

Supporting Information for

Insights into the ruthenium-catalysed selective reduction of cardanol derivatives via transfer hydrogenation: a density functional theory study

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Step	ΔE	δ_{D3}	δE_{solv}	δE_G	δE_H	ΔG	ΔH	ΔG_1	ΔH_1
<i>Isomerisation</i>									
1 → TS1-2	7.7	0.3	0.3	-1.4	-1.2	6.8	7.0	6.8	7.0
1 → 2	4.3	0.8	0.4	0.9	0.7	6.4	6.3	6.4	6.3
2 → TS2-3	20.0	7.1	-6.5	-4.3	-1.8	16.4	18.9	22.8	25.2
2 → 3	13.6	3.1	-0.9	-3.3	-1.4	12.5	14.5	18.9	20.7
3 → TS3-4'	2.9	-0.4	-0.1	-1.3	-2.1	1.1	0.2	20.0	21.0
3 → 4'	-2.2	-2.1	-1.1	-0.7	-0.9	-6.0	-6.3	12.9	14.5
4' → TS4'-4	11.4	1.1	0.5	-0.4	-0.4	12.7	12.6	25.6	27.1
4' → 4	-2.1	3.3	2.3	0.9	1.2	4.3	4.6	17.3	19.1

^a B3PW91/ECP2 energies; ^b model solvent MeOH, ^c B3PW91/ECP1 energies; ^d free energies and enthalpies of the respective products relative to that of **1** set to 0 kcal mol⁻¹.

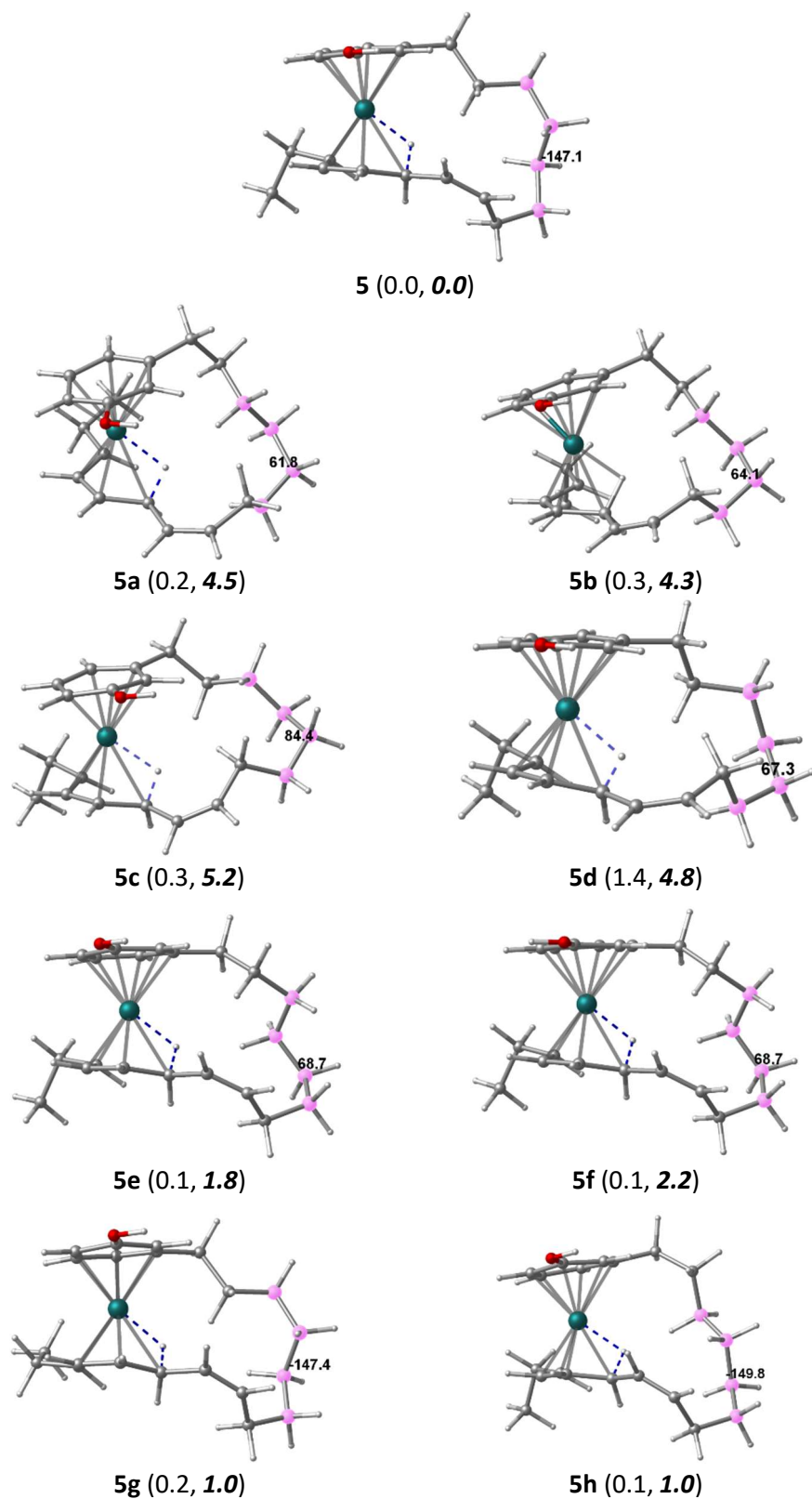


Figure S1. Geometries of isomers of intermediate **5** with selected dihedral angles, calculated at the B3PW91/ECP1 level. Energies (ΔH and ΔG) are in kcal mol⁻¹ relative to **5** calculated at the B3PW91-D3BJ/ECP2/PCM level, *i*PrOH as the model solvent.

Table S2. Reaction energies in the gas phase (ΔE)^a; DFT-D3BJ corrections (δ_{D3}), Solvation (δE_{solv})^{a,b} and thermochemistry (δE_G and δE_H)^c; Final free energies (ΔG) and enthalpies (ΔH) in kcal/mol. $\delta E_{\text{solv}} = (\Delta E_{\text{PCM}} - \Delta E)$; ΔG_1 = relative free energies and ΔH_1 = relative enthalpies ^d.

Step	ΔE	δ_{D3}	δE_{solv}	δE_G	δE_H	ΔG	ΔH	ΔG_1	ΔH_1
<i>Reduction to the diene</i>									
4 → 5	-32.1	-3.0	0.2	1.5	0.8	-33.4	-34.2	-16.1	-15.1
5 + 2<i>i</i>PrOH → 6	0.0	-20.7	8.0	23.1	4.2	10.5	-8.4	-0.7	-18.7
6 → TS6-7	16.5	-1.7	-0.2	-0.9	-3.7	13.7	10.9	12.9	-7.8
6 → 7	5.7	-2.0	-0.4	0.6	-0.2	3.9	3.1	3.2	-15.5
7 → 8	-7.8	16.6	-1.9	-8.4	-0.2	-1.5	6.8	1.7	-8.8
8 → TS8-9	11.3	-4.1	0.1	-0.2	-3.4	7.1	3.9	8.8	-4.9
8 → 9	9.6	-3.6	0.7	0.1	-2.2	6.8	4.5	8.5	-4.3
9 → TS9-10	-0.1	-0.5	0.7	-1.8	-0.9	-1.6	-0.8	6.8	-5.0
9 → 10	-11.0	3.5	1.0	-3.3	-0.1	-9.8	-6.5	-1.3	-10.8
10 → 11 + acetone	6.7	-6.9	-2.7	-4.1	-0.8	-7.1	-3.8	-8.4	-14.6

^a B3PW91/ECP2 energies; ^b model solvent MeOH, ^c B3PW91/ECP1 energies; ^d free energies and enthalpies of the respective products relative to that of **1** set to 0 kcal mol⁻¹.

Section S1: Reduction to the cardanol diene

After the inclusion of dispersion, solvation, and thermodynamic corrections, **TS9–10** is lower in free energy than the intermediate **9** that it connects to. Several studies,^{1–8} including some most recent ones,^{9–18} report such submerged transition states, where geometry optimisations and energy refinements are performed at different levels of theory. Such transition states are, in fact, artifacts of the lower level of theory employed in the optimisation. In these cases, the transition states, and the intermediates below which they fall probably would cease to be proper stationary points at the higher level of theory. They would rather denote non-equilibrium structures along a continuous reaction pathway as they might be expected to be visited along with an IRC at the higher level (if that were practicable to trace). Such “vanishing” transition states and intermediates might safely be omitted from the final profiles, but we kept them on the energy profile in the main text for illustrative purposes (to follow the transformations that take place).

Table S3. Reaction energies in the gas phase (ΔE)^a; DFT-D3BJ corrections (δ_{D3}), Solvation (δE_{solv})^{a,b} and thermochemistry (δE_G and δE_H)^c; Final free energies (ΔG) and enthalpies (ΔH) in kcal/mol. $\delta E_{\text{solv}} = (\Delta E_{\text{PCM}} - \Delta E)$; ΔG_1 = relative free energies and ΔH_1 = relative enthalpies ^d.

Step	ΔE	δ_{D3}	δE_{solv}	δE_G	δE_H	ΔG	ΔH	ΔG_1	ΔH_1
<i>Reduction to the monoene</i>									
11 → TS11-12	0.8	-0.1	0.1	0.7	-1.0	1.6	-0.1	-6.8	-14.7
11 → 12	-3.5	0.4	0.0	1.9	1.0	-1.2	-2.1	-9.6	-16.6
12 → TS12-13	17.4	4.0	-0.6	-3.7	-1.6	17.1	19.3	7.5	2.6
12 → 13	2.0	7.8	0.9	-4.1	-1.3	6.7	9.4	-3.0	-7.2
13 → TS13-14	2.3	-0.4	0.4	-1.8	-2.1	0.5	0.2	-2.5	-7.0
13 → 14'	-7.6	-0.3	-0.1	-1.4	-0.9	-9.4	-8.9	-12.4	-16.1
14a → 14	8.3	0.8	0.6	-0.7	0.3	8.9	10.0	-3.4	-6.1
14 → TS14-15	7.8	-0.3	-0.8	0.0	-1.2	6.7	5.5	3.3	-0.6
14 → 15'	-6.7	2.0	0.0	0.8	0.8	-4.0	-4.0	-7.4	-10.1
15' → 15	-16.8	-6.9	-3.6	3.9	1.7	-23.3	-25.6	-30.8	-35.7
15 → 15''	18.4	0.4	1.5	-1.1	-1.0	19.1	19.2	-11.7	-16.5
15'' → TS15-16	13.6	-0.9	-1.1	-1.6	-3.3	10.1	8.4	-1.6	-8.1
15'' → 16	-4.5	2.4	-2.1	-0.2	0.8	-4.4	-3.3	-16.0	-19.8
16 + iPrOH → 17	-2.0	3.7	1.2	5.2	0.1	8.2	3.1	-7.9	-16.8
17 → TS17-18	2.9	-0.6	0.4	-2.0	-2.1	0.8	0.7	-7.1	-16.1
17 → 18	0.1	-0.5	0.9	-1.2	-0.8	-0.6	-0.2	-8.5	-17.0
18 → TS18-19	0.1	1.2	0.5	-1.9	-1.0	-0.1	0.8	-8.6	-16.2
18 → 19	-10.4	3.2	1.0	-3.0	-0.2	-9.3	-6.4	-17.8	-23.4
19 → 20 + acetone + iPrOH	31.6	0.8	-7.7	-16.9	-3.1	7.7	21.5	-10.0	-1.9

^a B3PW91/ECP2 energies; ^b model solvent MeOH, ^c B3PW91/ECP1 energies; ^d free energies and enthalpies of the respective products relative to that of **1** set to 0 kcal mol⁻¹.

