927900	4.33475000
H	8.63051500	-2.88226100	-2.59106600	C	1.02749300	-2.55168500	1.15595600
H	8.32131100	-5.34932100	-2.49220100	C	2.07763800	-3.00803400	1.96499800
H	6.09750300	-6.28669500	-1.88489800	H	2.37560900	-2.43540900	2.83750800
H	4.20298600	-4.76977700	-1.38654700	C	2.75149500	-4.19945900	1.66820800
O	0.06181000	0.87933900	-2.93986500	C	2.34701900	-4.93479500	0.54700300
O	1.75557200	-0.57885900	-1.31809400	H	2.85445700	-5.87051000	0.31519800
H	3.52864100	-2.46795300	-0.64431800	C	1.30567100	-4.50090800	-0.28226600
H	-0.50508200	1.62818400	-3.17354500	C	0.65415900	-3.30205000	0.03218200

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C	1.00053900	-0.27166000	2.98049500	H	4.86830500	-4.41561800	2.08161100
C	2.06361100	0.61643800	2.77711000	H	3.88393700	-5.76331000	2.65640600
H	2.35122600	0.88618400	1.76894200	H	3.86933600	-4.21737200	3.52445000
C	2.77240200	1.15330700	3.86216600	C	0.90977900	-5.29015800	-1.50976400
C	2.39806000	0.78878800	5.15723800	H	-0.16101200	-5.19340000	-1.71706200
H	2.94346600	1.20231900	6.00466200	H	1.14507600	-6.35422600	-1.39624600
C	1.33812400	-0.09727100	5.39329900	C	-2.04382800	1.17183900	-2.80953600
C	0.64864900	-0.62122200	4.29640100	C	-0.90790100	1.06864600	-3.62688400
H	-0.16966800	-1.31015300	4.47744700	H	-0.04291500	0.51214100	-3.27953100
C	3.90880900	2.12119000	3.62007100	C	-0.86775300	1.67804600	-4.88786000
H	3.53985600	3.08325100	3.24172000	C	-1.98197500	2.40348500	-5.31955000
H	4.60984900	1.73430300	2.87144000	H	-1.95945200	2.87949200	-6.29892200
H	4.46991100	2.31928200	4.53947700	C	-3.12489100	2.53550700	-4.52188800
C	0.94899100	-0.47040700	6.80661200	C	-3.14482400	1.91069300	-3.26996200
H	0.55313800	0.39418400	7.35536400	H	-4.03388700	2.00668000	-2.65646000
H	1.80995800	-0.84285700	7.37554800	C	0.37456700	1.57318200	-5.74342800
H	0.17902100	-1.24861800	6.81647000	H	1.16074200	2.24711800	-5.37876600
C	-1.44159300	-1.59633100	2.33101300	H	0.16832800	1.83818300	-6.78587700
C	-1.60832900	-2.93125700	2.72411900	H	0.78937500	0.55904500	-5.72530600
H	-0.84150900	-3.66259800	2.48908600	C	-4.30648900	3.35055200	-4.99870400
C	-2.74465100	-3.33837400	3.43471300	H	-4.53763900	3.14512900	-6.05055100
C	-3.71578200	-2.37967300	3.74966200	H	-4.10823900	4.42774200	-4.91775900
H	-4.59637900	-2.68239500	4.31380400	H	-5.20374700	3.13765700	-4.40846800
C	-3.57770000	-1.03846400	3.37268300	C	-3.60430300	0.96038000	-0.40302100
C	-2.43241800	-0.66231000	2.65895200	C	-4.86531900	0.40933700	-0.67033900
H	-2.30654600	0.37549200	2.36313700	H	-4.94598800	-0.48085900	-1.28589300
C	-2.91887800	-4.78303400	3.84626400	C	-6.03655700	0.99681900	-0.17233700



C	-5.92849000	2.16279600	0.59428300	H	3.09558000	-1.92977400	-2.57249100
H	-6.83367400	2.63555600	0.97232800	H	3.74778000	-0.30593600	-2.77123000
C	-4.68532600	2.74042400	0.88017500	H	4.90756800	-0.45983400	-0.56987400
C	-3.53351400	2.12643200	0.37451700	H	5.07677800	-4.01283200	-1.59393300
H	-2.56618800	2.57371000	0.57669700	H	6.95511100	-5.02058000	-2.85908800
C	-7.38670100	0.37526500	-0.45055900	H	8.73652600	-3.56856200	-3.81455200
H	-7.40055600	-0.13574200	-1.41904400	H	8.62100900	-1.10433600	-3.48639300
H	-8.18224100	1.12812100	-0.45151900	H	6.74182100	-0.10597900	-2.22075700
H	-7.64492500	-0.37050400	0.31317900	O	1.04793100	-0.77550000	-1.67600100
C	-4.58926200	3.98625400	1.73144100	O	2.37995600	0.31500900	-0.30563100
H	-5.43454500	4.65982000	1.55259300	H	4.24747200	-2.06805800	-0.30962900
H	-3.66653200	4.54023800	1.53013100	C	-0.03024900	3.30210000	-0.77662300
H	-4.59430600	3.73795100	2.80131800	C	0.63251100	4.58352000	-0.33701600
C	-2.47947200	-1.44145900	-1.60980300	C	2.09340500	4.39422300	0.10561600
C	-3.10090000	-2.28510300	-0.67033700	C	2.73030600	5.68492600	0.57230400
H	-3.35871700	-1.90539500	0.31262400	C	2.55704800	6.13471600	1.88992100
C	-3.41191700	-3.61112000	-0.98246400	C	3.12110200	7.33652300	2.32073100
C	-3.07069400	-4.10147300	-2.25180100	C	3.87257600	8.11489100	1.43737400
H	-3.31320500	-5.13235400	-2.50583400	C	4.05473500	7.67979400	0.12322000
C	-2.43759400	-3.29532400	-3.19928000	C	3.48833900	6.47650700	-0.30179700
C	-2.15355000	-1.96196800	-2.86629300	H	-0.97179300	2.20621600	1.54890200
H	-1.67918600	-1.33009900	-3.60875700	H	0.57417400	5.28981400	-1.18175900
C	-2.06264200	-3.83267000	-4.56202500	H	0.03168000	5.01981800	0.46956400
H	-0.97303200	-3.88515900	-4.68152900	H	2.09761600	3.64944300	0.90784600
H	-2.44227800	-3.18851900	-5.36414600	H	1.97542400	5.53114800	2.58415300
H	-2.46358000	-4.83914800	-4.72033600	H	2.97791400	7.66308800	3.34791000
C	-4.10962800	-4.50449500	0.01790900	H	4.31574400	9.04944500	1.77146600
H	-5.05538100	-4.89038000	-0.38352500	H	4.64277200	8.27496700	-0.57118500
H	-4.32868300	-3.96772900	0.94527800	H	3.64091700	6.14053900	-1.32553600
H	-3.49149600	-5.37488600	0.27301100	O	0.60318000	2.39562300	-1.35930700
Ru	0.08646200	0.54954400	-0.24981400	O	-0.15808600	2.21134400	1.02290100
P	0.10625300	-0.98412000	1.51088500	H	2.66207000	3.96522800	-0.72535300
P	-2.03123800	0.30786300	-1.15735800				
H	1.44406800	-4.92988400	-2.39920000				
H	-1.12818600	3.33510200	-0.84967200	<b>Int14</b>			
C	2.22821400	-0.46769400	-1.28881800	C	2.46255600	0.89472900	2.49337400
C	3.42343800	-1.04217200	-2.02237900	C	1.69751600	1.93756300	3.03976100
C	4.60099900	-1.37666000	-1.08355300	H	0.86043800	2.33685400	2.47820800
C	5.77088600	-1.98775500	-1.82403700	C	2.00764100	2.48270100	4.29319600
C	5.85169100	-3.37465800	-2.01449900	C	3.09673500	1.96684100	5.00240700
C	6.90953100	-3.94235400	-2.72647600	H	3.34065000	2.38049400	5.98015500
C	7.91005100	-3.12868400	-3.26244800	C	3.88164900	0.93123300	4.48356000
C	7.84388000	-1.74599300	-3.07848800	C	3.55612400	0.40677700	3.22700800
C	6.78371200	-1.18371600	-2.36528000	H	4.16693100	-0.39414800	2.82562000
				C	1.19224500	3.62745400	4.85216000

H	1.12152200	3.57505000	5.94449900	C	-4.74326100	-1.70355700	-2.64344800
H	0.17663900	3.62869400	4.44353000	H	-5.73029200	-1.63936000	-3.09979400
H	1.64491900	4.59680200	4.60287200	C	-4.33556300	-2.90813600	-2.06358900
C	5.04061200	0.36941600	5.27648100	C	-3.06430000	-2.97677100	-1.47524400
H	4.69425300	-0.33962700	6.04048000	H	-2.75197900	-3.91048500	-1.02066300
H	5.59203300	1.16045700	5.79768300	C	-4.36217300	0.71568000	-3.29359800
H	5.74478800	-0.16588500	4.63110800	H	-3.82803500	1.57592700	-2.87783000
C	3.07314300	-1.31060800	0.80109500	H	-5.43674900	0.88236100	-3.15715800
C	4.32941400	-1.36942600	0.18324900	H	-4.17244900	0.70464800	-4.37560300
H	4.69186600	-0.52167300	-0.39007400	C	-5.23256100	-4.12608600	-2.08927900
C	5.13982300	-2.50348200	0.31423900	H	-5.11721200	-4.72833900	-1.18137900
C	4.66474600	-3.57869400	1.07693300	H	-4.99568800	-4.77803900	-2.94107500
H	5.29289800	-4.46011900	1.19763300	H	-6.28774900	-3.84589100	-2.17924500
C	3.41356600	-3.54577800	1.70498800	C	-0.49224700	-3.60213400	0.07038100
C	2.61995300	-2.39918200	1.55834500	C	-0.33854300	-4.76861800	-0.69830000
H	1.65158100	-2.32977200	2.04982500	H	-0.13901200	-4.69392000	-1.76325000
C	6.49654300	-2.56683600	-0.35115300	C	-0.44480200	-6.03550800	-0.11615100
H	6.91481500	-1.56571200	-0.49985500	C	-0.72538200	-6.11932600	1.25533100
H	6.43755400	-3.04419200	-1.33817100	H	-0.81867800	-7.10169900	1.71707600
H	7.20852400	-3.14671800	0.24680200	C	-0.88424100	-4.97567400	2.04410800
C	2.93538600	-4.71147700	2.54022100	C	-0.75650200	-3.71371100	1.44218000
H	3.69216900	-5.50132100	2.59218700	H	-0.82207100	-2.80832000	2.04408000
H	2.01737600	-5.14559700	2.12852800	C	-0.24781400	-7.28823200	-0.94053500
H	2.70754200	-4.39699300	3.56620400	H	-0.34712900	-7.08170800	-2.01114800
C	2.91875900	1.36208400	-0.34259100	H	-0.97762200	-8.06231700	-0.67611300
C	3.85716100	2.30561300	0.10462600	H	0.75000400	-7.71871900	-0.78132100
H	4.08191300	2.38369600	1.16375600	C	-1.20760100	-5.08694300	3.51764000
C	4.51420700	3.15099800	-0.79584400	H	-0.83195300	-6.02351700	3.94449100
C	4.22418700	3.02829900	-2.16179800	H	-2.29251100	-5.06406200	3.68853800
H	4.73816100	3.67398300	-2.87262500	H	-0.77569500	-4.25352800	4.08131300
C	3.29427400	2.09778700	-2.63618400	C	0.58875200	-2.09591600	-2.17632300
C	2.64056700	1.27145200	-1.71197600	C	1.80865000	-2.79028300	-2.08312000
H	1.89978800	0.56043000	-2.06312500	H	2.10316300	-3.24527100	-1.14337900
C	5.50330000	4.18570400	-0.30712700	C	2.64885800	-2.93018400	-3.19129200
H	5.88105000	3.93748200	0.69009400	C	2.26640900	-2.34433000	-4.40645500
H	5.04181200	5.18021100	-0.24341500	H	2.91172700	-2.45460900	-5.27687600
H	6.36181200	4.27171600	-0.98321600	C	1.06966900	-1.63632300	-4.52870300
C	2.98083400	1.98748800	-4.11117100	C	0.23808800	-1.52331600	-3.40451800
H	3.03598100	0.94691000	-4.45095400	H	-0.70213500	-0.99380400	-3.50889300
H	3.67506700	2.58159900	-4.71481700	C	0.66160700	-1.00706100	-5.84224800
C	-2.20977300	-1.86730800	-1.46126300	H	0.71740800	0.08813500	-5.79516900
C	-2.65514500	-0.66551900	-2.03905000	H	-0.37150200	-1.26425700	-6.10430800
H	-2.02408900	0.21666600	-1.99176400	H	1.30877100	-1.33646100	-6.66185000
C	-3.91295100	-0.57477100	-2.64449600	C	3.93553300	-3.71845300	-3.09873800