Section S2: Reduction to the cardanol monoene

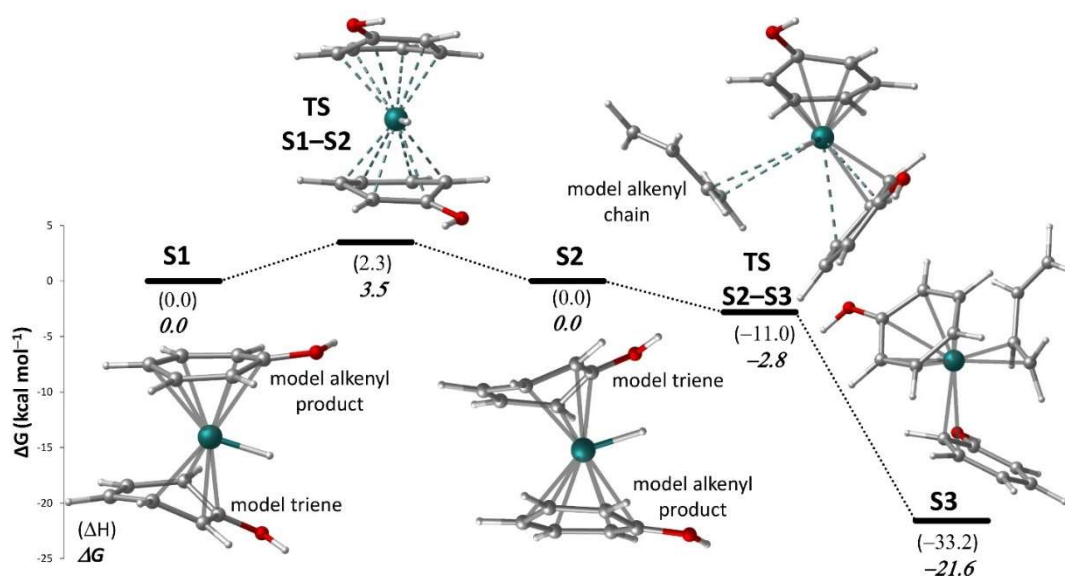
There is a facile hydride transfer to C_(SP²)#12, where Ru forms a η^1 - coordination with C#11 and an agostic interaction with the H on C#12 ($\Delta G_{11 \rightarrow 12} = -1.2 \text{ kcal mol}^{-1}$ and $\Delta G^\ddagger_{11 \rightarrow 12} = 1.6 \text{ kcal mol}^{-1}$, see Scheme 7 in the main text). *i*PrOH is still coordinated to Ru in intermediate **12**. The next step is kinetically demanding with a barrier of $17.1 \text{ kcal mol}^{-1}$, where Ru forms a β -agostic interaction with the hydrogen of C#10 at first. Although in the transition state, **TS12–13**, *i*PrOH is coordinated to the Ru metal, it eventually rearranges to form a hydrogen bond with the –OH of phenol in the resulting optimised complex, **13** ($\Delta G_{12 \rightarrow 13} = 6.7 \text{ kcal mol}^{-1}$ and $\Delta G^\ddagger_{12 \rightarrow 13} = 17.1 \text{ kcal mol}^{-1}$). Again, followed by a low kinetic barrier via **TS13–14**, intermediate **14'** is formed, where the β -agostic interaction between the hydrogen at C#10 is lost ($\Delta G_{13 \rightarrow 14'} = -9.4 \text{ kcal mol}^{-1}$ and $\Delta G^\ddagger_{13 \rightarrow 14} = 0.5 \text{ kcal mol}^{-1}$). However, it is still a β -agostic intermediate, with agostic interaction at C#12 (see Scheme 7 in the main text).

In intermediate **14'**, the hydride bonded to Ru is facing toward C#10. To initiate the reduction to the monoene, however, this hydride needs to be transferred to C#11. We therefore modelled another isomer of **14'**, i.e., **14**, where now Ru–H is positioned towards C#11 ($\Delta G_{13 \rightarrow 14'} = 8.9 \text{ kcal mol}^{-1}$, see Scheme 8 in the main text). For the hydrogen transfer to C#11, a transition state, **TS14–15**, is associated with a kinetic barrier of $6.7 \text{ kcal mol}^{-1}$, which gives rise to intermediate **15'** ($\Delta G_{14 \rightarrow 15'} = -4.0 \text{ kcal mol}^{-1}$ and $\Delta G^\ddagger_{14 \rightarrow 15} = 6.7 \text{ kcal mol}^{-1}$). In **15'**, there is a β -agostic interaction between Ru–H and C#11, which when broken gives rise to η^3 -allyl complex, **15**.

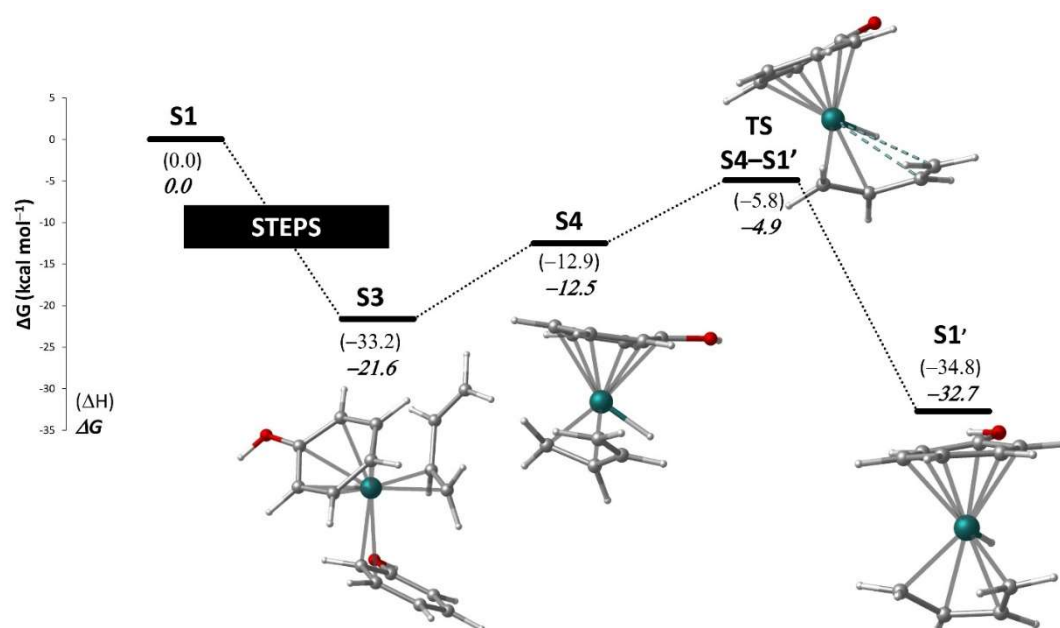
Section S3: Model studies for associative interchange mechanism

In these model studies, we have used a truncated system with phenol and 1,3-butadiene. Since we are doing these model studies to see the kinetics involved in the product exchange with fresh triene, and; therefore, phenol with 1,3-butadiene precisely illustrates the formation of model complex **1**. However, such a model system does not count the steric effects, making some intermediates much more stable than the actual system.

We start the reaction profile with a model intermediate **S1**, where the “model alkenyl product” is still associated, whereas the new reactant, illustrated as “model triene,” is associated via η^4 -coordination. **TS-S1-S2** allows interchanging η^6 - and η^4 -coordination of the “model alkenyl product” and “model triene.” Via the next low kinetic barrier, the **S3** intermediate is obtained with a η^2 -coordinated “model alkenyl product” and η^2 -coordinated “model alkenyl chain.” **S3** seems to be a very stable intermediate; however, it is missing the steric effects from the actual alkenyl chain in the actual system. Even if we agree on the stability of **S3**, the next kinetic barrier via **TS-S4-S1'** of 16.7 kcal mol⁻¹ is much lower than the overall barrier, 29.2 kcal mol⁻¹, for reduction to the cardanol monoene product, which eventually gives the **S1'** intermediate comparable to our proposed entry (complex **1**) into the catalytic cycle (Schemes S1 and S2).



Scheme S1. Model studies for associative interchange mechanism (B3PW91-D3BJ/ECP2/PCM level, *i*PrOH as the model solvent). Energies (ΔH and ΔG) are in kcal mol⁻¹ relative to **S1**. Table S5 shows the reaction energies of individual steps.



Scheme S2. Model studies for associative interchange mechanism (B3PW91-D3BJ/ECP2/PCM level, *i*PrOH as the model solvent). Energies (ΔH and ΔG) are in kcal mol⁻¹ relative to **S1**. Table S5 shows the reaction energies of individual steps.

Table S4. Reaction energies in the gas phase (ΔE)^a; DFT-D3BJ corrections (δ_{D3}), Solvation (δE_{solv})^{a,b} and thermochemistry (δE_G and δE_H)^c; Final free energies (ΔG) and enthalpies (ΔH) in kcal/mol. $\delta E_{\text{solv}} = (\Delta E_{\text{PCM}} - \Delta E)$; ΔG_1 = relative free energies and ΔH_1 = relative enthalpies ^d.

Step	ΔE	δ_{D3}	δE_{solv}	δE_G	δE_H	ΔG	ΔH	ΔG_1	ΔH_1
<i>Reduction to the diene HETS and MARI</i>									
15' → 15	-16.8	-6.9	-3.6	3.9	1.7	-23.3	-25.6	-30.8	-35.7
19 → 20 + acetone + iPrOH	31.6	0.8	-7.7	-16.9	-3.1	7.7	21.5	-10.0	-1.9
20 → 21	-0.3	1.8	-2.8	1.2	0.7	-0.2	-0.7	-10.2	-2.6
21 → 22	-9.1	-11.1	7.5	13.6	2.8	0.9	-9.9	-9.4	-12.5
22 → TS22-23	30.6	-1.4	-0.8	-3.1	-4	25.2	24.3	15.8	11.9

^a B3PW91/ECP2 energies; ^b model solvent MeOH, ^c B3PW91/ECP1 energies; ^d free energies and enthalpies of the respective products relative to that of **1** set to 0 kcal mol⁻¹.

Section S4: Derivation of the pressure correction

The use of elevated pressure in the expressions for evaluating the thermodynamic corrections from the partition function of an ideal gas only affects the translational part of the entropy (and therefore only affects the computed free energies when the number of particles changes along a reaction step). The rationale for this comes from the restricted translational degrees of freedom in a condensed phase compared to the gas phase. The derivation of the correctional term for the solvent, *i*PrOH, is shown below:

$$p = \frac{\rho RT}{M} = 381.0 \text{ atm},$$

where, p = *i*PrOH pressure, ρ = density of *i*PrOH (0.786 g/cm³), M = molar mass of *i*PrOH (60.1 g/mol), T = 355.65 K, p° = 1 atm, R = ideal gas constant (8.314 J/K.mol).

Section S5: References

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Gaussian full reference

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Atomic coordinates (in Å) of the intermediates and transition states, optimised at the B3PW91/ECP1 level.