H	3.91476200	-4.59340000	-3.76151300
H	4.11281500	-4.07196700	-2.07915800
H	4.79794700	-3.11023100	-3.39953900
Ru	-0.26837600	0.06485100	0.54216300
P	2.02780600	0.21352800	0.80511000
P	-0.51008800	-1.90856200	-0.68177800
H	1.96408300	2.34145400	-4.32567200
H	-2.38628700	-0.40823900	2.61184200
C	-0.51883900	2.49483100	-0.35174200
C	-0.67613700	3.89299800	-0.91680700
C	0.30929800	4.89487900	-0.27368000
C	0.19673000	6.28166400	-0.86865200
C	0.99188400	6.66008300	-1.95956600
C	0.87059400	7.92731800	-2.53223300
C	-0.05214600	8.84226600	-2.02101400
C	-0.84939300	8.47978200	-0.93321800
C	-0.72361800	7.21138100	-0.36439300
H	-0.53356900	3.84762900	-2.00055700
H	-1.70607500	4.22929900	-0.73551300
H	0.11776600	4.92376600	0.80406700
H	1.71682200	5.95286500	-2.35780900
H	1.50001900	8.20173700	-3.37520400
H	-0.14606600	9.83062000	-2.46330200
H	-1.56634500	9.18697900	-0.52347900
H	-1.34377300	6.93871300	0.48733600
O	-0.42970800	1.49629900	-1.13535900
O	-0.45782600	2.31592800	0.90704100
H	1.33060200	4.51705700	-0.40316900
C	-3.03072000	0.01849500	1.82302900
C	-4.48803600	0.25781700	2.09135700
C	-5.26852200	0.89996100	0.93292600
C	-6.73810100	1.06605700	1.25691300
C	-7.20476400	2.20966100	1.92011800
C	-8.55351500	2.34722500	2.25190300
C	-9.46202400	1.33872900	1.92381600
C	-9.01156700	0.19573300	1.26015400
C	-7.66162600	0.06331100	0.93025400
H	0.14725200	-0.32161500	3.01677200
H	-4.92596300	-0.71355700	2.37128400
H	-4.55812400	0.86542500	3.00701900
H	-4.81802300	1.87245700	0.70280200
H	-6.50383700	3.00279400	2.17329600
H	-8.89550000	3.24394800	2.76241700
H	-10.51308800	1.44511200	2.17874600

H	-9.71232000	-0.59167100	0.99427900
H	-7.31762700	-0.82593700	0.40585000
O	-2.50898500	0.27169200	0.74032900
O	-0.37631600	-0.87150500	2.41257200
H	-5.14149900	0.28129300	0.03823000

### Int15

C	-0.95718100	-2.77861500	-1.38647100
C	-1.55326100	-2.31355500	-2.57150500
H	-1.82066500	-1.26484800	-2.65977000
C	-1.84302700	-3.18819300	-3.62577100
C	-1.52649500	-4.54411000	-3.47864700
H	-1.75118600	-5.23366600	-4.29143700
C	-0.93544300	-5.03782000	-2.31047200
C	-0.65948700	-4.14348400	-1.26779400
H	-0.20968300	-4.52236100	-0.35540000
C	-2.46895400	-2.67476700	-4.90299700
H	-1.71856300	-2.56593200	-5.69753800
H	-2.93074100	-1.69403800	-4.75290500
H	-3.23744800	-3.36082700	-5.27783700
C	-0.58342300	-6.50310400	-2.18130000
H	-0.56915900	-6.82074600	-1.13332700
H	0.41135900	-6.71250100	-2.59769100
H	-1.29795000	-7.13669500	-2.71839000
C	0.52324400	-2.49880000	1.06615200
C	0.15833900	-2.91864100	2.34929000
H	-0.82752800	-2.68108400	2.73666100
C	1.04529800	-3.65116300	3.15255200
C	2.30259600	-3.97864000	2.63848700
H	2.99064600	-4.56366400	3.24734600
C	2.69890000	-3.57306000	1.35573500
C	1.80414300	-2.82228000	0.58973200
H	2.10932900	-2.49447400	-0.40011300
C	0.64682000	-4.06125300	4.55234100
H	1.22666200	-4.92327200	4.89927300
H	-0.41569100	-4.32316100	4.60633800
H	0.81484200	-3.24416800	5.26676500
C	4.05294300	-3.96054900	0.80459400
H	4.82715300	-3.92758900	1.57968500
H	4.35850600	-3.29414100	-0.00863400
H	4.04205100	-4.98358100	0.40456600
C	-2.18068900	-1.46799600	0.90864800
C	-3.24725400	-2.35265200	0.69420500
H	-3.16141000	-3.12889900	-0.05995400

C	-4.42969800	-2.25100900	1.43593300	H	3.58731800	-1.78547100	-4.84431100
C	-4.52385500	-1.25142000	2.41362800	H	3.02290400	-2.85634800	-3.56099000
H	-5.43605400	-1.17062600	3.00338800	H	4.72226200	-2.89469200	-4.06716900
C	-3.47557500	-0.35566400	2.65357500	C	2.25175100	0.90633400	1.45471800
C	-2.31036800	-0.46801200	1.88292600	C	3.30445500	0.15839300	1.98600300
H	-1.49754900	0.23581000	2.03614500	H	4.06225500	-0.25716200	1.32876500
C	-5.58872700	-3.18716100	1.17645400	C	3.40534000	-0.06451400	3.36879300
H	-6.35411700	-2.70880600	0.55105600	C	2.43816000	0.49073300	4.20849500
H	-6.07747100	-3.49039400	2.10947600	H	2.51834000	0.33766900	5.28386200
H	-5.26084700	-4.09256200	0.65568000	C	1.36681500	1.24283600	3.70330200
C	-3.58721300	0.69969400	3.73105500	C	1.28088000	1.43705700	2.32312500
H	-3.09787700	0.37510300	4.65940800	H	0.45554500	2.01447100	1.91258400
H	-4.63285800	0.91715600	3.97330700	C	0.32630400	1.81818700	4.63754400
C	2.48881900	3.07110400	-0.39970200	H	-0.27098300	2.59050900	4.14256200
C	2.07987400	3.86482800	-1.47550400	H	0.78827800	2.26563500	5.52552500
H	1.43585800	3.43200600	-2.23529700	H	-0.36531500	1.04190800	4.99136200
C	2.46777900	5.20861200	-1.57525900	C	4.52954500	-0.90614800	3.92742700
C	3.27708900	5.74883300	-0.57290900	H	5.47118500	-0.72469600	3.39669200
H	3.58401500	6.79164700	-0.64150600	H	4.30041100	-1.97526500	3.82760600
C	3.69725900	4.98336300	0.52310700	H	4.69502800	-0.70149200	4.99060400
C	3.29719600	3.64589100	0.59683000	Ru	0.01059500	0.65220300	-1.22423900
H	3.61407400	3.05145000	1.44836600	P	-0.59972800	-1.53254600	-0.05245100
C	1.99084200	6.05501400	-2.73404200	P	2.02424600	1.26658400	-0.34584900
H	2.06129100	5.51091100	-3.68265000	H	-3.10793800	1.63588200	3.42475100
H	2.57630400	6.97593600	-2.82620700	H	0.20935000	1.89745600	-2.23141400
H	0.93903800	6.34318100	-2.60677400	C	-2.31491900	1.59712000	-0.82847100
C	4.55167500	5.59956900	1.60840900	C	-3.61810300	2.29506300	-0.50646900
H	3.98610900	6.33844500	2.19118200	C	-4.85697500	1.48282200	-0.93163300
H	5.42110000	6.12041900	1.18881500	C	-6.15253900	2.20235600	-0.62252100
H	4.91862300	4.84086400	2.30710400	C	-6.84130100	1.96100800	0.57422600
C	3.46331000	0.47623700	-1.20938200	C	-8.02113200	2.64407200	0.87537900
C	4.79655800	0.87803700	-1.03574600	C	-8.53437300	3.58477800	-0.01958600
H	5.03015600	1.69057400	-0.35355600	C	-7.85987900	3.83414300	-1.21692700
C	5.83490900	0.25969700	-1.73901800	C	-6.68154700	3.14757300	-1.51320100
C	5.51648900	-0.76389900	-2.64365600	H	-3.63814800	2.51625500	0.56576200
H	6.31803700	-1.24489900	-3.20233200	H	-3.61222000	3.26613400	-1.02162200
C	4.19755900	-1.17257400	-2.86072800	H	-4.78246000	1.27378000	-2.00388400
C	3.18182900	-0.54282500	-2.12683600	H	-6.44835900	1.22400800	1.27170600
H	2.14914700	-0.85621200	-2.28448700	H	-8.54194600	2.43845800	1.80742700
C	7.27305300	0.67729200	-1.52971900	H	-9.45418500	4.11572200	0.21143600
H	7.33924200	1.59952400	-0.94403800	H	-8.25457500	4.55987900	-1.92367500
H	7.78359900	0.84782300	-2.48488900	H	-6.16590700	3.34190100	-2.45165700
H	7.84015900	-0.09650800	-0.99569700	O	-1.27294400	1.86384500	-0.12378900
C	3.86681200	-2.23627700	-3.88284400	O	-2.20969500	0.77418900	-1.77991700

H	-4.83519300	0.51368400	-0.42073000	C	-3.83346000	-0.02423900	2.09432900
				H	-3.43231700	-0.94899100	1.68716000
<b>Int16</b>				C	-5.40216500	3.63624400	3.74491200
C	-2.18843700	2.96183500	-0.41085500	H	-5.69555300	4.34424500	2.96110200
C	-1.13432100	3.85885300	-0.22544800	H	-4.64248900	4.13544700	4.36047400
H	-0.24364200	3.53068300	0.29710700	H	-6.27480200	3.45458600	4.38076000
C	-1.20536900	5.17030500	-0.72483000	C	-5.21481600	-1.42173200	3.69224800
C	-2.35473500	5.56633000	-1.40821300	H	-6.30605400	-1.47273400	3.78712900
H	-2.41897300	6.58173300	-1.79708300	H	-4.79681700	-1.58976600	4.69341500
C	-3.42989500	4.68686200	-1.61345600	C	1.31657100	-2.72940100	1.51477200
C	-3.33119900	3.38831900	-1.11378600	C	1.97749800	-2.13084900	2.59665200
H	-4.15454800	2.69922000	-1.27838300	H	2.12889900	-1.05619400	2.60248700
C	-0.04738900	6.12053600	-0.51921400	C	2.46480700	-2.90331400	3.66036000
H	0.87145500	5.72880600	-0.97282000	C	2.26888200	-4.28719400	3.63068800
H	0.16145400	6.27038000	0.54738400	H	2.63575700	-4.89363700	4.45777200
H	-0.24935600	7.10129300	-0.96229100	C	1.61064600	-4.91361500	2.56459600
C	-4.65860300	5.14066100	-2.36939100	C	1.14254200	-4.12285700	1.50965700
H	-5.09489800	6.04328600	-1.92344300	H	0.63275000	-4.60270300	0.68001900
H	-5.43062000	4.36469800	-2.37766100	C	3.20437400	-2.24562300	4.80377500
H	-4.41986000	5.38260600	-3.41311900	H	2.76675400	-1.27343700	5.05466300
C	-2.86381200	0.30925700	-1.15737400	H	4.25671500	-2.06705100	4.54522900
C	-4.21071200	-0.08126600	-1.20300500	H	3.18968200	-2.86985800	5.70370200
H	-4.85936300	0.10626500	-0.35299900	C	1.39008500	-6.40991500	2.56833600
C	-4.74433000	-0.70061900	-2.33945200	H	2.28606800	-6.94735200	2.90049100
C	-3.90687100	-0.91830000	-3.44068500	H	1.12545300	-6.77759200	1.57159100
H	-4.31440000	-1.39271300	-4.33210400	H	0.57543600	-6.69163100	3.24893500
C	-2.56171200	-0.53763800	-3.42646800	C	2.14208400	-1.59296600	-1.02828400
C	-2.05413000	0.07451400	-2.27393300	C	3.25439200	-2.44007100	-0.90235800
H	-1.01192600	0.38384500	-2.25189800	H	3.29560500	-3.15891300	-0.08997200
C	-6.19368300	-1.13209600	-2.37910800	C	4.32013000	-2.37259000	-1.80556600
H	-6.67440500	-0.83859700	-3.31982800	C	4.25804000	-1.43801000	-2.84846800
H	-6.76536200	-0.68999400	-1.55667300	H	5.08685200	-1.37158000	-3.55172000
H	-6.28890200	-2.22315200	-2.29769600	C	3.16313100	-0.58274900	-3.00390500
C	-1.66438800	-0.79239100	-4.61554700	C	2.11275000	-0.66598600	-2.07872000
H	-1.09843400	0.10553300	-4.89076400	H	1.28083900	0.02583600	-2.16228200
H	-2.23971400	-1.10931500	-5.49164900	C	5.50963900	-3.29725800	-1.67283000
H	-0.93397800	-1.57982200	-4.39051400	H	5.52372400	-3.79180700	-0.69648700
C	-3.41205300	1.20872500	1.56658500	H	6.45482900	-2.75418800	-1.79029600
C	-3.93491100	2.38549300	2.10868200	H	5.49331500	-4.08238000	-2.44051100
H	-3.61730500	3.34756400	1.71883400	C	3.10351400	0.41522200	-4.13847200
C	-4.86865100	2.34955700	3.15670300	H	2.40469200	0.08918400	-4.92037400
C	-5.27922800	1.10873300	3.64613300	H	4.08367600	0.54706200	-4.60824600
H	-6.01014700	1.07054200	4.45237000	H	2.75999900	1.39488700	-3.78763800
C	-4.76947600	-0.09141500	3.12791400	C	-0.47577300	-2.78245200	-0.72519000

C	-0.17066800	-3.44035400	-1.92491800
H	0.79213900	-3.27861300	-2.39954500
C	-1.08190800	-4.32361600	-2.51796800
C	-2.30778000	-4.55016600	-1.88172600
H	-3.01891400	-5.24304900	-2.32876300
C	-2.64163800	-3.90969600	-0.68347300
C	-1.71519300	-3.02562000	-0.11973600
H	-1.96001600	-2.52988000	0.81679600
C	-3.98180000	-4.14253200	-0.02408100
H	-3.88604900	-4.21929500	1.06536900
H	-4.45341800	-5.06228800	-0.38585600
H	-4.66954100	-3.31250800	-0.23245300
C	-0.75282600	-5.01252300	-3.82353700
H	-1.22402800	-4.50069900	-4.67343900
H	-1.11132300	-6.04817600	-3.83276400
H	0.32634500	-5.02621200	-4.00820400
Ru	-0.02671200	0.63774100	1.08304300
P	-2.09488400	1.22999300	0.26166900
P	0.70318600	-1.63995000	0.13788000
H	-4.89304300	-2.25390700	3.05760700
C	2.30897100	1.52934000	0.49852300
C	3.64602800	2.09129100	0.06001700
C	4.64242800	2.29823800	1.21630900
C	5.98911100	2.79271900	0.73238500
C	6.98688800	1.88847900	0.34110200
C	8.21829300	2.33881000	-0.13722500
C	8.47509100	3.70822700	-0.23260900
C	7.49172600	4.62045100	0.15511300
C	6.26185800	4.16404100	0.63266900
H	4.06725600	1.39101900	-0.67462200
H	3.46470500	3.02738500	-0.47979300
H	4.21628500	3.01063700	1.93292700
H	6.79523400	0.81996400	0.41700600
H	8.97961000	1.62010900	-0.43044800
H	9.43471300	4.06113800	-0.60125300
H	7.68338600	5.68866700	0.09057600
H	5.50261200	4.88110300	0.93855500
O	1.28052300	1.71331400	-0.24052500
O	2.19192100	0.85822400	1.56614400
H	4.75456500	1.35013300	1.75192900
H	-0.23141100	2.04616700	1.84766500
H	-0.85725000	-0.45861700	2.14960900
H	-0.68600300	0.26511300	2.61707000

**Int17**

C	1.54138000	-2.38552700	-2.63522900
C	0.38924100	-2.07098400	-3.35897100
H	-0.41403300	-1.53341800	-2.86909300
C	0.26562100	-2.42490500	-4.71288600
C	1.31707500	-3.10588200	-5.32574400
H	1.23004100	-3.38421300	-6.37517600
C	2.48869800	-3.43628400	-4.62592300
C	2.58913200	-3.06577200	-3.28477200
H	3.49675400	-3.30772200	-2.73952700
C	-0.98725400	-2.06196500	-5.47754000
H	-1.13977400	-0.97571500	-5.49525700
H	-1.87900400	-2.50260300	-5.01467800
H	-0.94025100	-2.41117700	-6.51422200
C	3.61322600	-4.17252200	-5.31904200
H	3.28169000	-5.14834200	-5.69632200
H	4.45459000	-4.34542900	-4.64058200
H	3.99007800	-3.60740900	-6.18088100
C	3.49530700	-1.45990100	-0.80463800
C	4.51095700	-2.29400800	-0.31549500
H	4.26033200	-3.25581300	0.12105400
C	5.85689900	-1.91577500	-0.39764400
C	6.17374700	-0.68635900	-0.98796600
H	7.21797200	-0.38772900	-1.06539200
C	5.18314700	0.16588100	-1.48597800
C	3.84618100	-0.23589700	-1.38525500
H	3.06684300	0.40901400	-1.78462500
C	6.94723000	-2.81267000	0.14522900
H	7.81972700	-2.83060600	-0.51802300
H	6.59477300	-3.84214100	0.26753400
H	7.29739100	-2.46700400	1.12722800
C	5.53654400	1.49634900	-2.10960500
H	5.04646400	1.62691600	-3.08183300
H	6.61647200	1.59392900	-2.26179900
H	5.21170900	2.32578900	-1.46865200
C	1.64678200	-3.55685100	0.03526500
C	1.23618500	-4.73107800	-0.60206400
H	0.98806000	-4.71487100	-1.65865500
C	1.13606400	-5.94105600	0.10223400
C	1.46714800	-5.95664700	1.45841900
H	1.40148300	-6.89244000	2.01114400
C	1.87835200	-4.79521100	2.12851100
C	1.95932100	-3.60387500	1.40448100
H	2.27666500	-2.69850600	1.91625800

C	0.66164100	-7.19378200	-0.59899600	C	5.12779400	2.56224300	1.83915200
H	1.11331500	-7.29304300	-1.59263500	C	5.57359100	1.44692800	2.55733500
H	-0.42709800	-7.17991000	-0.74034400	H	6.60041400	1.42316500	2.91872800
H	0.90682300	-8.09253800	-0.02358200	C	4.73076100	0.36296100	2.82625200
C	2.19799300	-4.83011000	3.60591400	C	3.41274000	0.41175300	2.36016700
H	2.73589500	-5.74501900	3.87941100	H	2.74513500	-0.41994500	2.57472700
H	1.28139600	-4.80045500	4.20974200	C	5.23044900	-0.84414600	3.58658300
C	0.33778800	1.79694500	2.80026800	H	4.51560600	-1.15786000	4.35656400
C	-0.94640500	1.29391200	3.04082300	H	6.18694700	-0.64072800	4.07923700
H	-1.46036100	0.71777000	2.27852600	H	5.37785100	-1.69846000	2.91318900
C	-1.58650000	1.51537500	4.27185600	C	6.06332500	3.71300600	1.54269500
C	-0.91048700	2.23870900	5.25730300	H	6.67505100	3.51024000	0.65316600
H	-1.39567600	2.40394500	6.21853400	H	6.75409100	3.89375000	2.37400000
C	0.37661200	2.75298500	5.04599400	H	5.51137000	4.63981600	1.35400300
C	0.98844200	2.52619800	3.81118700	Ru	0.07487400	-0.47165900	-0.09929700
H	1.98762300	2.91545300	3.63905800	P	1.69685000	-1.92352900	-0.83989100
C	-2.98453200	0.99328700	4.51412100	P	1.14246400	1.49996800	1.15418100
H	-3.14343000	0.03703200	4.00790500	H	2.81265400	-3.97416200	3.90376700
H	-3.73628700	1.69477300	4.12621400	C	-1.33801600	1.23616300	-1.43089100
H	-3.18130900	0.86573900	5.58446800	C	-2.14242800	2.16094400	-2.31841600
C	1.08687600	3.52187500	6.13773200	C	-3.07759300	3.10996800	-1.54444500
H	0.48182700	4.36463300	6.49466300	C	-3.87034200	4.01004900	-2.46840700
H	2.04375000	3.92121600	5.78651400	C	-3.33148400	5.22090200	-2.92661300
H	1.29224400	2.88444900	7.00749000	C	-4.04683100	6.03946600	-3.80195400
C	0.93752700	3.12365000	0.28241700	C	-5.31879200	5.65940000	-4.23612000
C	0.29129100	4.22583800	0.86155400	C	-5.86773100	4.45673300	-3.78720300
H	-0.09673900	4.15284600	1.87223000	C	-5.14813500	3.64185700	-2.91125800
C	0.13333700	5.42537700	0.15682500	H	-1.44125400	2.72077600	-2.94562300
C	0.63600600	5.50782100	-1.14860200	H	-2.73196700	1.53263700	-3.00180400
H	0.51827500	6.43628900	-1.70592000	H	-3.75529500	2.51227300	-0.92623300
C	1.28199500	4.42551700	-1.75659900	H	-2.34188100	5.52222700	-2.58841300
C	1.41504600	3.23457000	-1.03136200	H	-3.61315800	6.97679600	-4.14184200
H	1.87802100	2.37603500	-1.50777200	H	-5.87879700	6.29722000	-4.91497400
C	-0.54554900	6.61584500	0.79706200	H	-6.85935200	4.15437800	-4.11452900
H	-1.10970000	6.32173500	1.68756500	H	-5.58501300	2.70908700	-2.56039000
H	-1.24018300	7.10339000	0.10327200	O	-0.24646400	0.74332700	-1.85428400
H	0.18691300	7.37356300	1.10596400	O	-1.74558700	0.92143300	-0.26060200
C	1.83331000	4.53396700	-3.16068700	H	-2.47434000	3.71385300	-0.85694900
H	2.91045200	4.74879000	-3.15057300	H	-0.84863000	-1.58570800	-0.82032600
H	1.34624000	5.33842300	-3.72174700	H	0.26644400	-1.17539600	1.47813700
H	1.69482500	3.60005800	-3.71647800	H	-0.43158000	-1.55911700	1.12361700
C	2.93152900	1.51673900	1.64661800	C	-3.96231600	-1.36935900	1.15678000
C	3.80003700	2.58732100	1.39283100	C	-5.17210600	-2.28229300	1.23805300
H	3.44105900	3.45986500	0.85571100	C	-6.51457600	-1.51369800	1.19464100

C	-7.70738600	-2.44194300	1.28300800	C	-4.32109200	0.79741000	0.31058700
C	-8.29694500	-2.96569800	0.12415700	H	-4.13287200	-0.10946300	-0.25630600
C	-9.37358700	-3.85055400	0.20342500	C	-5.10652000	4.37487300	2.58504800
C	-9.88083100	-4.22733000	1.44862400	H	-6.17313300	4.62723200	2.59018000
C	-9.30445500	-3.71146300	2.61124600	H	-4.55717800	5.23505300	2.18825700
C	-8.22806700	-2.82709600	2.52619300	H	-4.80124500	4.24660300	3.63251500
H	-5.13342000	-2.98176600	0.39341400	C	-6.44253000	-0.29087000	1.15104500
H	-5.08877000	-2.86335200	2.15999100	H	-6.45436300	-0.85823000	0.21418600
H	-6.53999500	-0.79652100	2.02475400	H	-7.46571700	0.03779800	1.36446000
H	-7.90987200	-2.67278600	-0.84972700	H	-6.14538000	-0.98711800	1.94605600
H	-9.81903300	-4.24200300	-0.70769100	C	-1.29535900	3.44422500	-0.87341400
H	-10.72103100	-4.91372900	1.51238100	C	-1.82493100	4.36547500	-1.78999700
H	-9.69545700	-3.99427400	3.58535500	H	-2.58309600	4.04933900	-2.50023100
H	-7.78672300	-2.42560500	3.43624600	C	-1.38199800	5.69144300	-1.82005200
O	-3.08920400	-1.31978900	2.00668700	C	-0.40081800	6.09249100	-0.90271800
O	-3.96705300	-0.62227400	0.04697600	H	-0.04730200	7.12254900	-0.91890200
H	-6.55432100	-0.93105800	0.26862300	C	0.14184800	5.19999100	0.02509700
H	-3.14312800	-0.06380900	0.01847900	C	-0.31522600	3.87462400	0.02590400

**Int18**

C	-2.58664200	1.37912400	-2.48459900	H	0.11570500	3.16267900	0.72317300
C	-1.75790300	0.75349300	-3.42710700	C	-1.93022700	6.66947700	-2.83507800
H	-0.73716000	0.49736000	-3.15248700	H	-2.84179300	6.28734700	-3.30583700
C	-2.21918600	0.44424600	-4.71370700	H	-1.20375800	6.86371300	-3.63537400
C	-3.53502800	0.78183000	-5.04773100	H	-2.16732100	7.63620400	-2.37498900
H	-3.90982700	0.54032000	-6.04153800	C	1.20902900	5.63384300	1.00413600
C	-4.38648800	1.41777900	-4.13366600	H	1.56951900	6.64413500	0.78403500
C	-3.90201200	1.70469100	-2.85230100	H	2.06523800	4.95012000	0.97154300
H	-4.56490600	2.17329700	-2.13095600	C	-0.01374900	-2.67550800	1.69734400
C	-1.30104700	-0.22716100	-5.71015000	C	0.54241000	-3.71329000	0.92802700
H	-0.61078600	-0.91330200	-5.20810600	H	0.17744500	-3.89069000	-0.08005900
H	-0.69366000	0.51246200	-6.24929800	C	1.54926500	-4.53541500	1.43785700
H	-1.86596000	-0.79305600	-6.45889800	C	2.02132500	-4.29345400	2.73710200
C	-5.79618100	1.79551100	-4.53107100	H	2.80722100	-4.92752800	3.14498600
H	-5.80719600	2.70677200	-5.14415400	C	1.50398400	-3.25980300	3.51891200
H	-6.42241900	1.98452300	-3.65311500	C	0.48106600	-2.45894000	2.98647600
H	-6.27212700	1.00508400	-5.12297400	H	0.06504500	-1.66395600	3.59890900
C	-3.40963400	1.86066900	0.24929000	C	2.11545700	-5.67423200	0.61884400
C	-3.68050500	3.01878100	0.99091800	H	1.92092600	-6.64429600	1.09438800
H	-2.99599400	3.85989600	0.95038000	H	3.20341300	-5.58757500	0.50534300
C	-4.83622500	3.12531600	1.77639100	H	1.67381800	-5.70325400	-0.38258200
C	-5.73050500	2.05072200	1.80320900	C	2.02150500	-3.00183100	4.91656100
H	-6.63847000	2.12800600	2.39966800	H	2.76445000	-3.74961200	5.21258600
C	-5.48629600	0.87744700	1.08020300	H	1.21022000	-3.02426700	5.65466700
				H	2.49474000	-2.01441000	4.99171300
				C	-2.41291200	-2.79176100	0.11714200