2-propanol

C	0.0015000	0.0451740	0.3632140
H	-0.0054560	0.0828040	1.4669740
C	1.3209200	-0.5596750	-0.0882360
H	1.3533200	-0.6220480	-1.1808840
H	1.4504210	-1.5653210	0.3231330
H	2.1564680	0.0633510	0.2424230
C	-1.2009570	-0.7712320	-0.1026780
H	-1.1697030	-1.7899040	0.2982880
H	-1.2188510	-0.8277990	-1.1960320
H	-2.1413740	-0.3151840	0.2298770
O	-0.0357060	1.3652090	-0.1656050
H	-0.8679540	1.7668310	0.1072560

acetone

C	-0.0000030	0.1844920	-0.0000040
C	1.2881810	-0.6134740	0.0001800
H	2.1431920	0.0637030	0.0095250
H	1.3390650	-1.2577590	-0.8851710
H	1.3309960	-1.2735460	0.8741560
C	-1.2881740	-0.6134760	-0.0001820
H	-1.3390650	-1.2577170	0.8852040
H	-1.3309810	-1.2736080	-0.8741140
H	-2.1432010	0.0636800	-0.0095700
O	-0.0000040	1.3987490	0.0000000

triene_cardanol

H	2.0361570	4.8307340	-0.6846830
C	-2.7209520	-0.8520460	0.4165400
C	-3.6556750	-1.7358620	0.9651980
C	-4.9918970	-1.3562320	1.0894140
C	-5.4195850	-0.0993430	0.6752790
C	-4.4903710	0.7891650	0.1282930
C	-3.1516060	0.4120590	0.0008360
H	-3.3351760	-2.7194610	1.2992490
H	-5.7116550	-2.0475410	1.5200030
H	-6.4550220	0.2113550	0.7701520
H	-2.4306710	1.1118660	-0.4223110
C	2.1171940	2.3800780	1.3740890
H	1.3440110	2.7901430	2.0269850
C	2.2369600	2.8710160	0.1383270
H	2.9993850	2.4599560	-0.5240900
C	1.3914250	3.9774660	-0.4196710
H	0.7158960	4.3614830	0.3587770
C	0.5797910	3.6218890	-1.6395710
H	0.0883670	4.4644280	-2.1283690
C	0.4249480	2.4003940	-2.1505660
H	-0.1734880	2.2310640	-3.0411380
H	0.8967180	1.5317490	-1.6991180
C	2.9563750	1.2862680	1.9857030
H	2.3218530	0.4077490	2.1608870
H	3.2590130	1.6175220	2.9916970
C	4.1918880	0.9165880	1.2166370
H	4.9165940	1.7235450	1.1038700
C	4.5000650	-0.2741730	0.6884720
H	5.4655530	-0.3637740	0.1870010
C	3.6696410	-1.5247100	0.6883210
H	4.1290390	-2.2700640	1.3561740
H	2.6759760	-1.3200950	1.0993750
C	3.5416580	-2.1428610	-0.7123000
H	4.5446180	-2.4033500	-1.0760020
H	3.1637750	-1.3822110	-1.4065910
C	2.6569740	-3.3947030	-0.7676970
H	3.0681440	-4.1503520	-0.0841930
H	2.7272160	-3.8283300	-1.7746710
C	1.1761420	-3.1731030	-0.4289870
H	0.6681910	-4.1472750	-0.4261040
H	1.0877480	-2.7904330	0.5954870
C	0.4493210	-2.2399200	-1.4000130
H	0.9546820	-1.2651410	-1.4246580
H	0.5378050	-2.6504830	-2.4153830
C	-1.0317180	-2.0057350	-1.0867330
H	-1.5708500	-2.9624380	-1.0664190

H	-1.4793210	-1.4242750	-1.9024660
C	-1.2784070	-1.2563610	0.2342820
H	-0.9674360	-1.8819040	1.0793030
H	-0.6436430	-0.3608940	0.2570270
O	-4.9429630	2.0135700	-0.2610740
H	-4.2028050	2.5186260	-0.6163070

diene_product

H	3.9540690	0.7787690	1.4949810
C	-2.0167870	2.5741720	0.5079290
C	-0.9904630	2.7686600	1.4396040
C	0.2760620	3.1686720	1.0176090
C	0.5465670	3.3826750	-0.3303020
C	-0.4712310	3.1895340	-1.2664910
C	-1.7426560	2.7891550	-0.8459180
H	-1.1877010	2.6155690	2.4976660
H	1.0646750	3.3236400	1.7491690
H	1.5254130	3.7022360	-0.6727830
H	-2.5336120	2.6481760	-1.5821540
C	2.8634100	-1.8508790	0.7939620
H	3.3582200	-1.5175970	1.7059080
C	3.0533070	-1.1762690	-0.3425800
H	2.5360360	-1.5228410	-1.2385320
C	3.9128150	0.0422230	-0.5305200
H	4.6325030	-0.1603240	-1.3392490
C	4.6706670	0.5361030	0.6997640
H	5.2979110	-0.2760140	1.0897780
C	5.5395950	1.7566930	0.4045730
H	6.2905250	1.5334610	-0.3618380
H	6.0707830	2.0965780	1.2995540
H	4.9365130	2.5953170	0.0382370
C	1.9867900	-3.0698320	0.9523720
H	1.1005500	-2.8038530	1.5438990
H	2.5305790	-3.8006080	1.5721350
C	1.5968690	-3.7393790	-0.3327480
H	2.4386640	-4.0555850	-0.9499060
C	0.3654450	-4.0032280	-0.7850500
H	0.2879940	-4.5270020	-1.7400100
C	-0.9530300	-3.6787710	-0.1447240
H	-1.4257020	-4.6155760	0.1908130
H	-0.8085350	-3.0720370	0.7550830
C	-1.9177250	-2.9754590	-1.1114710
H	-1.9843110	-3.5724370	-2.0312030
H	-1.4886450	-2.0114370	-1.4125220
C	-3.3333120	-2.7847150	-0.5535190
H	-3.7100870	-3.7626650	-0.2229820
H	-3.9969900	-2.4682370	-1.3700560
C	-3.4714670	-1.7829370	0.5997610
H	-4.4779880	-1.8847380	1.0286520
H	-2.7778550	-2.0425640	1.4111310
C	-3.2604620	-0.3219640	0.1958400
H	-2.2504220	-0.1782140	-0.2070330
H	-3.9537870	-0.0757150	-0.6224830
C	-3.4851190	0.6513820	1.3527660
H	-2.7611400	0.4430570	2.1519890
H	-4.4789290	0.4735930	1.7864020
C	-3.3903310	2.1357970	0.9599460
H	-4.1206270	2.3428040	0.1674340
H	-3.6906310	2.7443460	1.8221990
O	-0.1717750	3.4101690	-2.5766380
H	-0.9575470	3.2423460	-3.1088330
H	3.2806060	0.8564040	-0.9171460

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O	3.0761120	-3.7750320	-0.0179460
H	2.2219150	-3.5716180	-0.4152600
C	4.2227740	-0.3116980	-0.5716210
C	5.4968610	-0.4061870	-0.0045900
C	5.9362230	-1.6125400	0.5418450
C	5.1209300	-2.7381060	0.5357990
C	3.8450530	-2.6510810	-0.0285120
C	3.4038780	-1.4463100	-0.5787030
H	6.1467860	0.4650570	0.0051940
H	6.9301530	-1.6775040	0.9767430
H	5.4489520	-3.6837060	0.9551280
H	2.4088120	-1.3888550	-1.0199520
C	-1.8544700	-0.5779180	0.9693170
C	-1.2486820	0.3520150	1.7210100
H	-1.1118450	0.0766720	2.7689190
C	-3.7682660	-0.4861570	-0.7096370

H	-3.9542990	-0.4370210	-1.7919360
C	-4.5680440	-1.6528070	-0.1244540
H	-4.1260220	-2.5945740	-0.4796310
C	-6.0577250	-1.6433080	-0.4847220
H	-6.1672770	-1.6285090	-1.5790560
C	-6.8567570	-0.4852680	0.1172260
H	-6.4577600	0.4713750	-0.2426600
C	-8.3473560	-0.5617620	-0.2064610
H	-8.5196430	-0.5360810	-1.2885480
H	-8.8990390	0.2737260	0.2367020
H	-8.7883940	-1.4902580	0.1739880
C	-2.2466980	-0.5814310	-0.4828640
H	-4.1247290	0.4625740	-0.2898890
H	-1.8923270	-1.5202280	-0.9352060
H	-2.1320010	-1.4894620	1.5006690
C	-0.7030590	1.7282000	1.4409160
H	-1.2458790	2.4317430	2.0930190
H	0.3256820	1.7429920	1.8298630
C	-0.7078060	2.2881360	0.0191150
H	-1.7377920	2.3174130	-0.3566110
H	-0.1551440	1.6187800	-0.6515880
C	-0.1262130	3.7046570	-0.0804040
H	-0.6967830	4.3666970	0.5861360
H	-0.3053880	4.0783980	-1.0977300
C	1.3686820	3.8697240	0.2304630
H	1.5932750	4.9414680	0.1646610
H	1.5732630	3.5950080	1.2738310
C	2.3261050	3.0991750	-0.6989490
H	1.8517260	2.9611100	-1.6816200
H	3.2180780	3.7112610	-0.8871690
C	2.7908420	1.7442210	-0.1586850
H	1.9304140	1.1064410	0.0775570
C	3.3219030	1.8956660	0.7906050
C	3.7143250	0.9948250	-1.1311700
H	3.1725340	0.8114510	-2.0687830
H	4.5658870	1.6374270	-1.3876390
H	-6.5070090	-2.5888790	-0.1509280
H	-4.4649790	-1.6617040	0.9688260
H	-6.7168240	-0.4810140	1.2071330
H	-1.7587340	0.2261390	-1.0307220

intermediate-1

Ru	-1.8072470	0.1241580	-0.0322570
H	-3.0442510	3.3018580	-0.8901280
C	-0.0641230	-1.4535800	0.0350380
C	-0.4306390	-1.1658820	1.3820210
C	-1.7796780	-1.2592810	1.7693530
C	-2.7662270	-1.7391260	0.8595000
C	-2.3998490	-2.1054700	-0.4546050
C	-1.0658310	-1.8533660	-0.8927680
H	0.3231090	-0.8425080	2.0915910
H	-2.0779770	-0.9951510	2.7788430
H	-3.8001950	-1.8543850	1.1630060
H	-0.7820560	-2.0734310	-1.9179680
C	-0.1349790	1.4919670	-0.6901230
H	0.4533280	0.9245110	-1.4098420
C	-1.3382590	2.0015210	-1.1883790
H	-1.5657410	1.8820710	-2.2437610
C	-2.1568910	2.9592410	-0.3511350
H	-1.5902520	3.8450440	-0.0491490
C	-2.5358050	2.0673550	0.8133350
H	-2.1012150	2.2542360	1.7925840
C	-3.6139950	1.1945110	0.6860730
H	-2.7482180	0.3145360	-1.2651050
H	-4.0003880	0.6959370	1.5703480
H	-4.3310800	1.3099730	-0.1209390
C	0.7066090	2.1235830	0.4045590
H	1.1591290	1.3542700	1.0356180
H	0.0876110	2.7398900	1.0646110
C	1.7803270	2.9688400	-0.2388910
H	1.4150100	3.8343700	-0.7908850
C	3.1021130	2.7508070	-0.2145380
H	3.7265750	3.4661110	-0.7509070
C	3.8524910	1.6407120	0.4600000
H	4.6082040	2.0808420	1.1254980
H	3.1874960	1.0602210	1.1095730
C	4.5692480	0.7113570	-0.5375760
H	5.2926820	1.3041370	-1.1104660
H	3.8433040	0.3422030	-1.2753880
C	5.2969140	-0.4654460	0.1260650
H	5.9483250	-0.0767680	0.9191900

H	5.9653860	-0.9328420	-0.6079410
C	4.3762390	-1.5443320	0.7137350
H	4.9615180	-2.1831470	1.3840570
H	3.6295310	-1.0661260	1.3632010
C	3.6720770	-2.4320660	-0.3365860
H	3.7878570	-1.9989150	-1.3393060
H	4.1657230	-3.4084860	-0.3810830
C	2.1768370	-2.6519950	-0.0698890
H	2.0240840	-2.9333090	0.9801730
H	1.7983170	-3.4850390	-0.6740610
C	1.3725240	-1.3790090	-0.3968720
H	1.8503960	-0.5268990	0.0950880
H	1.4269470	-1.1975570	-1.4760290
O	-3.3472330	-2.6261270	-1.2351750
H	-3.0310630	-2.7516280	-2.1396060

intermediate-2

Ru	-1.8177890	0.1092910	-0.0237820
H	-2.6964650	3.6890940	-0.5168230
C	-0.0921410	-1.4446190	0.0111650
C	-0.3753140	-0.9033400	1.3139050
C	-1.6703130	-0.9841960	1.8778540
C	-2.7216870	-1.5503980	1.1147890
C	-2.4490890	-2.0743250	-0.1822800
C	-1.1367200	-2.0249140	-0.7338740
H	0.4245830	-0.4403420	1.8798090
H	-1.8666630	-0.5882500	2.8683150
H	-3.7384980	-1.5900030	1.4900490
H	-0.9413590	-2.4327150	-1.7213790
C	0.0022140	1.6239530	-0.6526580
H	0.5287530	1.0919380	-1.4441830
C	-1.2306540	2.1358710	-0.9857750
H	-1.5630840	2.0323440	-2.0178760
C	-2.0979890	2.9175570	-0.0158190
H	-1.5006480	3.4116450	0.7526480
C	-2.9227080	1.7848060	0.5581200
H	-3.2973330	1.8660150	1.5767930
C	-3.8245980	1.1596190	-0.4470140
H	-3.2304790	0.3890690	-1.1429800
H	-4.6724350	0.6076990	-0.0445040
H	-4.1368370	1.8245560	-1.2610770
C	0.8965080	2.0932020	0.4725510
H	1.3657520	1.2449920	0.9729660
H	0.3227200	2.6302170	1.2348300
C	1.9676020	2.9801060	-0.1189930
H	1.6038880	3.8851200	-0.6038640
C	3.2870230	2.7463740	-0.1156740
H	3.9178030	3.4888730	-0.6052090
C	4.0211150	1.5857740	0.4883800
H	4.8187110	1.9749520	1.1358770
H	3.3604840	1.0109400	1.1471990
C	4.6595550	0.6536040	-0.5588060
H	5.4046610	1.2204210	-1.1298350
H	3.8961730	0.3504980	-1.2887840
C	5.3235060	-0.5858400	0.0569740
H	5.9993920	-0.2631820	0.8591930
H	5.9603780	-1.0669890	-0.6958240
C	4.3367650	-1.6230580	0.6112490
H	4.8678720	-2.2988500	1.2906570
H	3.5973690	-1.1126490	1.2446680
C	3.6141270	-2.4628710	-0.4638540
H	3.7124450	-1.9871830	-1.4491960
H	4.1062720	-3.4365640	-0.5579040
C	2.1225370	-2.6821530	-0.1743370
H	1.9841270	-2.9367130	0.8845570
H	1.7360950	-3.5307870	-0.7506580
C	1.3103290	-1.4199640	-0.5270590
H	1.8323590	-0.5461000	-0.1262420
H	1.2889830	-1.3058720	-1.6168830
O	-3.4972540	-2.5849350	-0.8444960
H	-3.2446670	-2.8626170	-1.7350330

intermediate-3

Ru	1.6091090	-0.0801600	-0.0555150
H	3.2045810	2.0969300	-1.2427790
C	0.1757080	-1.8312550	-0.0029490
C	0.3645640	-1.4933230	-1.3555090
C	1.6888380	-1.3029580	-1.8518540
C	2.8413090	-1.5912150	-1.0699890
C	2.6663600	-2.0643360	0.2607890
C	1.3494170	-2.0677890	0.8029430
H	-0.4875380	-1.2590560	-1.9838620

H	1.8257830	-0.9167020	-2.8572350
H	3.8413240	-1.4785100	-1.4734560
H	1.2138370	-2.2916150	1.8589020
C	0.4404190	3.8158670	-0.4940150
H	0.2407630	4.8823740	-0.3854000
C	1.7291450	3.4586720	-0.4495320
H	2.4702490	4.2450860	-0.3103550
C	2.3659430	2.0939010	-0.5419270
H	1.5265740	1.4502300	-1.0864510
C	2.7356670	1.3973280	0.7388540
H	3.7757560	1.3035360	1.0359840
C	1.6512880	1.4145430	1.7535320
H	0.7241830	0.7916410	1.3538760
H	1.9195350	0.9873450	2.7185970
H	1.1330060	2.3742570	1.8576320
C	-0.8002540	2.9815680	-0.6611370
H	-0.5686480	1.9133600	-0.7637990
H	-1.2749320	3.2747880	-1.6102180
C	-1.7794310	3.2091250	0.4750020
H	-1.5067900	3.9912950	1.1829340
C	-2.9485590	2.5844010	0.6613020
H	-3.5470840	2.9013580	1.5161420
C	-3.5694330	1.5188120	-0.1967960
H	-4.2304120	1.9979740	-0.9357930
H	-2.7976930	1.0055220	-0.7857380
C	-4.4044450	0.5150220	0.6141310
H	-5.1883130	1.0722940	1.1420450
H	-3.7797180	0.0720260	1.4027450
C	-5.0600170	-0.5898720	-0.2250700
H	-5.5851890	-0.1267950	-1.0704330
H	-5.8353470	-1.0842030	0.3737030
C	-4.0872700	-1.6520470	-0.7531610
H	-4.5663250	-2.2132330	-1.5633950
H	-3.2336350	-1.1445140	-1.2254710
C	-3.5817180	-2.6481210	0.3110810
H	-3.7196760	-2.2340300	1.3190710
H	-4.1901220	-3.5580610	0.2804170
C	-2.1028030	-3.0159850	0.1308050
H	-1.9103270	-3.2411060	-0.9261460
H	-1.8511440	-3.9233790	0.6911140
C	-1.2066410	-1.8517790	0.5955280
H	-1.6926430	-0.9091330	0.3213150
H	-1.1381020	-1.8550430	1.6889510
O	3.7604240	-2.3980650	0.9529760
H	3.5353590	-2.6964570	1.8437870
intermediate-4'			
Ru	-1.1153380	-0.3977550	0.2563590
H	-0.3379870	-3.0871970	-0.0416660
C	-1.7791100	1.6421240	-0.5615920
C	-0.8196900	1.0835440	-1.4345120
C	-0.9615070	-0.2440250	-1.9212570
C	-2.1353970	-0.9878230	-1.6179730
C	-3.2130060	-0.3660690	-0.9207550
C	-2.9701550	0.8735170	-0.2954300
H	0.0942230	1.6245350	-1.6482810
H	-0.1751720	-0.6928880	-2.5168420
H	-2.2644560	-1.9994750	-1.9886310
H	-3.7297750	1.3042130	0.3542310
C	2.3022530	-2.6851720	0.7868310
H	3.1965330	-2.6934480	1.4076420
C	1.1410520	-2.3796310	1.3913080
H	1.1822570	-2.1292600	2.4501140
C	-0.2008170	-2.3947340	0.7871880
H	0.4199560	-0.2073970	0.4523040
C	-1.3895540	-2.0573520	1.4936750
H	-2.3239350	-2.5884500	1.3357430
C	-1.3224070	-0.9740610	2.4933000
H	-1.0244900	0.0916780	1.9803750
H	-2.2600720	-0.7723000	3.0097170
H	-0.4818480	-1.0112490	3.1905330
C	2.5166940	-3.0340460	-0.6503190
H	1.5577760	-3.1057770	-1.1811230
H	2.9395550	-4.0502860	-0.6880600
C	3.4396120	-2.1530590	-1.4677560
H	3.6772410	-2.6056030	-2.4308520
C	4.0011570	-0.9603960	-1.2274540
H	4.6320480	-0.5763920	-2.0313640
C	3.9080660	-0.0346520	-0.0478030
H	3.3573500	-0.4903890	0.7797780
H	4.9243540	0.1655980	0.3212550
C	3.2415460	1.2995690	-0.4168990
H	2.2040910	1.0814360	-0.7057820
H	3.7207000	1.7196160	-1.3117300
C	3.2607900	2.3521330	0.6989680
H	4.2722390	2.7661700	0.7857430
H	3.0459350	1.8765490	1.6669270
C	2.2466960	3.4808510	0.4574980
H	2.5104260	4.3632860	1.0508790
H	2.3147640	3.7964990	-0.5933210
C	0.8075430	3.0414300	0.7790830
H	0.7404420	1.9558410	0.6502580
H	0.5963030	3.2217410	1.8417350
C	-0.2794960	3.7070230	-0.0718060
H	0.0380340	3.7453000	-1.1227360
H	-0.4004580	4.7549360	0.2253510
C	-1.6568200	3.0380220	0.0179900
H	-1.9953280	3.0103700	1.0614660
H	-2.3910140	3.6580350	-0.5154500
O	-4.3471610	-1.0664860	-0.8002690
H	-5.0122090	-0.5757440	-0.2995620
intermediate-4			
Ru	-1.5141240	-0.2813740	-0.0018970
H	-0.6872470	-2.8020310	-0.9637330
C	-1.3595180	2.0229670	-0.0892210
C	-0.7503920	1.3770330	-1.2165120
C	-1.4679900	0.4765680	-2.0480880
C	-2.8072960	0.1404570	-1.7204140
C	-3.4176010	0.7575560	-0.5921600
C	-2.6910910	1.6736540	0.2255190
H	0.2941660	1.5651620	-1.4344270
H	-0.9779760	0.0143500	-2.8980630
H	-3.3806840	-0.5730200	-2.3018690
H	-3.1703120	2.1147050	1.0956770
C	1.6132480	-1.6757060	0.5970590
H	2.1912980	-0.8603860	1.0236430
C	0.2727720	-1.5465420	0.5836990
H	-0.1072250	-0.6861870	1.2686280
C	-0.8302610	-2.2269180	-0.0540290
H	-1.0446830	-2.6275330	2.7397620
C	-2.0328970	-2.4491950	0.8002760
H	-2.8499010	-2.9055380	0.2373140
C	-1.8439890	-3.1076750	2.1701260
H	-2.4644860	-1.3775550	1.1232490
H	-2.7646110	-3.0731730	2.7585330
H	-1.5720640	-4.1570980	2.0233020
C	2.3893790	-2.8748160	0.1312880
H	1.7111190	-3.7169270	-0.0314600
H	3.0718610	-3.1743030	0.9390480
C	3.1884150	-2.6171000	-1.1388600
H	2.9006160	-3.2210940	-1.9972520
C	4.1986760	-1.7509420	-1.2830900
H	4.6774650	-1.6971910	-2.2605460
C	4.6932820	-0.7830460	-0.2478710
H	4.4230490	-1.1301820	0.7577130
H	5.7885920	-0.7319130	-0.2675200
C	4.1004470	0.6200480	-0.4831820
H	3.0383110	0.4904300	-0.7280980
H	4.5538400	1.0654370	-1.3778010
C	4.2354380	1.5874940	0.6973550
H	5.2656230	1.9561660	0.7608870
H	4.0501560	1.0543780	1.6416160
C	3.2614220	2.7688910	0.5903150
H	3.5697320	3.5743790	1.2674160
H	3.3193890	3.1885060	-0.4240220
C	1.8103350	2.3792050	0.9030620
H	1.5822720	1.4131420	0.4348470
H	1.7041810	2.2195870	1.9853610
C	0.7906320	3.4214800	0.4444330
H	0.9123740	3.6201580	-0.6291590
H	1.0106920	4.3753610	0.9383200
C	-0.6730000	3.0869780	0.7458350
H	-0.7894880	2.8293580	1.8060280
H	-1.2711980	3.9963430	0.5967740
O	-4.6801720	0.3919610	-0.3220640
H	-5.0021010	0.8191070	0.4825800
intermediate-5			
Ru	1.1943340	-0.1111330	0.0972020
H	0.8607970	2.3708420	-0.8703460
C	0.4182590	-2.0240530	-0.8935470
C	1.4784380	-1.4987240	-1.6704640
C	2.7128110	-1.1767030	-1.0429900