C	-2.68514400	-4.06639000	0.64290700	C	7.64071900	-2.22081300	-2.01546700
H	-2.22074400	-4.37604000	1.57491000	C	6.31426700	-2.16779900	-1.58563800
C	-3.52055800	-4.96562600	-0.02723200	H	3.04405400	-2.13222000	-3.52965000
C	-4.08332700	-4.57344200	-1.24951700	H	3.64056100	-0.90195400	-2.39976400
H	-4.72711100	-5.27071100	-1.78438100	H	3.86687500	-2.69120700	-0.61582400
C	-3.82367500	-3.31953100	-1.80944000	H	5.00215200	-4.59739100	-3.56479900
C	-2.97766600	-2.44197400	-1.11560700	H	7.35397900	-4.69328000	-4.33327800
H	-2.73712100	-1.47882400	-1.55772700	H	9.05455600	-3.17242700	-3.34062000
C	-3.81352300	-6.33269800	0.54992900	H	8.37905900	-1.55761300	-1.57181800
H	-3.17193700	-6.54845900	1.41027200	H	6.01876700	-1.46154800	-0.81257300
H	-3.65652800	-7.12358800	-0.19342900	O	0.68714000	-1.93608100	-2.56182300
H	-4.85595700	-6.41087200	0.88586000	O	1.60751600	-1.18995800	-0.68613300
C	-4.44546700	-2.91304500	-3.12641200	H	3.41008100	-3.90232000	-1.80899000
H	-5.46033100	-2.51863000	-2.98039500	H	0.65788900	1.19889000	-1.35345400
H	-4.52565300	-3.76531400	-3.81064800	H	0.19715000	0.87198800	0.86255300
H	-3.86165400	-2.13016500	-3.62015000	H	1.78838100	1.68143100	-0.47627400
C	-2.24325000	-1.02995000	2.46173800	C	3.64111400	1.47547300	0.14950900
C	-3.24771500	-1.80739400	3.06152900	C	4.80469700	2.29607000	0.67106500
H	-3.54854400	-2.74760200	2.61162300	C	6.10223400	1.49417800	0.85895900
C	-3.88182700	-1.39130200	4.23522700	C	7.22564200	2.34972300	1.40714000
C	-3.49613100	-0.17282500	4.81257500	C	8.08010300	3.05185200	0.54599700
H	-3.98372800	0.15905200	5.72825000	C	9.09592600	3.86598800	1.04956700
C	-2.50792400	0.62732300	4.23700400	C	9.27425700	3.99128800	2.42876700
C	-1.89024200	0.18569100	3.05712000	C	8.43122800	3.29611600	3.29814200
H	-1.12956300	0.80196400	2.58589800	C	7.41720600	2.48303700	2.78926600
C	-2.12027100	1.95551300	4.84589100	H	4.95637700	3.14123000	-0.01082500
H	-1.03555800	2.03078400	4.98996600	H	4.48634500	2.74272200	1.62264600
H	-2.60007700	2.10739200	5.81849400	H	5.90394500	0.65135300	1.52978400
H	-2.41565000	2.78577000	4.19175400	H	7.95114000	2.95479200	-0.53022600
C	-4.96557700	-2.23122700	4.87459400	H	9.75058600	4.39865000	0.36457800
H	-5.93845400	-1.72336900	4.84384000	H	10.06664700	4.62196900	2.82280700
H	-4.74508000	-2.43486600	5.92985300	H	8.56594400	3.38218200	4.37329800
H	-5.07801300	-3.19367500	4.36519400	H	6.76882700	1.93853700	3.47291100
Ru	-0.25788600	0.12041900	-0.44671400	O	2.59643900	2.21627100	-0.14747400
P	-1.87404700	1.67961400	-0.79061200	O	3.70012800	0.24618800	0.03530200
P	-1.29824100	-1.55390600	0.94544200	H	6.39511100	1.06158800	-0.10490000
H	0.83286800	5.63314100	2.03567000	H	2.43509300	-0.70864100	-0.37822600
C	1.70164800	-1.67282800	-1.95208000				
C	3.11217100	-1.86015000	-2.47365400	<b>II-cation</b>			
C	3.90554800	-2.93247600	-1.68335200	C	1.23861500	3.13382100	0.13182800
C	5.34678100	-3.01971000	-2.13771900	C	2.13870700	2.99229500	1.19948800
C	5.74018700	-3.92574800	-3.13083000	H	2.01672400	2.17654600	1.90880500
C	7.06641200	-3.98085500	-3.56430600	C	3.19333600	3.89378600	1.36640000
C	8.02108300	-3.12797600	-3.00741000	C	3.33273000	4.93411700	0.43597500

H	4.15099100	5.64175900	0.55709300	H	-3.94330500	1.37686300	4.89010300
C	2.45469600	5.09320800	-0.64077000	C	-1.64051400	-2.14293400	1.80408000
C	1.39883400	4.18121300	-0.78208500	C	-0.54546600	-2.05718800	2.68026600
H	0.70530500	4.29728400	-1.61003700	H	0.38617600	-1.61515900	2.34130300
C	4.15678000	3.76541300	2.52371500	C	-0.64185800	-2.54503900	3.98893900
H	4.06403700	4.61531100	3.21108400	C	-1.85481100	-3.11028700	4.40472900
H	5.19663400	3.74539200	2.17725200	H	-1.94141100	-3.48233500	5.42423400
H	3.97516300	2.85263800	3.09959700	C	-2.95955000	-3.21251400	3.55037700
C	2.65130900	6.20979700	-1.64012600	C	-2.84064800	-2.71910400	2.24449900
H	1.72903400	6.42577400	-2.18858200	H	-3.69239000	-2.78419300	1.57488200
H	3.41916700	5.94623900	-2.37894400	C	0.53702800	-2.47358300	4.93229000
H	2.97824100	7.13263700	-1.14950100	H	0.96583800	-3.46899900	5.10430100
C	-0.93623000	2.07409100	-1.61919300	H	0.24319600	-2.07795000	5.91116200
C	-2.31358000	2.29331900	-1.80359000	H	1.33125700	-1.83593400	4.53254000
H	-2.93266300	2.56903000	-0.95605000	C	-4.24168900	-3.86081500	4.01995300
C	-2.89098900	2.16919400	-3.06744800	H	-4.47173300	-3.58964600	5.05587200
C	-2.07149500	1.80594900	-4.15185200	H	-4.16599500	-4.95523600	3.98207000
H	-2.52021300	1.71258700	-5.13879600	H	-5.09173300	-3.56940900	3.39526100
C	-0.70249600	1.58003800	-4.00862500	C	-0.57518200	-2.81685200	-0.86971600
C	-0.13419200	1.71144500	-2.72700200	C	-0.03040900	-3.96682100	-0.27200700
H	0.94208100	1.61103200	-2.61387200	H	-0.25171700	-4.19029500	0.76668900
C	-4.37074600	2.39016000	-3.26996400	C	0.78595200	-4.83173800	-1.00203300
H	-4.57987400	2.82975300	-4.25062200	C	1.07806300	-4.51549800	-2.34084500
H	-4.78538800	3.05272100	-2.50380700	H	1.71781900	-5.18615100	-2.91110000
H	-4.91404900	1.43807100	-3.21232700	C	0.56760700	-3.37690000	-2.96449300
C	0.16974100	1.25321400	-5.19805300	C	-0.26916200	-2.52766100	-2.21718200
H	0.71981200	2.14073900	-5.53621500	H	-0.73330600	-1.67848600	-2.71542300
H	-0.42442500	0.89380600	-6.04360500	C	1.33548400	-6.09425300	-0.38094100
H	0.91401400	0.48848000	-4.95108600	H	1.15665100	-6.12186100	0.69784000
C	-1.31889200	2.49166700	1.31697900	H	2.41470200	-6.18372500	-0.54928000
C	-1.80397500	3.81099900	1.29667200	H	0.86692800	-6.98410800	-0.81981700
H	-1.48932300	4.49667500	0.51412500	C	0.90557400	-3.05256700	-4.40074900
C	-2.68866100	4.25848000	2.28084900	H	0.03464900	-2.66415300	-4.94024400
C	-3.06281000	3.36460000	3.29689900	H	1.26863000	-3.93548000	-4.93505400
H	-3.74882900	3.70622500	4.06995400	H	1.69184400	-2.28845700	-4.45608000
C	-2.57350000	2.05668600	3.35710000	C	-3.16037000	-1.37795900	-0.56249200
C	-1.69824000	1.62535700	2.34742600	C	-3.66475200	-2.26111200	-1.52342200
H	-1.30676800	0.61349900	2.37948900	H	-3.03834600	-3.05665700	-1.91538900
C	-3.22766600	5.67007500	2.26454100	C	-4.98477700	-2.14078700	-1.98549700
H	-2.93909600	6.21355700	3.17216100	C	-5.78541400	-1.12344700	-1.45850200
H	-4.32338200	5.67776500	2.22039900	H	-6.81273600	-1.02769300	-1.80558400
H	-2.85282900	6.23338500	1.40488300	C	-5.30858300	-0.22907200	-0.48686900
C	-2.95128900	1.13593900	4.49461300	C	-3.98699100	-0.36075900	-0.05426600
H	-2.95065800	0.08687400	4.18234000	H	-3.60652800	0.32641100	0.69695100

C	-6.21093100	0.84392100	0.07855900	H	-1.36936900	5.05263800	1.44908200
H	-5.68692200	1.46165500	0.81448700	H	-0.92336900	6.61437500	0.73260200
H	-7.08563800	0.40491800	0.57349100	H	-0.25235000	6.13192500	2.29037200
H	-6.58936400	1.50562700	-0.70981400	C	3.83604900	6.16072400	-1.19591900
C	-5.53334600	-3.11644800	-3.00135700	H	3.58341300	6.42144700	-2.23212500
H	-5.89267100	-4.03229400	-2.51432200	H	4.80143000	5.64484800	-1.21558200
H	-4.76838800	-3.41436000	-3.72618500	H	3.96330700	7.09967800	-0.64761500
H	-6.37634200	-2.68863200	-3.55279300	C	2.49573100	0.97714400	1.68845400
Ru	0.32521400	-0.17473200	-0.54964300	C	3.68304500	1.58508000	2.13777800
P	-0.14594600	1.94399200	0.02599700	H	4.29345400	2.16317400	1.44985200
P	-1.45110900	-1.51624500	0.09058800	C	4.08877700	1.47035900	3.46795300
H	-2.23932200	1.22935600	5.32508900	C	3.27337500	0.74834500	4.35465800
C	2.75827200	-0.34970200	0.06965000	H	3.57877000	0.65674100	5.39541100
O	1.78669600	-0.75561800	0.81756200	C	2.07854200	0.15602100	3.94448100
O	2.45212400	0.20422500	-1.02897100	C	1.70172900	0.27721400	2.59713700
C	4.18436100	-0.53099600	0.51293900	H	0.77794300	-0.17728400	2.26057700
H	4.19693100	-1.13351800	1.42590400	C	5.36941200	2.10978200	3.95313500
H	4.57668200	0.46250500	0.76785800	H	5.17906800	2.79965000	4.78380300
C	5.07639100	-1.16083700	-0.58367800	H	5.86346200	2.67394100	3.15627200
H	4.68309600	-2.15478400	-0.83171000	H	6.07757000	1.35578100	4.31854700
H	4.99746200	-0.55027200	-1.48899000	C	1.19430900	-0.58141200	4.92325000
C	6.52118300	-1.26981500	-0.14382900	H	0.32975300	0.02928400	5.21493900
C	6.96759800	-2.38187100	0.58288600	H	1.73737100	-0.83647800	5.83853700
C	7.43375700	-0.24472600	-0.42682900	H	0.80552200	-1.50779000	4.48651100
C	8.29066200	-2.46780800	1.01854600	C	3.35784400	0.84730700	-1.14097600
H	6.27424700	-3.19140100	0.80312300	C	3.26535800	1.22543100	-2.49579600
C	8.75803100	-0.32631900	0.00689400	H	2.39661800	1.78023800	-2.84389600
H	7.10594700	0.62058200	-0.99960200	C	4.29839800	0.94476000	-3.40140500
C	9.18986100	-1.43843000	0.73236100	C	5.43101300	0.27012400	-2.92937400
H	8.62075900	-3.34030400	1.57591500	H	6.24297300	0.05254500	-3.62090400
H	9.45376200	0.47481900	-0.22772800	C	5.55396300	-0.11931600	-1.59059300
H	10.22128000	-1.50554200	1.06686600	C	4.50267000	0.16566200	-0.70601800
<b>H-cation-w</b>				H	4.59312000	-0.13052000	0.33372300
C	1.84355800	3.09572500	-0.07571100	C	4.20960100	1.39282300	-4.84209100
C	0.73349000	3.70779200	0.53801100	H	4.83318100	2.27914200	-5.01516300
H	-0.04418100	3.09376400	0.98423100	H	3.18381200	1.65300700	-5.12087400
C	0.62615600	5.10344500	0.60491200	H	4.56257900	0.61360600	-5.52633600
C	1.64565300	5.88074000	0.03887500	C	6.80363900	-0.82376500	-1.11385200
H	1.57153200	6.96563700	0.08425500	H	7.70258900	-0.26328000	-1.39489600
C	2.76004600	5.30029000	-0.57457400	H	6.89591700	-1.82145600	-1.56083500
C	2.84893800	3.90074900	-0.62345700	C	-0.73419900	-2.83211500	-1.49091400
H	3.71587300	3.44932800	-1.09467000	C	-1.62092200	-2.41051600	-2.50181400
C	-0.54518300	5.75756300	1.30119800	H	-2.12715000	-1.45430000	-2.41012300
				C	-1.88617700	-3.22169700	-3.61400300