C	2.9264590	-1.4497340	0.3351830
C	1.9001250	-2.0712470	1.1008190
C	0.6335480	-2.2767130	0.5004140
H	1.3271310	-1.2858310	-2.7224280
H	3.5027980	-0.7053520	-1.6170820
H	3.8689690	-1.2089740	0.8146240
H	-0.1814630	-2.6822910	1.0940970
C	0.8746930	1.2914310	1.6497510
H	0.9871290	1.0627490	2.7050060
C	1.9731550	1.7533860	0.8743580
H	2.9672660	1.7603850	1.3168450
C	1.7944460	1.9240170	-0.5259260
H	2.3465910	4.2408010	-1.9769880
C	2.9692750	2.2216140	-1.4257400
H	2.7829780	1.7974940	-2.4196850
C	3.2205820	3.7284010	-1.5620910
H	3.8710350	1.7327610	-1.0359960
H	3.4471390	4.1825860	-0.5924330
H	4.0657350	3.9194570	-2.2294610
C	-0.4758260	1.3046550	1.0311540
H	-0.4492100	0.6360300	0.0120420
H	-0.6933880	2.2558070	0.5288070
C	-1.6063530	0.8011340	1.8644610
H	-1.3327170	0.0740890	2.6277980
C	-2.8929500	1.1676530	1.7565780
H	-3.5850030	0.7185900	2.4700990
C	-3.5145260	2.1615880	0.8226990
H	-3.8335980	3.0169000	1.4363070
H	-2.7796500	2.5573920	0.1113810
C	-4.7501130	1.6695530	0.0393920
H	-5.1951450	2.5534240	-0.4306320
H	-5.5058940	1.2918310	0.7407960
C	-4.4623170	0.6163520	-1.0418360
H	-3.5010220	0.8612940	-1.5148120
H	-5.2054970	0.7144180	-1.8411550
C	-4.4636360	-0.8429590	-0.5477660
H	-4.2226520	-0.8763390	0.5232910
H	-5.4779200	-1.2484350	-0.6338130
C	-3.4782150	-1.7623300	-1.2831870
H	-3.6990750	-2.8087090	-1.0372940
H	-3.6032310	-1.6651700	-2.3699630
C	-2.0425100	-1.4346970	-0.8787160
H	-1.9787850	-1.4888660	0.2153150
H	-1.8249960	-0.3924390	-1.1420580
C	-0.9407200	-2.3044320	-1.4927740
H	-1.1654740	-3.3661970	-1.3244730
H	-0.8980310	-2.1596420	-2.5768790
O	2.1860310	-2.3756750	2.3726810
H	1.4184910	-2.7524830	2.8221210

intermediate-6

Ru	0.5582510	-0.6850700	-0.4415290
H	4.3354800	3.3125370	0.1925600
C	-0.8089100	-2.3387780	-1.0698640
C	-0.8933630	-1.2545340	-1.9829060
C	0.2906220	-0.7275970	-2.5703870
C	1.5496030	-1.3050490	-2.2712840
C	1.6063500	-2.5159540	-1.5055120
C	0.4541030	-2.9935050	-0.8686040
H	-1.8486180	-0.7887170	-2.1856670
H	0.2402800	0.1395140	-3.2188620
H	2.4624270	-0.9037020	-2.6959730
H	0.5056010	-3.8663810	-0.2229650
C	0.2077860	1.4442820	-0.4062270
H	0.0171780	1.6512210	0.6594320
C	1.4424160	2.1727130	-0.7941310
H	1.7163010	2.1273060	-1.8521850
C	2.2447590	2.8837080	0.0273760
H	1.9457300	3.0002740	1.0732520
C	3.4688010	3.6429410	-0.3979170
H	3.6993760	3.4140480	-1.4453080
C	3.3072470	5.1577260	-0.2178940
H	2.4858330	5.5394900	-0.8314900
H	4.2215980	5.6825170	-0.5092540
H	3.0938510	5.4137760	0.8251000
C	-1.0127080	1.9325230	-1.2168810
H	-1.8133460	1.1905150	-1.1785110
H	-0.7269420	2.0273610	-2.2754020
C	-1.5381720	3.2521470	-0.7177830
H	-0.7951530	4.0399130	-0.5953450
C	-2.8124680	3.5225690	-0.4033870

H	-3.0386270	4.5184760	-0.0226750
C	-3.9788950	2.5781020	-0.5078620
H	-4.8577810	3.1240230	-0.8741050
H	-3.7738390	1.8082230	-1.2595680
C	-4.3301510	1.9114270	0.8333310
H	-4.6788580	2.6773570	1.5367670
H	-3.4085820	1.5101510	1.2776800
C	-5.3843820	0.8018340	0.7405170
H	-6.3308030	1.2295010	0.3864970
H	-5.5833160	0.4315230	1.7548960
C	-5.0205360	-0.3895230	-0.1584650
H	-5.8123760	-1.1443560	-0.0680350
H	-5.0266390	-0.0831660	-1.2131570
C	-3.6716970	-1.0350180	0.1660400
H	-2.8703220	-0.3083010	-0.0189320
H	-3.6255340	-1.2742220	1.2378780
C	-3.3955000	-2.3095160	-0.6347560
H	-3.5424530	-2.1267730	-1.7075500
H	-4.1513430	-3.0578060	-0.3680550
C	-2.0214930	-2.9449360	-0.3929710
H	-1.8225840	-2.9984700	0.6843880
H	-2.0529800	-3.9865140	-0.7415590
O	2.8181350	-3.0803190	-1.3712200
H	2.7602980	-3.8851570	-0.8397340
C	3.5244820	-0.7499670	1.0139400
C	4.0038850	-0.3819100	2.4101760
H	3.2527510	-0.6239980	3.1658440
H	4.2322130	0.6871140	2.4764920
H	4.9180660	-0.9328670	2.6510080
C	4.5534160	-0.4290120	-0.0573650
H	5.4765430	-0.9823060	0.1384530
H	4.8020950	0.6378100	-0.0546500
H	4.2036130	-0.7084630	-1.0523060
O	2.2614920	-0.0673520	0.7592450
H	2.4417930	0.8624990	0.4825880
H	3.2696730	-1.8129350	0.9779790
C	0.0103740	-0.6560490	2.8201180
H	0.8710020	0.0209750	2.8211720
C	0.4688430	-2.0768920	3.0755770
H	0.9840600	-2.1377550	4.0383470
H	1.1604540	-2.4060840	2.2950930
H	-0.3839520	-2.7623590	3.1000650
C	-1.0354860	-0.1759020	3.8113370
H	-0.6166850	-0.1758790	4.8217560
H	-1.9141500	-0.8284080	3.8076090
H	-1.3562050	0.8494990	3.5946570
O	-0.5611580	-0.6263010	1.4739240
H	-1.1494560	0.1388650	1.4181850

intermediate-7

Ru	0.8327770	-0.5431440	-0.4752800
H	1.3261460	4.0138190	-0.2617330
C	-0.3905790	-2.4801110	-0.4538500
C	-0.6926990	-1.8005210	-1.6520240
C	0.3538170	-1.3029760	-2.4608770
C	1.7227570	-1.5904540	-2.1641790
C	2.0159130	-2.4634190	-1.0822150
C	0.9918890	-2.7376870	-0.1425220
H	-1.7200150	-1.5724820	-1.9063680
H	0.1188630	-0.7022340	-3.3322690
H	2.5242640	-1.2555280	-2.8125790
H	1.2331360	-3.2686670	0.7750510
C	-0.0911320	1.5582670	-0.9445060
H	-0.1045650	2.0217120	0.0388870
C	1.0969980	1.6043120	-1.6456230
H	1.0507300	1.3008440	-2.6924450
C	2.3219600	2.4067470	-1.2985820
H	2.5500770	2.9853090	-2.2071730
C	2.2019570	3.3673340	-0.1165410
H	2.0302040	2.7891810	0.7966020
C	3.4486280	4.2342430	0.0451440
H	4.3409810	3.6235400	0.2212740
H	3.3457170	4.9206650	0.8906330
H	3.6345420	4.8384080	-0.8496360
C	-1.4434060	1.4298720	-1.6204190
H	-2.0473430	0.6536620	-1.1459170
H	-1.2950120	1.1240000	-2.6662660
C	-2.2057260	2.7327540	-1.5707870
H	-1.6292100	3.6339160	-1.7759760
C	-3.5149600	2.8459980	-1.3131750
H	-3.9411570	3.8483670	-1.2981580
C	-4.4657330	1.7129570	-1.0331920

H	-5.4447890	1.9448400	-1.4700670
H	-4.1247330	0.8033120	-1.5405190
C	-4.6404910	1.4354710	0.4703350
H	-5.1217560	2.3006000	0.9418240
H	-3.6463790	1.3729370	0.9330830
C	-5.4516870	0.1759920	0.7995380
H	-6.4754350	0.2943810	0.4234220
H	-5.5409450	0.1014850	1.8913000
C	-4.8867430	-1.1455820	0.2576590
H	-5.5071760	-1.9686730	0.6342060
H	-4.9840750	-1.1797030	-0.8354810
C	-3.4267540	-1.4103270	0.6341710
H	-2.8044970	-0.6279780	0.1763450
H	-3.3082170	-1.3165010	1.7240480
C	-2.9135080	-2.7837490	0.1967670
H	-3.1256150	-2.9466920	-0.8679760
H	-3.4907280	-3.5524780	0.7233510
C	-1.4308270	-3.0485560	0.4862010
H	-1.1801910	-2.7335560	1.5068980
H	-1.2608020	-4.1343420	0.4665450
O	3.2765390	-2.8610990	-0.9394930
H	3.4025740	-3.3482430	-0.1137950
C	3.3823430	-0.3589610	1.0979870
C	3.7239000	0.1710060	2.4913060
H	2.9375150	-0.0648000	3.2126050
H	3.8522220	1.2575060	2.4586300
H	4.6585280	-0.2706150	2.8519180
C	4.5540810	-0.1366800	0.1408110
H	5.4246710	-0.7234150	0.4524830
H	4.8486550	0.9174930	0.1389110
H	4.3035230	-0.4293200	-0.8820250
O	2.2015730	0.2831620	0.6604980
H	3.1779390	1.7414480	-1.1515690
H	3.2082930	-1.4471750	1.1924460
C	-0.0342630	0.5739740	2.6824150
H	0.9645920	0.9541470	2.4563530
C	0.0256830	-0.3972700	3.8506480
H	0.3883000	0.1108950	4.7497240
H	0.7044500	-1.2265460	3.6330410
H	-0.9646460	-0.8088460	4.0757220
C	-1.0023020	1.7214950	2.9197340
H	-0.6926070	2.2947520	3.7984760
H	-2.0168940	1.3529830	3.1161640
H	-1.0401240	2.4108880	2.0716220
O	-0.3964100	-0.1615990	1.4777110
H	-1.3494870	-0.1034390	1.3356570