C	-1.24456400	-4.46281900	-3.70519400	H	1.27954900	-4.35658900	4.83916300
H	-1.44104100	-5.09816000	-4.56709100	H	1.79239200	-5.84173900	4.03450300
C	-0.36136000	-4.91183600	-2.71647400	H	0.10995000	-5.29749100	3.90940700
C	-0.11394600	-4.08589900	-1.61159200	Ru	-0.14231400	0.46568100	-0.90432400
H	0.56398200	-4.43421800	-0.84044600	P	1.91958200	1.23648300	-0.04279500
C	-2.86199700	-2.77724700	-4.67925400	P	-0.44280500	-1.71299000	-0.03230000
H	-3.07580700	-1.70668500	-4.60548900	H	6.80830400	-0.94352300	-0.02666400
H	-3.81570100	-3.31222000	-4.58602900	C	-2.53744600	1.15027800	-0.34295300
H	-2.47700400	-2.98002700	-5.68475200	C	-3.92594600	1.56993000	0.06571900
C	0.32047200	-6.25457800	-2.84682600	C	-4.79967500	2.05964700	-1.10918900
H	-0.39576300	-7.04052600	-3.11122300	C	-6.20426700	2.41170100	-0.66529800
H	0.81353100	-6.54628300	-1.91468200	C	-7.21594400	1.44191500	-0.65989100
H	1.08354100	-6.23704800	-3.63545400	C	-8.50325300	1.75352500	-0.21976400
C	-1.96368700	-1.91396300	0.99486200	C	-8.79878500	3.04461900	0.22252600
C	-2.91591300	-2.90498400	0.71631300	C	-7.80014200	4.02046500	0.21984700
H	-2.78326700	-3.56388800	-0.13539400	C	-6.51418200	3.70392100	-0.22092300
C	-4.04847600	-3.06340100	1.52531000	H	-4.39777800	0.69460400	0.53324500
C	-4.20482200	-2.21701400	2.62930600	H	-3.84319100	2.33316900	0.84587300
H	-5.08085800	-2.33310800	3.26502500	H	-4.32549600	2.93747300	-1.56782600
C	-3.26669400	-1.22446600	2.93928300	H	-6.99525600	0.43603900	-1.01189900
C	-2.14999900	-1.07833900	2.10714200	H	-9.27709100	0.99063100	-0.22940600
H	-1.43601300	-0.29062900	2.32244300	H	-9.80157300	3.29018100	0.56058600
C	-5.08790100	-4.11351000	1.20612600	H	-8.02345200	5.02975200	0.55493900
H	-4.71121500	-4.84511700	0.48467000	H	-5.74349000	4.47241700	-0.22789200
H	-5.98986000	-3.65968400	0.77573200	O	-1.53566500	1.38756100	0.41802500
H	-5.39902300	-4.65488700	2.10642500	O	-2.31674300	0.53679700	-1.44183800
C	-3.44743200	-0.34232800	4.15364800	H	-4.82591200	1.27800600	-1.87536600
H	-3.12125500	-0.85545600	5.06782600	O	0.76692500	-0.38098100	-2.71481200
H	-4.49801500	-0.06796900	4.29707700	H	0.46166800	-1.30032600	-2.84185400
H	-2.86480000	0.58046000	4.06812200	H	1.74365900	-0.38018000	-2.71393900
C	0.84956700	-2.63162700	0.91337500	O	-0.22420400	2.35282000	-2.13743200
C	0.52691700	-3.39548400	2.04089700	H	-1.13422000	2.31089500	-2.48446300
H	-0.49193500	-3.40986500	2.41343100	H	-0.17707900	3.12387400	-1.53845400
C	1.50187800	-4.16403700	2.69535500				
C	2.80023800	-4.17012200	2.18010900	<b>TS8-w</b>			
H	3.55993400	-4.77890700	2.66705000	C	1.46344000	2.60700600	-1.28039800
C	3.15179900	-3.42301600	1.04656700	C	1.84471300	2.12542200	-2.54362400
C	2.16759500	-2.64540300	0.42957700	H	1.74716500	1.06521500	-2.76474600
H	2.42948600	-2.05961600	-0.44838000	C	2.40044900	2.97498400	-3.51361200
C	4.56270900	-3.47808000	0.50907800	C	2.56944000	4.32499100	-3.19457400
H	4.65637400	-2.92164100	-0.42755400	H	2.99270800	4.99647900	-3.93937200
H	4.87407500	-4.51230300	0.32039200	C	2.21762000	4.83781800	-1.93796400
H	5.27858300	-3.05486900	1.22484600	C	1.66238900	3.96911900	-0.99185300
C	1.15142200	-4.96046600	3.93113300	H	1.38186600	4.36451400	-0.02075400

C	2.83586500	2.43564500	-4.85652300	C	-1.44487900	-3.79403000	-2.86776900
H	2.34101100	1.48785300	-5.09155200	C	-1.39622900	-4.96180900	-2.10116000
H	3.91777500	2.25201100	-4.87140700	H	-1.13054300	-5.89994100	-2.58415500
H	2.61726800	3.14379300	-5.66275400	C	-1.69647900	-4.96447000	-0.72717400
C	2.44124400	6.29732400	-1.61598500	C	-2.02496200	-3.75437900	-0.10890100
H	3.51182900	6.53457900	-1.58577800	H	-2.24032300	-3.74235900	0.95455600
H	2.01329300	6.56556300	-0.64555800	C	-1.10376100	-3.80717900	-4.33931400
H	1.99092000	6.94634000	-2.37594000	H	-1.19867200	-4.81105400	-4.76355000
C	-0.48938000	2.47221100	0.88015500	H	-0.06989600	-3.47552800	-4.50060400
C	-0.77844000	2.20047100	2.22217100	H	-1.75488600	-3.13355500	-4.90663700
H	-0.24816300	1.41170000	2.74505800	C	-1.68124200	-6.25687000	0.05414300
C	-1.73822000	2.94335500	2.92551000	H	-2.55347900	-6.87468900	-0.19472300
C	-2.39017600	3.98643400	2.26421300	H	-1.70093500	-6.07434200	1.13250800
H	-3.11757000	4.58641800	2.80747100	H	-0.79012100	-6.85158600	-0.17508500
C	-2.12009100	4.29214500	0.92267800	C	-3.73851700	-0.18308600	-0.90351200
C	-1.18593900	3.51074300	0.23444300	C	-4.73031900	-1.01100300	-1.45299600
H	-0.97115200	3.75110400	-0.80251000	H	-4.64445200	-2.08951200	-1.36324600
C	-2.04228200	2.61771900	4.36939700	C	-5.83020900	-0.46959700	-2.12625300
H	-2.73015500	3.34694800	4.80763200	C	-5.91832100	0.92432900	-2.24706500
H	-1.12893900	2.61075700	4.97586200	H	-6.76370700	1.35501900	-2.78036900
H	-2.50037600	1.62513600	4.46043800	C	-4.95649400	1.77865600	-1.70042900
C	-2.79111300	5.47333000	0.25937000	C	-3.86059300	1.21102300	-1.02811700
H	-2.59787600	5.49746300	-0.81786500	H	-3.12563600	1.86533500	-0.56212400
H	-2.42299700	6.41788500	0.67933200	C	-6.90059100	-1.35909400	-2.71391300
H	-3.87648700	5.45937900	0.40971500	H	-6.65519500	-2.41803800	-2.59151900
C	2.11304500	1.20256800	1.21554000	H	-7.03406900	-1.16499300	-3.78465000
C	3.25747100	2.01523100	1.21971100	H	-7.86991200	-1.18168100	-2.23229100
H	3.39201400	2.77469100	0.45781400	C	-5.11257100	3.27739200	-1.81101600
C	4.24794700	1.85712100	2.19553900	H	-5.64856200	3.68123100	-0.94223200
C	4.06549000	0.87769500	3.18005700	H	-5.68389500	3.55458800	-2.70242900
H	4.82403800	0.75513600	3.95095200	H	-4.14366400	3.78381000	-1.85647200
C	2.94245900	0.04346800	3.19375100	C	-2.71210600	-1.14682100	1.67917900
C	1.97504900	0.20779600	2.19362500	C	-3.98822400	-0.83587000	2.15999200
H	1.12086900	-0.45802200	2.16434800	H	-4.74202300	-0.43947700	1.48677900
C	5.50105300	2.70125600	2.17021600	C	-4.31235100	-1.03082500	3.51101400
H	5.34954800	3.63028100	1.61179800	C	-3.33087800	-1.54521200	4.36336500
H	6.32659200	2.15996900	1.68991100	H	-3.57374700	-1.70404900	5.41255100
H	5.82850300	2.96246300	3.18216700	C	-2.04300000	-1.86805500	3.90802800
C	2.76995000	-1.00961700	4.26458500	C	-1.73878600	-1.65059800	2.56098400
H	2.03512500	-0.69594900	5.01720100	H	-0.74452400	-1.88770400	2.18976800
H	3.71057700	-1.20626100	4.78787100	C	-1.01730200	-2.43615200	4.86175900
C	-2.08065600	-2.56226600	-0.84693800	H	-0.07462000	-2.65729200	4.35273400
C	-1.79415700	-2.59114800	-2.22719400	H	-1.37558800	-3.36512600	5.32125600
H	-1.88173600	-1.68821600	-2.82660400	H	-0.80301900	-1.73772100	5.68006100

C	-5.70202800	-0.72345500	4.01997700
H	-6.37579100	-1.57602300	3.86398800
H	-6.13951400	0.13490300	3.49942200
H	-5.69696800	-0.50490200	5.09241300
Ru	-0.06876300	-0.46706600	-0.97520900
P	0.75863600	1.43751500	-0.02084800
P	-2.25142200	-0.89346100	-0.07671400
H	2.41648500	-1.95558700	3.83900800
C	1.84203900	-1.94653800	-0.91504000
C	3.32584600	-1.61179300	-0.83541100
C	4.08755500	-2.68088700	-0.01246700
C	5.58160600	-2.43474300	-0.02379200
C	6.38722300	-2.98772800	-1.02898600
C	7.76085800	-2.74285400	-1.06192600
C	8.35243800	-1.93840600	-0.08571500
C	7.56096500	-1.38301400	0.92169600
C	6.18706300	-1.62933600	0.95029300
H	3.72891900	-1.57488400	-1.85212300
H	3.44973100	-0.62822400	-0.37929000
H	3.70583100	-2.66831100	1.01464800
H	5.93494100	-3.62345500	-1.78758800
H	8.36990800	-3.18659000	-1.84492700
H	9.42259900	-1.75199300	-0.10609200
H	8.01559700	-0.76474000	1.69167600
H	5.57666200	-1.19629900	1.73943500
O	1.63764000	-2.99965800	-1.76603400
O	1.06627500	-1.86581200	0.12930300
H	3.86867300	-3.66949700	-0.43039500
H	1.43947300	-0.73227500	-1.75957600
H	0.76395100	-3.38260100	-1.56066600
O	-1.01722900	0.71534300	-2.61081600
H	-1.87839500	1.09263300	-2.34577200
H	-0.43995800	1.45992000	-2.86462000

**TS8**

C	-0.33415800	-2.46184500	-1.64365000
C	-0.65146300	-1.81945000	-2.85735000
H	-1.16135500	-0.85663600	-2.84400400
C	-0.36625300	-2.41914800	-4.09034000
C	0.22116700	-3.69077700	-4.08637500
H	0.43665400	-4.17533500	-5.03696200
C	0.52977000	-4.36480900	-2.89704400
C	0.25986500	-3.73084600	-1.67656500
H	0.51395800	-4.23555600	-0.75015800

C	-0.69159300	-1.72332900	-5.39154000
H	0.21890400	-1.50890600	-5.96423300
H	-1.21005200	-0.77485700	-5.22137600
H	-1.33103700	-2.34740200	-6.02646300
C	1.11468700	-5.75776300	-2.92846700
H	1.69466600	-5.97078000	-2.02508800
H	1.76719500	-5.89953200	-3.79605100
H	0.32112500	-6.51348900	-2.99306100
C	0.35920100	-2.38914300	1.20028500
C	-0.20517500	-2.92533700	2.36566000
H	-1.27447200	-2.86489800	2.53282200
C	0.59337500	-3.56262500	3.32554000
C	1.96933800	-3.65406800	3.09641600
H	2.59750800	-4.14838900	3.83553200
C	2.56243100	-3.13378600	1.93850200
C	1.74429400	-2.49995300	0.99976100
H	2.20047800	-2.10291300	0.09902500
C	-0.02439700	-4.16672200	4.56612100
H	-1.03994800	-3.79410000	4.73193900
H	0.56991500	-3.94251800	5.45882600
H	-0.08447500	-5.25966100	4.48565500
C	4.05359500	-3.24415100	1.72109100
H	4.59980200	-2.60969600	2.42986200
H	4.33595600	-2.93073300	0.71147500
H	4.40437700	-4.27195900	1.86930900
C	-2.39975800	-1.94998800	0.40436900
C	-3.12434300	-2.95027700	-0.25708400
H	-2.67838900	-3.48930300	-1.08706600
C	-4.42538300	-3.27705500	0.14702700
C	-4.98172200	-2.58478800	1.22852400
H	-5.99158300	-2.83225100	1.55046300
C	-4.28093800	-1.57982800	1.90786500
C	-2.98533000	-1.26594300	1.48109000
H	-2.43769700	-0.47528000	1.98675400
C	-5.20069900	-4.37197100	-0.54882400
H	-5.21201300	-5.29037400	0.05210200
H	-4.76192800	-4.61940200	-1.52032300
H	-6.24400500	-4.08073800	-0.71189100
C	-4.92823000	-0.82922800	3.04897200
H	-5.49111600	-1.50410100	3.70285000
H	-5.63646600	-0.07887800	2.67378700
C	1.98338700	2.92752700	-0.20446300
C	2.36430200	3.49073400	-1.43532100
H	2.73676500	2.85413100	-2.23215500