intermediate-8

Ru	0.7939170	1.1928850	-0.2358530
H	-4.7531830	0.6506630	-1.7097800
C	1.1937920	0.3729120	-2.3296780
C	-0.0301230	-0.1112330	-1.8057930
C	-1.0321990	0.7730850	-1.2964620
C	-0.8213470	2.1712990	-1.3114040
C	0.4071340	2.6793820	-1.8292840
C	1.4172540	1.7755560	-2.2749370
H	-0.1976660	-1.1781910	-1.7228160
H	-1.9309880	0.3515620	-0.8522090
H	-1.5468820	2.8645630	-0.9012660
H	2.3894090	2.1682180	-2.5631700
C	-3.9423020	-1.7881100	-0.2672240
H	-4.4713270	-1.6790110	-1.2140990
C	-3.9667100	-0.7776500	0.6102640
H	-3.4512070	-0.9057720	1.5632690
C	-4.6965940	0.5292330	0.4489070
H	-5.4043840	0.6269050	1.2860940
C	-5.4486520	0.7409540	-0.8637330
H	-6.1847700	-0.0624290	-0.9907640
C	-6.1552800	2.0931810	-0.9250050
H	-6.8862760	2.1959550	-0.1159530
H	-6.6899400	2.2195770	-1.8709410
H	-5.4445210	2.9228910	-0.8329970
C	-3.2956700	-3.1363020	-0.0628790
H	-2.5168480	-3.2893610	-0.8222320
H	-4.0575390	-3.8967860	-0.3002260
C	-2.7717480	-3.4131410	1.3161540
H	-3.4639020	-3.1740920	2.1234410
C	-1.6062050	-3.9800210	1.6529310
H	-1.4276100	-4.1570390	2.7147530
C	-0.5086890	-4.4539220	0.7439890
H	-0.5383340	-5.5531260	0.6913770

H	-0.6806420	-4.1031030	-0.2798260
C	0.8863080	-4.0348320	1.2288700
H	1.0289290	-4.4075190	2.2512200
H	0.9205550	-2.9390770	1.3126620
C	2.0423630	-4.5511520	0.3615070
H	2.0056560	-5.6476620	0.3450450
H	2.9941670	-4.2934020	0.8459770
C	2.0656170	-4.0460560	-1.0870960
H	2.8657500	-4.5623200	-1.6319550
H	1.1332130	-4.3285790	-1.5932540
C	2.2695680	-2.5352170	-1.2228220
H	1.5408680	-2.0211200	-0.5799180
H	3.2707040	-2.2713880	-0.8498350
C	2.1258820	-2.0358680	-2.6633480
H	1.1610000	-2.3613360	-3.0747530
H	2.8825120	-2.5301020	-3.2837390
C	2.2894350	-0.5259550	-2.8613010
H	3.2457810	-0.1935210	-2.4380820
H	2.3544200	-0.3200870	-3.9384810
O	0.5760990	4.0070310	-1.7902560
H	1.4536640	4.2587490	-2.1067130
C	-0.5906400	2.2835670	2.1781630
C	-0.2471500	3.7590200	2.3479690
H	-0.0294000	4.2269200	1.3827820
H	0.6274340	3.8759660	2.9954720
H	-1.0846650	4.2936860	2.8065070
C	-0.8882540	1.5926840	3.5027390
H	-1.7557430	2.0532820	3.9851970
H	-0.0338080	1.6793960	4.1812080
H	-1.1025130	0.5315680	3.3486900
O	0.5150860	1.6134670	1.5701050
H	-3.9868300	1.3596330	0.6003840
H	-1.4660060	2.1891930	1.5188270
C	3.3638960	0.8590990	1.7530960
H	2.5872660	0.9255310	2.5202250
C	3.9260610	2.2346640	1.4636420
H	4.3923570	2.6394480	2.3662650
H	3.1325420	2.9243990	1.1624570
H	4.6840800	2.1904950	0.6751960
C	4.4198280	-0.1609290	2.1375740
H	4.9122250	0.1497130	3.0633270
H	5.1849920	-0.2534150	1.3602130
H	3.9807720	-1.1479350	2.3240660
O	2.7039270	0.4006210	0.5201090
H	2.6299920	-0.5632980	0.5572180

intermediate-9

Ru	-1.2386170	-0.4803470	-0.1347210
H	3.5159760	-3.3596700	-1.5017220
C	-1.0792190	0.5422380	-2.1030030
C	0.2119320	0.2008280	-1.6200580
C	0.4896810	-1.1382260	-1.2205700
C	-0.5150460	-2.1307350	-1.3447260
C	-1.7495300	-1.8235890	-2.0115970
C	-2.0447060	-0.4975120	-2.3502140
H	0.9631520	0.9649930	-1.4745980
H	1.4504200	-1.3801820	-0.7764410
H	-0.3363770	-3.1499570	-1.0227290
H	-3.0039320	-0.2418460	-2.7923760
C	4.4531960	-0.9047660	-0.1720380
H	4.7700960	-1.3579310	-1.1114050
C	3.8493000	-1.6653880	0.7482000
H	3.5497600	-1.1997500	1.6883670
C	3.5742640	-3.1420230	0.6487490
H	4.0633300	-3.6374400	1.5014780
C	4.0049050	-3.8371400	-0.6415060
H	5.0823710	-3.6913910	-0.7866380
C	3.6896250	-5.3312060	-0.6389390
H	4.1978160	-5.8429450	0.1854640
H	4.0096690	-5.8073550	-1.5704150
H	2.6142750	-5.5147020	-0.5266590
C	4.8036630	0.5562300	-0.0291860
H	4.2369680	1.1432370	-0.7645090
H	5.8545550	0.6687590	-0.3415030
C	4.6606670	1.1293040	1.3507360
H	5.1204400	0.5334380	2.1393720
C	4.1064240	2.2956340	1.7040190
H	4.1501460	2.5664030	2.7603070
C	3.4532120	3.3196260	0.8212180
H	4.1316920	4.1797810	0.7115100
H	3.3113160	2.9211170	-0.1894860

C	2.1208230	3.8291140	1.3890050
H	2.2954610	4.2097790	2.4037020
H	1.4352670	2.9786530	1.5088620
C	1.4630780	4.9415450	0.5618390
H	2.1594250	5.7874540	0.4968540
H	0.5863850	5.3182400	1.1063820
C	1.0361570	4.5515240	-0.8589640
H	0.6934410	5.4516470	-1.3853410
H	1.9081850	4.1947600	-1.4232870
C	-0.0679830	3.4935270	-0.9146970
H	0.2275810	2.6254440	-0.3123050
H	-0.9787920	3.8927190	-0.4466950
C	-0.3944730	3.0491700	-2.3435630
H	0.5229090	2.7277320	-2.8551890
H	-0.7466060	3.9213510	-2.9075130
C	-1.4633630	1.9595540	-2.4748750
H	-2.3517000	2.2355860	-1.8931480
H	-1.7929750	1.9161000	-3.5218130
O	-2.5994780	-2.8493090	-2.1742160
H	-3.4296300	-2.5454910	-2.5641340
C	-2.3264820	-2.5119740	1.9482670
C	-3.5017030	-3.0321530	2.7158280
H	-4.4263860	-2.5557500	2.3899330
H	-3.3486410	-2.8401030	3.7849670
H	-3.5782300	-4.1190200	2.6046690
C	-1.0042180	-3.1822510	2.1279560
H	-0.9940880	-4.1057000	1.5349120
H	-0.8581620	-3.4787910	3.1706320
H	-0.1958020	-2.5311740	1.7916450
O	-2.4916660	-1.5441490	1.1920690
H	2.4983080	-3.3184870	0.8143280
H	-0.2693590	-0.2963840	1.1062590
C	-3.4803920	1.3333950	1.4401860
H	-3.4380770	0.5453590	2.2002660
C	-4.5833560	1.0287770	0.4485330
H	-5.5438650	0.9737410	0.9685280
H	-4.4067330	0.0689020	-0.0435470
H	-4.6506580	1.8132760	-0.3115790
C	-3.6226830	2.6921480	2.1039940
H	-4.5552780	2.7320480	2.6739690
H	-3.6431060	3.4929390	1.3585810
H	-2.8050280	2.8866370	2.8076350
O	-2.2165070	1.3045460	0.7047260
H	-1.5377870	1.7166030	1.2539280

intermediate-10

Ru	-1.2386170	-0.4803470	-0.1347210
H	3.5159760	-3.3596700	-1.5017220
C	-1.0792190	0.5422380	-2.1030030
C	0.2119320	0.2008280	-1.6200580
C	0.4896810	-1.1382260	-1.2205700
C	-0.5150460	-2.1307350	-1.3447260
C	-1.7495300	-1.8235890	-2.0115970
C	-2.0447060	-0.4975120	-2.3502140
H	0.9631520	0.9649930	-1.4745980
H	1.4504200	-1.3801820	-0.7764410
H	-0.3363770	-3.1499570	-1.0227290
H	-3.0039320	-0.2418460	-2.7923760
C	4.4531960	-0.9047660	-0.1720380
H	4.7700960	-1.3579310	-1.1114050
C	3.8493000	-1.6653880	0.7482000
H	3.5497600	-1.1997500	1.6883670
C	3.5742640	-3.1420230	0.6487490
H	4.0633300	-3.6374400	1.5014780
C	4.0049050	-3.8371400	-0.6415060
H	5.0823710	-3.6913910	-0.7866380
C	3.6896250	-5.3312060	-0.6389390
H	4.1978160	-5.8429450	0.1854640
H	4.0096690	-5.8073550	-1.5704150
H	2.6142750	-5.5147020	-0.5266590
C	4.8036630	0.5562300	-0.0291860
H	4.2369680	1.1432370	-0.7645090
H	5.8545550	0.6687590	-0.3415030
C	4.6606670	1.1293040	1.3507360
H	5.1204400	0.5334380	2.1393720
C	4.1064240	2.2956340	1.7040190
H	4.1501460	2.5664030	2.7603070
C	3.4532120	3.3196260	0.8212180
H	4.1316920	4.1797810	0.7115100
H	3.3113160	2.9211170	-0.1894860
C	2.1208230	3.8291140	1.3890050