C	2.27985200	4.86991300	-1.65521200	C	5.30218900	0.36513400	4.18257800
C	1.79332500	5.68494000	-0.62293000	H	6.01761800	0.15872100	3.38035200
H	1.72198600	6.75860800	-0.78562900	H	5.37397900	-0.44428900	4.91789400
C	1.39388400	5.15606400	0.60883500	H	5.62768900	1.28460400	4.68576100
C	1.48380200	3.76756500	0.80382600	Ru	-0.30379200	0.61713800	-0.75365200
H	1.18022200	3.34797400	1.75813200	P	-0.67420300	-1.55465500	-0.07648700
C	2.70442900	5.47499900	-2.97312600	P	1.95802800	1.08563400	0.01248500
H	2.98176100	4.70440400	-3.69854400	H	-4.18555000	-0.30679000	3.66040700
H	3.56812000	6.13852700	-2.84288800	H	-1.89453400	0.68373900	-1.34946800
H	1.89995100	6.07695600	-3.41149000	C	-1.88238400	2.09842300	-0.49450700
C	0.90524800	6.05668600	1.71965200	C	-3.33815200	2.44664900	-0.72126100
H	0.19291000	5.54099300	2.37191900	C	-4.35099500	1.48511800	-0.08666500
H	0.41948000	6.95427400	1.32394500	C	-5.77754100	1.95344500	-0.29146700
H	1.74091600	6.38896800	2.34909400	C	-6.51084900	1.55069800	-1.41564700
C	3.40080700	0.52683800	-0.98142900	C	-7.81485200	2.00495300	-1.61915100
C	4.64801500	1.16936900	-0.90215100	C	-8.40668500	2.87101300	-0.69736600
H	4.77455000	2.03160500	-0.25378300	C	-7.68747500	3.27795800	0.42809700
C	5.73450300	0.73172800	-1.66683100	C	-6.38353400	2.82132700	0.62754100
C	5.54827900	-0.35925000	-2.52710000	H	-3.45569200	3.45341600	-0.29382300
H	6.38781200	-0.70646100	-3.12703400	H	-3.50318100	2.54706700	-1.79786300
C	4.31399500	-1.00529400	-2.65011300	H	-4.21622300	0.48679700	-0.51720800
C	3.24406400	-0.54837400	-1.86718000	H	-6.05909200	0.86993600	-2.13470200
H	2.27759900	-1.03740100	-1.96213100	H	-8.37003900	1.67898700	-2.49453400
C	7.07668100	1.42116800	-1.58082000	H	-9.42264100	3.22275700	-0.85284300
H	7.07186000	2.21782200	-0.83100800	H	-8.14248100	3.94728100	1.15315000
H	7.35482900	1.86880500	-2.54269600	H	-5.83070000	3.13991400	1.50934900
H	7.87064500	0.71327800	-1.31506400	O	-1.38351100	1.77089000	0.64998200
C	4.13908400	-2.15244200	-3.61860200	H	-4.13227100	1.40037200	0.98230200
H	4.92549600	-2.90511100	-3.49009200	O	-1.01394300	2.87105500	-1.30507200
H	4.19671300	-1.80326700	-4.65730200	H	-0.36118900	3.30639300	-0.71178300
H	3.17163500	-2.64628000	-3.48737900				
C	2.35107700	0.81913200	1.79184200	<b>TSH_HOAc</b>			
C	3.65648500	0.65921700	2.27960900	C	-3.30919400	0.23500400	1.32689200
H	4.49917400	0.64574800	1.59683000	C	-3.60013000	-0.67265900	2.35054100
C	3.89442100	0.50568000	3.64942900	H	-2.94909400	-1.52605700	2.50760300
C	2.79910000	0.50530300	4.52406600	C	-4.70180400	-0.49328700	3.19874600
H	2.97582000	0.38411400	5.59128400	C	-5.51483100	0.62651900	3.01149500
C	1.48674400	0.65110200	4.06550700	H	-6.36911800	0.78053700	3.66910900
C	1.27465000	0.80741400	2.68902200	C	-5.25111500	1.56051300	2.00138100
H	0.26053400	0.91398100	2.31389100	C	-4.14913700	1.35166100	1.16646700
C	0.31698000	0.60224600	5.02101400	H	-3.94143100	2.08031400	0.38960600
H	0.62005100	0.85819800	6.04105700	C	-4.99968700	-1.50321500	4.28410400
H	-0.12091400	-0.40423900	5.05046200	H	-4.08980600	-1.78685100	4.82544800
H	-0.47722500	1.29391500	4.71936300	H	-5.42639100	-2.42454000	3.86582900

H	-5.71720600	-1.10993800	5.01182200	C	4.51572000	-2.63273000	-1.90017300
C	-6.12655800	2.78290100	1.83785100	C	3.60463800	-1.59495400	-1.67526500
H	-7.19091900	2.52489100	1.89109600	H	3.35998800	-0.92841100	-2.49538400
H	-5.94696700	3.27908000	0.87856300	C	4.61253700	-4.25460700	1.56856600
H	-5.93436700	3.51951600	2.62928800	H	3.74089900	-4.85539400	1.85845900
C	-1.63161400	1.62845400	-0.50936800	H	4.93172500	-3.70111200	2.45991700
C	-1.95962400	1.99933900	-1.81603400	H	5.41682900	-4.94547300	1.29494500
H	-2.34331100	1.25977700	-2.51134500	C	5.13184900	-2.83967600	-3.26596900
C	-1.81563500	3.32690800	-2.24766700	H	6.21682500	-2.98544400	-3.20025300
C	-1.33607300	4.27664600	-1.34263100	H	4.94627500	-1.98290400	-3.92193200
H	-1.23873500	5.31316300	-1.66230900	H	4.71836100	-3.72889000	-3.76017200
C	-0.98788000	3.93193200	-0.02875900	C	2.96197500	1.21739200	0.74571700
C	-1.14069400	2.60323200	0.37533400	C	4.33197900	1.24974200	0.44118900
H	-0.90044500	2.32330300	1.39782300	H	4.74577100	0.52919100	-0.25766900
C	-2.17577300	3.70987900	-3.66485900	C	5.18376700	2.19058900	1.02882900
H	-2.22408200	4.79709300	-3.78676100	C	4.64138400	3.11031800	1.93531300
H	-3.14669700	3.29376700	-3.95872900	H	5.29742700	3.84233400	2.40483900
H	-1.43235700	3.32626200	-4.37495400	C	3.28147300	3.10600300	2.26034700
C	-0.44619800	4.97293900	0.92411000	C	2.44948000	2.15151600	1.65639400
H	-0.73131500	4.75561000	1.95903100	H	1.39924900	2.11761700	1.92189600
H	-0.81103000	5.97524900	0.67408900	C	6.66389200	2.19653300	0.71858600
H	0.65092800	5.00530800	0.88972900	H	7.04642300	3.21733700	0.60308500
C	-2.69848500	-1.01235900	-1.20277700	H	6.88113300	1.64700600	-0.20285400
C	-3.98427100	-0.67836300	-1.66369700	H	7.24110600	1.72492200	1.52505700
H	-4.52729600	0.14255600	-1.20499300	C	2.71938300	4.11519100	3.23744400
C	-4.59064000	-1.39556100	-2.69738200	H	1.80116400	3.74724900	3.70671900
C	-3.89219100	-2.47213100	-3.26547500	H	2.47369300	5.06279700	2.73951000
H	-4.36174300	-3.04547800	-4.06382100	H	3.43841300	4.34635400	4.03139100
C	-2.62102000	-2.83974700	-2.81946300	C	1.52773800	0.69888500	-1.71644700
C	-2.03122500	-2.09803500	-1.78174400	C	1.91962800	1.99745000	-2.05867600
H	-1.06811800	-2.40287600	-1.38310400	H	2.41160200	2.62618100	-1.32346400
C	-5.97272700	-1.03235200	-3.19240100	C	1.69495800	2.50549900	-3.34501100
H	-6.39798700	-0.20490300	-2.61587700	C	1.08239600	1.68117900	-4.29412100
H	-6.66175900	-1.88256900	-3.11495300	H	0.92143600	2.05962100	-5.30245200
H	-5.95451200	-0.72990900	-4.24735300	C	0.67184300	0.37891100	-3.98061300
C	-1.88347400	-4.00783600	-3.43521500	C	0.89224000	-0.09506700	-2.68330300
H	-1.14802500	-3.66960900	-4.17744700	H	0.58198300	-1.10459300	-2.42914800
H	-2.57014100	-4.69256000	-3.94424500	C	0.01704500	-0.50456500	-5.01876900
C	3.01390500	-1.40762400	-0.41539600	H	0.67167400	-1.33870900	-5.30376000
C	3.36226600	-2.27332700	0.62814900	H	-0.21809300	0.05537300	-5.92994500
H	2.92503900	-2.12791400	1.60999500	H	-0.91406600	-0.94042400	-4.63813600
C	4.27278800	-3.31948100	0.42987600	C	2.09563000	3.92288300	-3.68431700
C	4.83788100	-3.48576300	-0.83697700	H	1.38470200	4.64274200	-3.25767800
H	5.54558800	-4.29713400	-1.00116300	H	2.12265600	4.08540700	-4.76699300



H	3.08435600	4.16836300	-3.27992300	C	-1.37553600	1.20183000	4.42198600
Ru	-0.03119100	-0.96574900	1.26258700	H	-1.27511700	1.48475100	5.46875500
P	-1.86807100	-0.07862300	0.17273700	C	-0.93238200	-0.06110200	4.01109600
P	1.82171700	-0.02737400	-0.03766800	C	-1.08079700	-0.41493000	2.66566200
H	-1.33359000	-4.57446000	-2.67608000	H	-0.75284500	-1.39799100	2.34038300
C	0.96813800	-0.27278200	3.53623700	C	-2.38878400	3.47949800	3.97276800
C	1.52590300	0.17600700	4.86310100	H	-2.56939900	3.51020900	5.05265200
H	2.47312000	0.70102800	4.68994000	H	-3.30779600	3.79407000	3.46580200
H	0.83303000	0.85942400	5.35939000	H	-1.61992900	4.22971300	3.74471000
O	0.10483700	0.43715000	2.92993500	C	-0.31103700	-1.02846400	4.99366600
O	1.38928600	-1.34932700	2.99181300	H	-0.26074500	-0.59981700	5.99990700
C	-0.55405200	-3.34336300	1.45414500	H	0.70845100	-1.29905900	4.69205200
C	-1.87414500	-4.07463000	1.29313400	H	-0.88699800	-1.96045000	5.05703400
H	-2.39455300	-4.16784300	2.24875400	C	-3.02771200	1.17176600	-0.70931500
H	-2.50446800	-3.56432800	0.56441500	C	-4.41446000	1.07173000	-0.51702500
O	0.13544900	-3.83680200	2.52702900	H	-4.82324700	0.22906800	0.03177400
O	0.08650400	-2.94451000	0.40532500	C	-5.28910400	2.03416200	-1.03133300
H	-1.11965800	-2.00287500	2.08338000	C	-4.75350900	3.10879500	-1.75323700
H	0.90130500	-3.24752600	2.68040300	H	-5.42704000	3.85611400	-2.17107000
H	1.72975700	-0.68836500	5.50071900	C	-3.37726500	3.23927400	-1.96115100
H	-1.64863500	-5.08149500	0.92038100	C	-2.52253600	2.25982000	-1.43312900

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C	-2.95423000	-1.57695400	0.14253600	H	-1.45717300	2.32362100	-1.62145800
C	-3.11537900	-2.39510300	-0.98194700	C	-6.78117200	1.92332900	-0.81060700
H	-2.58183200	-2.15804100	-1.89603200	H	-7.05309000	0.94091700	-0.41203300
C	-3.96291500	-3.51115700	-0.94858200	H	-7.33700100	2.07390400	-1.74375000
C	-4.64849600	-3.79863500	0.23405600	H	-7.13742800	2.67969000	-0.09867500
H	-5.30704500	-4.66539600	0.27005000	C	-2.82035400	4.41460700	-2.73413000
C	-4.51030000	-2.99767600	1.37547300	H	-2.65625800	5.28268100	-2.08134200
C	-3.66328200	-1.88649800	1.31514000	H	-3.50589500	4.73387200	-3.52711200
H	-3.56072500	-1.25892700	2.19445800	C	3.30041700	0.47778600	-1.20055300
C	-4.11488400	-4.38308800	-2.17441700	C	3.82672700	-0.49998700	-2.06160100
H	-3.15498400	-4.82926700	-2.46268300	H	3.39037000	-1.49364100	-2.08543200
H	-4.46902100	-3.80340300	-3.03572400	C	4.91767300	-0.22576700	-2.88938700
H	-4.82551100	-5.19836500	-2.00247200	C	5.48720700	1.05487400	-2.85006400
C	-5.25084500	-3.33959700	2.64934000	H	6.33886200	1.27857000	-3.49101900
H	-5.24534500	-2.50054400	3.35291100	C	4.98950400	2.04793500	-2.00535000
H	-4.79438300	-4.19877500	3.15905700	C	3.89791600	1.74304000	-1.17688800
H	-6.29572300	-3.60464800	2.44854500	H	3.52037900	2.51260800	-0.51241300
C	-1.67122700	0.46030600	1.74220400	C	5.46306700	-1.28224200	-3.82378700
C	-2.09848700	1.71802700	2.18374800	H	5.10133000	-2.27896400	-3.55235800
H	-2.56290900	2.40603100	1.48467400	H	6.55934200	-1.30281700	-3.81169800
C	-1.95014800	2.10524500	3.52164200	H	5.15587600	-1.09143200	-4.86070300
				C	5.59410500	3.43412200	-1.99063500
				H	5.01740000	4.12598900	-2.61925800