H	2.2954610	4.2097790	2.4037020
H	1.4352670	2.9786530	1.5088620
C	1.4630780	4.9415450	0.5618390
H	2.1594250	5.7874540	0.4968540
H	0.5863850	5.3182400	1.1063820
C	1.0361570	4.5515240	-0.8589640
H	0.6934410	5.4516470	-1.3853410
H	1.9081850	4.1947600	-1.4232870
C	-0.0679830	3.4935270	-0.9146970
H	0.2275810	2.6254440	-0.3123050
H	-0.9787920	3.8927190	-0.4466950
C	-0.3944730	3.0491700	-2.3435630
H	0.5229090	2.7277320	-2.8551890
H	-0.7466060	3.9213510	-2.9075130
C	-1.4633630	1.9595540	-2.4748750
H	-2.3517000	2.2355860	-1.8931480
H	-1.7929750	1.9161000	-3.5218130
O	-2.5994780	-2.8493090	-2.1742160
H	-3.4296300	-2.5454910	-2.5641340
C	-2.3264820	-2.5119740	1.9482670
C	-3.5017030	-3.0321530	2.7158280
H	-4.4263860	-2.5557500	2.3899330
H	-3.3486410	-2.8401030	3.7849670
H	-3.5782300	-4.1190200	2.6046690
C	-1.0042180	-3.1822510	2.1279560
H	-0.9940880	-4.1057000	1.5349120
H	-0.8581620	-3.4787910	3.1706320
H	-0.1958020	-2.5311740	1.7916450
O	-2.4916660	-1.5441490	1.1920690
H	2.4983080	-3.3184870	0.8143280
H	-0.2693590	-0.2963840	1.1062590
C	-3.4803920	1.3333950	1.4401860
H	-3.4380770	0.5453590	2.2002660
C	-4.5833560	1.0287770	0.4485330
H	-5.5438650	0.9737410	0.9685280
H	-4.4067330	0.0689020	-0.0435470
H	-4.6506580	1.8132760	-0.3115790
C	-3.6226830	2.6921480	2.1039940
H	-4.5552780	2.7320480	2.6739690
H	-3.6431060	3.4929390	1.3585810
H	-2.8050280	2.8866370	2.8076350
O	-2.2165070	1.3045460	0.7047260
H	-1.5377870	1.7166030	1.2539280

intermediate-11

Ru	-1.0604990	0.2378370	-0.3668780
O	-0.3254690	1.6018020	-3.3579900
H	0.6313350	1.5325120	-3.4661540
C	-0.4825960	-1.7116150	-1.7110250
C	-1.8303790	-1.6307420	-1.2247130
C	-2.6747480	-0.5368380	-1.5633670
C	-2.1658240	0.5450070	-2.3410020
C	-0.8041130	0.5480160	-2.6777610
C	0.0335390	-0.5641100	-2.3290530
H	-2.2436320	-2.4666400	-0.6705880
H	-3.7174680	-0.5462330	-1.2673760
H	-2.7869660	1.3861550	-2.6258780
H	1.0697920	-0.5494990	-2.6535210
C	-0.4865900	-0.7302880	1.5344840
H	-0.7781250	-1.7740350	1.4181720
C	-1.5393010	0.1691300	1.8000030
H	-1.2350620	1.1385450	2.1986740
C	-2.9296230	-0.1972930	2.2896590
H	-2.8741770	-0.1107410	3.3866860
C	-3.4995220	-1.5747070	1.9599560
H	-2.7825210	-2.3562260	2.2429220
C	-4.8256720	-1.8292750	2.6759730
H	-4.7030050	-1.7893200	3.7632920
H	-5.2283220	-2.8145310	2.4242950
H	-5.5776330	-1.0822070	2.3999910
C	0.9165860	-0.6273290	2.1187430
H	1.6184160	-1.1478660	1.4637360
H	0.8800370	-1.2315940	3.0424360
C	1.4684430	0.7237840	2.4826480
H	0.7777760	1.4402750	2.9283440
C	2.7698550	1.0632230	2.4232850
H	3.0478180	2.0592600	2.7676710
C	3.8904970	0.1717430	1.9630710
H	4.7888110	0.4027530	2.5462510
H	3.6415870	-0.8665840	2.2022290
C	4.2208100	0.2911170	0.4570540

H	4.9041640	1.1330690	0.2987530
H	3.3070110	0.5483710	-0.0931300
C	4.8371050	-0.9824820	-0.1403580
H	5.7458800	-1.2396790	0.4178590
H	5.1656730	-0.7653130	-1.1651070
C	3.9047030	-2.2033590	-0.1579380
H	4.4664800	-3.0765830	-0.5104830
H	3.6016800	-2.4527030	0.8682860
C	2.6512250	-2.0230970	-1.0227060
H	2.2409160	-1.0208090	-0.8512270
H	2.9354950	-2.0678950	-2.0842450
C	1.5609660	-3.0530820	-0.7279320
H	1.2496360	-2.9620260	0.3195660
H	1.9748470	-4.0636640	-0.8296900
C	0.3129550	-2.9964420	-1.6277630
H	0.6129610	-3.2359070	-2.6567610
H	-0.3693480	-3.7956770	-1.3212110
H	-3.6410740	0.5769280	1.9764700
H	-2.1252760	1.2421640	0.1725970
C	-0.0111000	3.2594670	0.3239790
H	-0.5234480	3.2480320	1.2955720
C	-0.9458070	3.8039150	-0.7348680
H	-1.1820070	4.8457100	-0.4996030
H	-1.8846990	3.2471950	-0.7688360
H	-0.4803120	3.7705200	-1.7235030
C	1.2765680	4.0610540	0.4257490
H	1.0491810	5.0898630	0.7190740
H	1.7935790	4.0864820	-0.5383790
H	1.9565230	3.6452850	1.1746310
H	-3.6545520	-1.6667580	0.8787660
O	0.3383770	1.8714400	-0.0016720
H	0.9988490	1.5838220	0.6626730

intermediate-12

Ru	-0.9598970	-0.1566660	0.4363920
O	-0.2003340	-1.9357950	3.1881800
H	0.7540630	-1.8544260	3.3091740
C	-0.4055420	1.5269320	1.8366350
C	-1.7955760	1.5367900	1.5176270
C	-2.5985980	0.3805350	1.7466570
C	-2.0845910	-0.7776090	2.3906570
C	-0.7090590	-0.8118110	2.6633060
C	0.1306980	0.2939580	2.3023380
H	-2.2447280	2.4267020	1.0900830
H	-3.6477160	0.4042180	1.4694940
H	-2.7071890	-1.6331250	2.6217650
H	1.1971640	0.2140410	2.4865200
C	-0.5380130	0.7626580	-1.4042820
H	-0.8173390	1.8148330	-1.3060910
C	-1.6964830	-0.0991190	-1.7749510
H	-1.3753840	-0.9687080	-2.3574110
C	-2.9462760	0.5174360	-2.4229550
H	-2.6341460	0.8649060	-3.4170870
C	-3.6265340	1.6663510	-1.6826160
H	-2.9062790	2.4723740	-1.4946800
C	-4.8167480	2.2275170	-2.4595130
H	-4.5043420	2.6220580	-3.4319410
H	-5.2982920	3.0420950	-1.9111690
H	-5.5730590	1.4567590	-2.6415450
C	0.7388850	0.6947330	-2.2474780
H	1.4759490	1.3610750	-1.7935660
H	0.4906400	1.1556820	-3.2200280
C	1.3678490	-0.6414720	-2.5357860
H	0.7119410	-1.4060530	-2.9567040
C	2.6772250	-0.9450470	-2.4463300
H	2.9796220	-1.9504980	-2.7420140
C	3.7826400	-0.0270080	-2.0140970
H	4.6141840	-0.1236510	-2.7229410
C	3.4446830	1.0088440	-2.0935190
H	4.3045310	-0.2953080	-0.5850060
H	5.0381280	-1.1092930	-0.6060080
H	3.4786400	-0.6600630	0.0383440
C	4.9363980	0.9379910	0.0780270
H	5.8087120	1.2571210	-0.5058500
H	5.3246550	0.6419340	1.0612110
C	3.9922510	2.1388910	0.2446820
H	4.5452560	2.9635210	0.7102210
H	3.6954780	2.5154780	-0.7435280
C	2.7312670	1.8464000	1.0656350
H	2.3239910	0.8740500	0.7670030
H	3.0030120	1.7655000	2.1284610

C	1.6411340	2.9006690	0.8761640
H	1.3049420	2.8836410	-0.1674510
H	2.0674160	3.8987000	1.0376640
C	0.4150280	2.7989700	1.7968820
H	0.7373500	2.9744960	2.8327810
H	-0.2624790	3.6237130	1.5533850
H	-3.6805240	-0.2789190	-2.5993660
H	-2.1366610	-0.6778930	-0.8134560
C	-0.1712530	-3.1911700	-0.5969890
H	-0.5772230	-3.0602200	-1.6099120
C	-1.2630050	-3.7000960	0.3196140
H	-1.5928970	-4.6835640	-0.0271650
H	-2.1305810	-3.0351190	0.3206090
H	-0.8956020	-3.8001950	1.3446330
C	1.0332700	-4.1172580	-0.6450550
H	0.7387830	-5.0911500	-1.0466890
H	1.4437560	-4.2690190	0.3577200
H	1.8239100	-3.7189310	-1.2877960
H	-3.9681910	1.3142100	-0.7004630
O	0.2779150	-1.8788920	-0.1283140
H	0.9681920	-1.5679330	-0.7518540

intermediate-13

Ru	-1.0396320	0.7606410	0.2513140
O	1.7493620	2.7869090	0.5115140
H	2.5681590	2.3209050	0.1765250
C	-0.4836670	1.0027220	-1.8975800
C	-1.6924550	1.7073130	-1.6226140
C	-1.7348260	2.6529740	-0.5624750
C	-0.5679000	3.0394190	0.1658240
C	0.6536510	2.4148310	-0.1287530
C	0.6273680	1.3029110	-1.0483220
H	-2.5925690	1.4887140	-2.1876030
H	-2.6806340	3.1230970	-0.3135860
H	-0.6103190	3.8012270	0.9353770
H	1.5481510	0.7397480	-1.1684990
C	-1.9873170	-1.0060980	0.5992820
H	-2.5351820	-1.5845320	-0.1395280
C	-2.7244910	-0.2108210	1.6182980
H	-2.4670870	-0.5044440	2.6421650
C	-4.2406030	-0.0634210	1.4817220
H	-4.6643740	-1.0563150	1.6831220
C	-4.7724350	0.4494070	0.1451950
H	-4.3881030	-0.1680910	-0.6765300
C	-6.2995530	0.4625810	0.1016400
H	-6.7085250	-0.5443200	0.2357630
H	-6.6656250	0.8440480	-0.8557460
H	-6.7143520	1.0965710	0.8923600
C	-0.6125700	-1.4267460	0.9880060
H	0.0277350	-0.4080590	1.1524370
H	-0.1351520	-1.9457050	0.1608060
C	-0.2925610	-2.1151880	2.2885160
H	-0.6065420	-1.6349860	3.2122630
C	0.3884040	-3.2689590	2.3366090
H	0.5874110	-3.6890870	3.3211000
C	0.8868950	-4.0453760	1.1416010
H	1.1103630	-5.0731520	1.4447140
H	0.0726350	-4.1285250	0.4121290
C	2.1331550	-3.4392330	0.4562680
H	3.0249640	-3.7143910	1.0308810
H	2.0837900	-2.3443340	0.5104670
C	2.3202300	-3.8783170	-1.0044700
H	2.3749080	-4.9735180	-1.0443220
H	3.2953710	-3.5172740	-1.3564470
C	1.2274540	-3.4085070	-1.9772260
H	1.3766100	-3.9024570	-2.9448050
H	0.2483350	-3.7635020	-1.6260850
C	1.1590500	-1.8892050	-2.1975370
H	1.3353030	-1.3768430	-1.2448020
H	1.9747400	-1.5758560	-2.8633070
C	-0.1870030	-1.4496550	-2.7801730
H	-0.9973930	-1.7726070	-2.1140170
H	-0.3482650	-1.9805570	-3.7267090
C	-0.3676850	0.0505510	-3.0704200
H	0.4631190	0.4010570	-3.6972890
H	-1.2717810	0.1705180	-3.6763280
H	-4.6022540	0.5852340	2.2885040
H	-2.2397920	0.8863330	1.6536310
C	5.0361930	1.4019520	0.5004370
H	5.7265590	0.7119720	-0.0031990
C	4.4717390	0.7305110	1.7374380