H	6.62138300	3.42778600	-2.37041600
H	5.60882700	3.85561600	-0.97911500
C	2.71932000	-1.06766600	1.14279400
C	4.04848900	-0.83061500	1.53267600
H	4.59641200	0.00024300	1.09749100
C	4.68634600	-1.65216500	2.46610900
C	3.97435600	-2.73391600	3.00571700
H	4.46747400	-3.38573000	3.72542800
C	2.65524100	-3.00460400	2.63415700
C	2.03525700	-2.15845800	1.69808200
H	1.02242100	-2.37238700	1.37137000
C	6.12216600	-1.40269600	2.86920900
H	6.24123400	-1.41839100	3.95918400
H	6.47666600	-0.43368600	2.50446400
H	6.78893300	-2.17361400	2.46158100
C	1.89922000	-4.17161500	3.22872200
H	1.22331000	-4.62345400	2.49477300
H	1.28381700	-3.85364000	4.08079700
H	2.58102700	-4.94865800	3.58994300
C	1.56431300	1.59378100	0.81370800
C	1.90604000	1.78245400	2.15605400
H	2.34964300	0.97015300	2.72282900
C	1.69283500	3.01540900	2.78830700
C	1.14137400	4.06244000	2.04425800
H	0.99105400	5.03025600	2.52046000
C	0.78164600	3.90113000	0.69964400
C	0.99382600	2.65770200	0.09577100
H	0.73718500	2.51657600	-0.95098500
C	0.15847900	5.03854200	-0.07713200
H	0.51112000	5.05682000	-1.11424700
H	0.38807200	6.00841700	0.37703900
H	-0.93463700	4.93971600	-0.10978600
C	2.04106100	3.19559900	4.24786400
H	2.99151700	2.71038100	4.49789100
H	1.27057700	2.74901600	4.88984800
H	2.12147700	4.25485100	4.51422500
Ru	0.08963000	-0.76360400	-1.36375700
P	-1.84760700	-0.09189300	-0.02077000
P	1.86060400	0.01460400	-0.10434000
H	-1.85792300	4.16902900	-3.19469700
H	1.22243600	-1.61380700	-2.32220100
C	-0.83807500	0.28585700	-3.52022500
C	-1.33332700	0.94638700	-4.78316700
H	-0.64903000	1.73755500	-5.09855700

H	-1.44466700	0.20361000	-5.57795200
O	-0.01097600	0.89556800	-2.76141700
O	-1.25826200	-0.86551100	-3.18584700
C	0.93489800	-3.04493000	-1.69374100
C	0.48781500	-3.71150800	-2.98148600
H	2.35053600	-3.17106000	-0.43254300
H	-0.39276100	-3.20197000	-3.37281600
H	1.28717900	-3.69601100	-3.72654000
O	0.09961600	-2.83946200	-0.73405200
O	2.21517000	-3.42900200	-1.36508500
H	-2.31953200	1.38621000	-4.59242800
H	0.24027400	-4.75538400	-2.75044500

### III

C	1.80309300	-2.75441500	0.17111700
C	1.52668100	-3.12697600	1.48333800
H	1.10886700	-2.40455900	2.17472100
C	1.79462000	-4.42638500	1.92717100
C	2.35029700	-5.33715200	1.03449900
H	2.56427200	-6.35020300	1.37243200
C	2.64193300	-4.98691500	-0.28883100
C	2.36239300	-3.69110900	-0.70845400
H	2.58227700	-3.40612600	-1.73414500
C	1.46324000	-4.81580800	3.34601500
H	1.91658000	-5.77472900	3.61563800
H	0.37908900	-4.90581900	3.48139800
H	1.81543000	-4.05891000	4.05455300
C	3.23192500	-6.00218800	-1.23626300
H	3.52928900	-5.53816400	-2.18131900
H	2.50831500	-6.79317800	-1.46602300
H	4.11545900	-6.48388700	-0.80286500
C	1.02593400	-1.33394100	-2.13162500
C	1.73488000	-0.85988700	-3.22848900
H	2.62988200	-0.26155000	-3.08200400
C	1.31999400	-1.16294300	-4.52891800
C	0.18293600	-1.94681800	-4.70387400
H	-0.14037500	-2.19307800	-5.71404500
C	-0.55517400	-2.42300500	-3.61655500
C	-0.11208300	-2.12054600	-2.33367300
H	-0.64166300	-2.51746000	-1.46981500
C	2.08989900	-0.62581100	-5.70726000
H	1.92756000	0.45401000	-5.80885200
H	1.77813000	-1.10039200	-6.64261300
H	3.16650600	-0.78595700	-5.58572700

C	-1.82762200	-3.20377800	-3.82276200	C	-3.31885700	-1.01592500	-0.88712600
H	-1.84715900	-3.69505100	-4.80063900	H	-2.46927400	-1.52875700	-1.32456400
H	-2.69878800	-2.53745000	-3.76803000	C	-6.61829800	0.91826600	1.07187800
H	-1.95641300	-3.97066400	-3.05219300	H	-6.74792000	0.46590100	2.06236400
C	3.16474600	-0.28723100	-0.41049800	H	-7.56050800	0.79419600	0.52717100
C	4.24712600	-0.91700100	0.20682400	H	-6.44336100	1.98901900	1.21210800
H	4.13194200	-1.91717800	0.61272700	C	-4.67242700	-3.10591500	-1.26153200
C	5.47062400	-0.26250600	0.34788500	H	-4.93353600	-3.13610500	-2.32667900
C	5.59762000	1.03524700	-0.14623600	H	-5.45332300	-3.64107200	-0.71207100
H	6.54127400	1.56176500	-0.01529800	H	-3.73389600	-3.65607600	-1.13731300
C	4.53308300	1.68887700	-0.76482200	C	-1.02584300	1.33418900	-2.13152200
C	3.31893900	1.01595800	-0.88670400	C	-1.73465000	0.86019600	-3.22849800
H	2.46937300	1.52893200	-1.32401100	H	-2.62964300	0.26181000	-3.08216200
C	6.61827500	-0.91892700	1.07179100	C	-1.31963600	1.16337600	-4.52886300
H	6.74729800	-0.46742000	2.06274900	C	-0.18259000	1.94730200	-4.70363300
H	7.56067700	-0.79399400	0.52761900	H	0.14081400	2.19367000	-5.71374900
H	6.44367700	-1.98987200	1.21097600	C	0.55536500	2.42346400	-3.61619300
C	4.67272200	3.10590900	-1.26071200	C	0.11214700	2.12088700	-2.33338900
H	4.93497600	3.13630100	-2.32557200	H	0.64161700	2.51776300	-1.46944800
H	5.45288500	3.64118400	-0.71032100	C	1.82776500	3.20436400	-3.82220900
C	-1.80322500	2.75442400	0.17125500	H	1.95656000	3.97097700	-3.05137100
C	-1.52684000	3.12692700	1.48349900	H	1.84720100	3.69600300	-4.79990300
H	-1.10905300	2.40447200	2.17485500	H	2.69897600	2.53806700	-3.76778300
C	-1.79480100	4.42631600	1.92737800	C	-2.08943200	0.62633600	-5.70731900
C	-2.35046200	5.33711700	1.03473700	H	-3.16599500	0.78711100	-5.58620900
H	-2.56444700	6.35015500	1.37270200	H	-1.92765400	-0.45360000	-5.80854400
C	-2.64207200	4.98693800	-0.28861700	H	-1.77706700	1.10048500	-6.64269300
C	-2.36250700	3.69115400	-0.70828900	Ru	-0.00003700	-0.00001500	1.03127000
H	-2.58237600	3.40620600	-1.73399300	P	1.48923400	-1.03146000	-0.38737100
C	-1.46344500	4.81567700	3.34624700	P	-1.48927100	1.03151700	-0.38733900
H	-1.91689300	5.77452600	3.61594600	H	3.73393700	3.65582800	-1.13739600
H	-0.37930200	4.90580600	3.48161900	C	-2.03329400	-0.98910200	2.20138800
H	-1.81553500	4.05868200	4.05473000	O	-1.66768500	0.16785400	2.55891800
C	-3.23204700	6.00225500	-1.23600900	O	-1.34035600	-1.63042000	1.34759600
H	-4.11543600	6.48411600	-0.80249800	C	2.03316400	0.98901200	2.20147800
H	-3.52963400	5.53823200	-2.18099700	O	1.66750400	-0.16792100	2.55901100
H	-2.50834500	6.79311500	-1.46592800	O	1.34027800	1.63035600	1.34765500
C	-3.16473700	0.28716100	-0.41065000	C	3.30419400	1.57597600	2.70286500
C	-4.24715300	0.91671400	0.20685900	C	3.68521900	2.86005100	2.31229700
H	-4.13202900	1.91681000	0.61297500	C	4.15075600	0.80853600	3.50268200
C	-5.47058100	0.26209000	0.34785100	C	4.90947700	3.37568500	2.72300300
C	-5.59749600	-1.03558100	-0.14653500	H	3.01911200	3.43519500	1.67780700
H	-6.54109300	-1.56220900	-0.01564100	C	5.37498100	1.32534000	3.91236000
C	-4.53294700	-1.68897700	-0.76532400	H	3.84072400	-0.19286400	3.78195100

C	5.75647100	2.60739400	3.51973900
H	5.20583300	4.37571800	2.41933600
H	6.03341900	0.72821200	4.53690600
H	6.71377000	3.01020300	3.83881400
C	-3.30432100	-1.57611400	2.70271800
C	-3.68534900	-2.86012200	2.31192900
C	-4.15087500	-0.80881100	3.50267100
C	-4.90960300	-3.37583000	2.72255300
H	-3.01924300	-3.43514600	1.67733100
C	-5.37509300	-1.32569000	3.91227300
H	-3.84085300	0.19254900	3.78209800
C	-5.75658400	-2.60767900	3.51943500
H	-5.20596700	-4.37580500	2.41870700
H	-6.03352700	-0.72867300	4.53693000
H	-6.71388000	-3.01054200	3.83845200

**TSIII**

C	2.94123300	-1.05803200	-1.51338300
C	3.32347300	-2.31107100	-1.03829500
H	2.88700300	-2.70108500	-0.12616400
C	4.25997400	-3.08838200	-1.72413000
C	4.80567900	-2.59176800	-2.90564500
H	5.52926300	-3.19450600	-3.45258400
C	4.43961600	-1.34279400	-3.40991100
C	3.50899400	-0.58466900	-2.70306900
H	3.21869000	0.38441800	-3.09769000
C	4.68256400	-4.42826200	-1.17720600
H	3.84029300	-4.94552500	-0.70787300
H	5.45109700	-4.30653800	-0.40499400
H	5.09085600	-5.07120500	-1.96345400
C	5.01583000	-0.83931200	-4.71022100
H	6.09300200	-1.02862900	-4.77043100
H	4.85266800	0.23622500	-4.82869200
H	4.54788200	-1.34015400	-5.56632900
C	1.23332300	1.15324500	-1.85904900
C	1.71553500	2.45372000	-1.97411100
H	2.39019200	2.85221000	-1.22276100
C	1.34247800	3.26163000	-3.05023700
C	0.48095400	2.73809500	-4.01188900
H	0.19621800	3.35562500	-4.86331000
C	-0.03180900	1.44324300	-3.90846400
C	0.35125600	0.65715600	-2.82394600
H	-0.03476900	-0.35592300	-2.72783400
C	1.87830000	4.66461000	-3.18109100

H	2.64228100	4.72449100	-3.96566600
H	2.33026600	5.00331300	-2.24417400
H	1.08155800	5.36942400	-3.44328300
C	-0.99551000	0.91858400	-4.94186500
H	-1.10850300	-0.16659000	-4.86149600
H	-0.65962500	1.15170000	-5.95806500
H	-1.98833600	1.36692800	-4.81351800
C	2.87889400	0.97397100	0.51526600
C	4.14081400	1.39728800	0.08397300
H	4.50460700	1.10058800	-0.89637600
C	4.94469900	2.19259100	0.89685400
C	4.46640900	2.56052400	2.15930700
H	5.08869000	3.18355100	2.80010300
C	3.22247000	2.13688400	2.62076600
C	2.43922800	1.33459800	1.78623600
H	1.49413200	0.94519500	2.15073700
C	6.31305600	2.63534900	0.44110200
H	6.45720100	2.44827400	-0.62702200
H	7.10049600	2.09673400	0.98171900
H	6.46652800	3.70474800	0.62224900
C	2.69944400	2.53928700	3.97624100
H	1.94968500	3.33499500	3.88267500
H	3.49870200	2.90955400	4.62544300
C	-2.13172800	1.11081500	2.26620000
C	-1.96332000	0.13793100	3.24687900
H	-1.42485500	-0.77231300	3.01485000
C	-2.44486700	0.33720100	4.54505000
C	-3.10201800	1.52805300	4.83716100
H	-3.47555000	1.69682000	5.84630300
C	-3.29209200	2.51997200	3.86790000
C	-2.80054400	2.30012400	2.58575800
H	-2.93856700	3.06284900	1.82393200
C	-2.25539700	-0.73525500	5.58869400
H	-1.28044100	-1.22028400	5.47769700
H	-3.02091900	-1.51477800	5.49165600
H	-2.32573700	-0.32629500	6.60154100
C	-4.02495700	3.79262300	4.21411100
H	-5.08778600	3.59764300	4.40025100
H	-3.95747900	4.52473300	3.40397800
H	-3.61481300	4.25247000	5.12009600
C	-3.14035300	0.39287400	-0.31071500
C	-4.30603100	0.10985500	0.40741900
H	-4.31141800	0.20156600	1.48870100
C	-5.46220100	-0.32046200	-0.23950300

C	-5.44524400	-0.45113200	-1.62819800
H	-6.33824700	-0.80662200	-2.13895900
C	-4.29989100	-0.17873800	-2.37066900
C	-3.14639200	0.23005400	-1.69819400
H	-2.23195700	0.38796600	-2.26282000
C	-6.69759500	-0.68753400	0.54246000
H	-6.58157900	-0.45669100	1.60545700
H	-6.90064500	-1.76138900	0.45001400
H	-7.58038100	-0.15451100	0.17214400
C	-4.29758000	-0.34880400	-3.86834500
H	-4.41123700	0.61535100	-4.37940700
H	-5.11691000	-0.99778200	-4.19192300
H	-3.36000700	-0.79564600	-4.21230100
C	-1.13531600	2.48833600	0.01487700
C	-1.71756100	3.13571100	-1.07173500
H	-2.48785900	2.64158100	-1.65488800
C	-1.32956700	4.42983800	-1.42562700
C	-0.34975100	5.07062300	-0.67020100
H	-0.04047600	6.07788700	-0.94390900
C	0.25056300	4.44527300	0.42309800
C	-0.16158900	3.15903700	0.75872300
H	0.28142800	2.67801600	1.62445000
C	1.33742100	5.12083800	1.22072700
H	1.03658700	5.25870600	2.26596600
H	1.58219800	6.10535700	0.81017100
H	2.25115500	4.51408500	1.22374000
C	-1.93765100	5.09305700	-2.63413000
H	-1.50272600	4.67747700	-3.55204500
H	-1.75848600	6.17284800	-2.63562400
H	-3.01890200	4.92658900	-2.68169200
Ru	-0.02274300	-1.09142800	0.43680300
P	1.75587900	-0.02028800	-0.54587700
P	-1.55938000	0.77907800	0.55125800
H	2.21315600	1.69418900	4.47428600
C	-1.95566300	-2.46642100	-0.48686100
O	-1.09735100	-1.93512200	-1.24974300
O	-1.82718000	-2.34975600	0.77749700
C	0.97403300	-2.38551400	2.20364100
O	0.07190700	-3.35065400	2.52430900
O	0.71855700	-1.15200400	2.45397200
H	0.93178400	-2.48387800	0.58668500
H	-0.79976100	-3.07440000	2.18050000
C	-3.14326500	-3.15031000	-1.05706200
C	-4.20014000	-3.51342500	-0.22260700

C	-3.23367800	-3.36223700	-2.43308900
C	-5.34749200	-4.08173800	-0.76493900
H	-4.11600300	-3.32555300	0.84231000
C	-4.38101600	-3.93016500	-2.97362500
H	-2.40429600	-3.06377600	-3.06591400
C	-5.44079100	-4.28553500	-2.14022500
H	-6.17139600	-4.36322500	-0.11535100
H	-4.45327600	-4.09245200	-4.04504400
H	-6.33910100	-4.72579000	-2.56376100
C	2.38509900	-2.88657800	2.33755900
C	2.67661300	-4.24582000	2.21528700
C	3.41057400	-1.97148100	2.56437500
C	3.99268800	-4.68336000	2.31614800
H	1.87048100	-4.94917700	2.03755000
C	4.72746900	-2.41066100	2.65208300
H	3.16885600	-0.92023000	2.66232900
C	5.02089600	-3.76618100	2.52890000
H	4.21768200	-5.74146200	2.21922500
H	5.52276900	-1.69023800	2.81825500
H	6.04894000	-4.11026700	2.60063900

#### IV

Ru	-0.19066200	-0.26660400	0.20757600
P	1.38040300	-0.28063100	-1.46606000
P	-1.39368300	1.45296300	-0.67842700
C	-2.95297300	1.71938500	0.24869100
C	-2.95519400	2.53094300	1.38665400
H	-2.05600800	3.07200000	1.66776900
C	-4.10029000	2.64173100	2.16751200
H	-4.09054600	3.27645700	3.04880400
C	-5.25162300	1.93412400	1.82837900
H	-6.14168600	2.01345300	2.44564000
C	-5.25426200	1.11746400	0.70246600
H	-6.13836100	0.54267800	0.44344300
C	-4.11159900	1.01308800	-0.08514500
H	-4.12220200	0.34499800	-0.94116600
C	3.09208000	-0.04391800	-0.84648600
C	3.82194500	-1.14115100	-0.37893300
H	3.39928600	-2.13843300	-0.44852100
C	5.07253500	-0.96208000	0.20404900
H	5.61628400	-1.82232600	0.58162200
C	5.60897500	0.31481800	0.33013500
H	6.57777700	0.45494100	0.79969000
C	4.88988100	1.41393300	-0.13269900

H	5.30119500	2.41445600	-0.03374500
C	3.63796100	1.23680500	-0.71313300
H	3.08405800	2.10862300	-1.04983300
C	-0.62837400	3.11538800	-0.68339500
C	0.61796000	3.30020700	-0.07873200
H	1.10391600	2.46491400	0.41887300
C	1.22376800	4.55588400	-0.09727700
H	2.19161700	4.69072700	0.37714000
C	0.59043800	5.63065800	-0.71318300
H	1.06575600	6.60707500	-0.72934100
C	-0.66134600	5.45595400	-1.30244700
H	-1.16318200	6.29555900	-1.77423500
C	-1.26906200	4.20595200	-1.28329700
H	-2.25015300	4.07799600	-1.73392400
C	1.49348000	-1.87263200	-2.36991600
C	0.52891700	-2.86103000	-2.16238600
H	-0.27220500	-2.69409300	-1.44860200
C	0.59115900	-4.05772100	-2.87597300
H	-0.16197900	-4.82151300	-2.70619700
C	1.61064800	-4.27451300	-3.79624900
H	1.65711500	-5.20885400	-4.34836500
C	2.57880600	-3.29244300	-4.00528000
H	3.38002600	-3.45906500	-4.71938500
C	2.52001900	-2.09939500	-3.29603200
H	3.28908600	-1.34636300	-3.44925900
C	1.30372100	0.92644400	-2.86814600
H	1.27459100	1.93677100	-2.44546200
H	2.25091800	0.83895500	-3.41146300
C	0.12036300	0.71798100	-3.83215300
H	-0.17802800	-0.33796100	-3.85567900
H	0.47764400	0.94590400	-4.84272600
C	-1.10859100	1.59654700	-3.58037400
H	-0.79351500	2.64313700	-3.48340100
H	-1.73262900	1.55184700	-4.48182500
C	-2.02125000	1.21531600	-2.40884300
H	-2.27988700	0.15121200	-2.46541800
H	-2.95553900	1.78183200	-2.49846300
C	1.69150700	-0.52450400	1.88740600
O	1.24310500	0.60963600	1.50935400
O	1.17837200	-1.57741200	1.41825800
C	-2.36349800	-1.46492300	0.72739900
O	-1.83609100	-1.52139000	-0.43832300
O	-1.79783900	-0.79018000	1.62697900
C	-3.66405900	-2.13897700	0.98080800

C	-4.29054500	-1.97853200	2.21752600
C	-4.28563800	-2.87337300	-0.02970800
C	-5.53529700	-2.55500700	2.44175600
H	-3.79599300	-1.38832400	2.98139800
C	-5.53132600	-3.44901000	0.19701800
H	-3.78612900	-2.98067800	-0.98698100
C	-6.15658500	-3.28899500	1.43231000
H	-6.02496100	-2.42902100	3.40286100
H	-6.01631000	-4.02059700	-0.58893400
H	-7.13015800	-3.73780100	1.60838100
C	2.85279000	-0.57758800	2.81266200
C	3.35041700	-1.81203100	3.23158000
C	3.49190900	0.60117300	3.19620900
C	4.48632100	-1.86555800	4.03094000
H	2.84313300	-2.71672700	2.91309200
C	4.62880200	0.54549200	3.99456200
H	3.09765000	1.54898800	2.84648300
C	5.12781200	-0.68717100	4.41045700
H	4.87517500	-2.82550300	4.35813900
H	5.12998700	1.46298200	4.28902500
H	6.01798600	-0.73030300	5.03200400

**TSIV**

Ru	-0.20779300	-0.56850100	-0.05444600
P	1.46562500	0.36504400	-1.46750600
P	-1.70367800	1.11171400	-0.34984000
C	-3.13216200	0.98027400	0.79994700
C	-2.81607900	0.87636300	2.16133800
H	-1.77303000	0.85841500	2.46828200
C	-3.82136200	0.77577900	3.11332900
H	-3.56207900	0.69739400	4.16506800
C	-5.15882500	0.76554200	2.71882900
H	-5.94591200	0.68039600	3.46247600
C	-5.47892600	0.85039300	1.36971400
H	-6.51664600	0.81739500	1.05122400
C	-4.47081300	0.96003700	0.41306000
H	-4.74847000	0.99442000	-0.63474600
C	2.92699200	1.07979300	-0.62404800
C	3.79495900	0.19930000	0.03364600
H	3.63504700	-0.87241500	-0.04691900
C	4.84739400	0.68022000	0.80239700
H	5.49030900	-0.01907500	1.32855900
C	5.05918200	2.05291100	0.91253800
H	5.87912000	2.43146800	1.51581600

C	4.21577200	2.93635000	0.24607600	H	-0.15090400	-3.32370900	0.22688500
H	4.37943600	4.00783400	0.32042500	H	-1.38042900	-1.27906000	0.90187000
C	3.15353000	2.45384600	-0.51621800	C	2.58765700	-1.36270400	2.74691500
H	2.49773400	3.16164900	-1.01276000	C	2.87702400	-0.36718500	3.68162500
C	-1.11171100	2.80712300	0.03805400	C	3.32171400	-2.54950300	2.73918200
C	0.08286500	2.97197200	0.74286900	C	3.89438200	-0.56116800	4.60816000
H	0.65052100	2.10036600	1.05636700	H	2.30633800	0.55483000	3.66140300
C	0.54871500	4.25056500	1.04513500	C	4.34095900	-2.74046200	3.66630000
H	1.48618700	4.36227600	1.58215700	H	3.08784300	-3.30773100	1.99916200
C	-0.17421500	5.37107500	0.64978500	C	4.62737600	-1.74713900	4.60087900
H	0.19325700	6.36710300	0.87943600	H	4.12045800	0.21304600	5.33528700
C	-1.37701700	5.21355200	-0.03806900	H	4.91175500	-3.66433800	3.66065900
H	-1.95053500	6.08516700	-0.33976000	H	5.42281300	-1.89722400	5.32540100
C	-1.84508500	3.93915600	-0.33677900	C	-3.17352300	-2.35246600	-0.16262400
H	-2.79130700	3.82709200	-0.85979300	C	-3.74019300	-2.56692300	1.09311700
C	2.24884000	-0.83544600	-2.61596200	C	-3.99356200	-2.14782600	-1.26954600
C	1.63814200	-2.06947000	-2.85014500	C	-5.12047000	-2.57005700	1.23983300
H	0.71430800	-2.31817900	-2.33637100	H	-3.08999800	-2.70938600	1.95050300
C	2.20354100	-2.96863100	-3.75345100	C	-5.37868500	-2.15975100	-1.12286000
H	1.72061700	-3.92539000	-3.92950600	H	-3.53603500	-1.99981600	-2.24228600
C	3.37915100	-2.64566100	-4.42229100	C	-5.94284300	-2.36907300	0.13109800
H	3.81887500	-3.34972700	-5.12310500	H	-5.55878300	-2.71889800	2.22179100
C	3.99469200	-1.41581700	-4.19082400	H	-6.01524000	-2.00951700	-1.99016000
H	4.91573000	-1.16094600	-4.70718500	H	-7.02274400	-2.37297000	0.24929600
C	3.43247700	-0.51622300	-3.29314900				
H	3.92346600	0.43553100	-3.10557600				
C	0.91382700	1.67476400	-2.64246500				
H	0.64107900	2.56062600	-2.05902500				
H	1.76030400	1.95639600	-3.27849400				
C	-0.28847000	1.20685400	-3.49562800				
H	-0.41039000	0.11744100	-3.44076700				
H	-0.06324000	1.42901900	-4.54375600				
C	-1.62493800	1.88233300	-3.15114400				
H	-1.45013000	2.94463400	-2.93871300				
H	-2.25891100	1.85561800	-4.04620000				
C	-2.46733400	1.26144200	-2.02521000				
H	-2.73344400	0.23169800	-2.28797500				
H	-3.39977700	1.83173100	-1.95130800				
C	1.53363100	-1.13281300	1.72329600				
O	0.90199900	-0.03254900	1.71147900				
O	1.29774000	-2.00601500	0.83033800				
C	-1.68391700	-2.37061100	-0.36011100				
O	-1.11483900	-3.46829000	0.20377200				
O	-1.19784500	-1.87227200	-1.44150000				