H	5.2821990	0.4734420	2.4246520
H	3.9453400	-0.1915230	1.4753390
H	3.7801270	1.3960760	2.2642120
C	5.7459550	2.7131090	0.7967450
H	6.6030780	2.5413880	1.4543540
H	5.0718860	3.4199280	1.2910270
H	6.1275390	3.1790110	-0.1189760
H	-4.3936560	1.4650080	-0.0266730
O	3.9203620	1.6226980	-0.4073690
H	4.2571440	2.1002200	-1.1764660

intermediate-14

Ru	-1.5614030	-0.2765380	0.4961220
O	0.9684290	-2.7233680	0.2662330
H	1.9233900	-2.4290540	0.2201690
C	-0.2107290	0.1885060	2.2685090
C	-1.4549520	-0.3506540	2.6943810
C	-1.9167440	-1.6049430	2.2137510
C	-1.1244600	-2.3053860	1.2746880
C	0.2229600	-1.8957130	0.9855140
C	0.6228390	-0.6177010	1.4116020
H	-2.0795970	0.2295350	3.3641170
H	-2.8919870	-1.9830540	2.4955340
H	-1.4800020	-3.2341660	0.8399830
H	1.5956170	-0.2466830	1.1054020
C	-2.0866680	0.9720250	-1.1552630
H	-2.8057440	1.7594010	-0.9554280
C	-2.5665420	-0.3355730	-1.6884760
H	-1.9108610	-0.7169640	-2.4760200
C	-4.0364340	-0.4265260	-2.1146610
H	-4.1650890	0.2803330	-2.9455280
C	-5.0839510	-0.1512770	-1.0375090
H	-4.9357280	0.8485300	-0.6098450
C	-6.5077510	-0.2629780	-1.5799520
H	-6.6861740	0.4587880	-2.3839380
H	-7.2433350	-0.0716280	-0.7938350
H	-6.7031420	-1.2629110	-1.9818080
C	-0.7149780	1.2440940	-1.0805870
H	-2.9555740	0.3686950	0.8072080
H	-0.4579990	2.2157520	-0.6688630
C	0.3234210	0.5757830	-1.8705140
H	0.1547490	-0.4644330	-2.1397920
C	1.4342610	1.1647340	-2.3588520
H	2.0801910	0.5429060	-2.9790640
C	1.8969320	2.5746790	-2.1700920
H	1.9941400	3.0474750	-3.1559320
H	1.1375920	3.1557900	-1.6409250
C	3.2531300	2.6551310	-1.4239230
H	4.0727660	2.7101080	-2.1485830
H	3.4132760	1.7230390	-0.8686320
C	3.3609140	3.8368630	-0.4498890
H	3.4048430	4.7790350	-1.0099880
H	4.3197040	3.7543230	0.0772190
C	2.2195650	3.9287840	0.5746490
H	2.4773240	4.6837670	1.3275990
H	1.3129190	4.3111650	0.0853400
C	1.8833360	2.6068250	1.2694010
H	1.7375920	1.8305300	0.5099090
H	2.7378730	2.2842330	1.8817090
C	0.6323260	2.6981490	2.1390510
H	-0.2356680	2.9715380	1.5255240
H	0.7580990	3.5168370	2.8588080
C	0.2911990	1.4454610	2.9555460
H	1.1788620	1.1456680	3.5315370
H	-0.4618490	1.7242490	3.6993970
H	-4.2070830	-1.4238890	-2.5370240
H	-2.4471080	-1.1692640	-0.8554670
C	4.4371000	-2.6252000	-0.6697010
H	5.3605930	-2.0321490	-0.6260240
C	3.8064050	-2.4659560	-2.0392430
H	4.5014230	-2.8028840	-2.8127990
H	3.5630180	-1.4176310	-2.2306400
H	2.8920440	-3.0628040	-2.1215230
C	4.7382800	-4.0711570	-0.3095900
H	5.4520450	-4.4996480	-1.0191940
H	3.8267960	-4.6769220	-0.3329020
H	5.1845030	-4.1523060	0.6882020
H	-4.9461050	-0.8597730	-0.2101700
O	3.5126270	-2.0433570	0.2901120
H	3.8702010	-2.2019020	1.1730880

intermediate-14'

Ru	-1.1569490	-0.5500280	-0.1207030
O	1.1339900	-3.0229470	0.2749920
H	2.0561930	-2.6253440	0.3327400
C	-0.5549510	-0.2677690	2.1057550
C	-1.8715450	-0.8005710	2.1202540
C	-2.1730970	-1.9419540	1.3547910
C	-1.1547070	-2.6569440	0.6604520
C	0.2018350	-2.2550270	0.7899740
C	0.4529190	-0.9671960	1.3609040
H	-2.6527960	-0.2977820	2.6803570
H	-3.1934120	-2.3085190	1.3078450
H	-1.3815560	-3.5615280	0.1084750
H	1.4692800	-0.5916020	1.3486440
C	-2.0785690	1.2076690	-0.8228870
H	-2.6736750	1.7349170	-0.0820900
C	-2.7242760	0.2114350	-1.6915040
H	-2.3262130	0.2214640	-2.7096890
C	-4.2498520	0.1012160	-1.7065770
H	-4.6084760	0.9789940	-2.2610060
C	-4.9645340	0.0286460	-0.3592440
H	-4.7152730	0.9048000	0.2520190
C	-6.4817310	-0.0553020	-0.5195440
H	-6.8740500	0.8226920	-1.0430210
H	-6.9785960	-0.1098050	0.4530900
H	-6.7735850	-0.9415360	-1.0927190
C	-0.7028590	1.5094340	-0.9839480
H	-0.2373410	0.8229920	-1.3566150
H	-0.3158320	2.1869680	-0.2292170
C	0.0526060	1.5077060	-2.2440340
H	-0.2953200	0.8421490	-3.0310810
C	1.1218120	2.2829240	-2.5078840
H	1.5731670	2.1797410	-3.4939930
C	1.7688470	3.2697810	-1.5817440
H	2.0194200	4.1791740	-2.1417560
H	1.0505980	3.5835820	-0.8194600
C	3.0428790	2.7282360	-0.8975810
H	3.8870650	2.7851390	-1.5945590
H	2.9048790	1.6607870	-0.6882140
C	3.4109660	3.4591670	0.4026760
H	3.6951030	4.4942750	0.1758950
H	4.3082580	2.9855910	0.8217940
C	2.3003730	3.4829620	1.4650200
H	2.6821230	3.9690830	2.3708890
H	1.4797480	4.1258060	1.1190230
C	1.7339320	2.1037760	1.8237860
H	1.6174890	1.5144660	0.9085190
H	2.4544810	1.5616220	2.4528350
C	0.3819920	2.1868600	2.5307840
H	-0.3495290	2.6718330	1.8711010
H	0.4710290	2.8474320	3.4023220
C	-0.2040370	0.8661040	3.0516910
H	0.5016290	0.4354730	3.7764330
H	-1.1080560	1.1016410	3.6228400
H	-4.5285270	-0.7683090	-2.3138130
H	-2.3102640	-0.9201340	-1.3955350
C	4.4232460	-2.1434800	-0.7240630
H	5.2117870	-1.3909210	-0.5907000
C	3.6058050	-1.8013270	-1.9547320
H	4.2530280	-1.7848680	-2.8357050
H	3.1405190	-0.8167550	-1.8564480
H	2.8219720	-2.5464450	-2.1247670
C	5.0404520	-3.5314460	-0.7778790
H	5.7304080	-3.6073910	-1.6232950
H	4.2683660	-4.2982130	-0.8972680
H	5.6140840	-3.7528990	0.1294340
H	-4.6056650	-0.8473860	0.1952710
O	3.5339600	-2.0284890	0.4238690
H	4.0146790	-2.3318610	1.2046640

intermediate-15'

Ru	-0.8800870	-0.4240580	0.4922020
O	1.4368460	-2.8046750	0.0730630
H	2.3661090	-2.4397990	0.0088310
C	0.3113120	-0.1153210	2.3866610
C	-0.9971340	-0.6142620	2.6511820
C	-1.4489190	-1.8316230	2.0509580
C	-0.6135830	-2.6050080	1.2118610
C	0.6743140	-2.1084270	0.9007370

C	1.0780800	-0.8281520	1.4217630
H	-1.6599550	-0.0679980	3.3151350
H	-2.4632830	-2.1680550	2.2423720
H	-0.9489060	-3.5364920	0.7720920
H	2.0434000	-0.4379460	1.1125100
C	-2.7209530	0.8195300	-0.3101150
H	-3.3138880	1.2378520	0.5077570
C	-3.5268460	0.7782190	-1.6208280
H	-3.6387700	1.8215640	-1.9408580
C	-4.9086400	0.1311850	-1.5084220
H	-5.4882520	0.6392290	-0.7246860
C	-4.9057550	-1.3773510	-1.2475550
H	-4.4297250	-1.5965790	-0.2807880
C	-6.3102700	-1.9773870	-1.2513410
H	-6.9405570	-1.5193100	-0.4814430
H	-6.2845180	-3.0546820	-1.0628820
H	-6.8026860	-1.8213660	-2.2169410
C	-1.3483370	1.4000030	-0.3421850
H	-2.6321480	-0.3460310	-0.0503460
H	-1.1635090	2.3720070	0.1011120
C	-0.4547260	0.8681400	-1.3507670
H	-0.6147880	-0.2506560	-1.5171620
C	0.5294600	1.4109110	-2.1000590
H	1.1918850	0.7321820	-2.6361600
C	0.7940070	2.8721120	-2.2807130
H	0.7512040	3.1052300	-3.3518020
H	0.0001950	3.4593070	-1.8090660
C	2.1905930	3.2796920	-1.7230010
H	2.8169210	3.6429360	-2.5442280
H	2.7020610	2.3897970	-1.3356330
C	2.1596160	4.3570670	-0.6294210
H	1.8143060	5.3029230	-1.0651930
H	3.1939130	4.5347980	-0.3077140
C	1.2980010	4.0494650	0.6014540
H	1.4415360	4.8556630	1.3322880
H	0.2344240	4.0976830	0.3283230
C	1.5786390	2.7027270	1.2701690
H	1.4161230	1.8949990	0.5459850
H	2.6370170	2.6502570	1.5637960
C	0.7031900	2.4624010	2.5001600
H	-0.3542520	2.6128560	2.2477090
H	0.9415910	3.2099510	3.2665420
C	0.8696190	1.0745300	3.1389030
H	1.9358470	0.8892540	3.3164100
H	0.3937920	1.0828550	4.1254300
H	-5.4455090	0.3239690	-2.4456990
H	-2.9342520	0.2803460	-2.3977080
C	4.7423620	-2.1409750	-1.1729750
H	5.6684190	-1.5698780	-1.0229950
C	3.9826660	-1.5571910	-2.3481050
H	4.5907760	-1.6198270	-3.2543340
H	3.7446930	-0.5048150	-2.1697170
H	3.0531140	-2.1083010	-2.5262170
C	5.0700730	-3.6161440	-1.3385490
H	5.7154180	-3.7668330	-2.2088960
H	4.1592550	-4.2062430	-1.4819790
H	5.6042450	-4.0089230	-0.4661220
H	-4.2909480	-1.8749540	-2.0104670
O	3.9186890	-1.9301310	0.0073600
H	4.3886180	-2.3048220	0.7636140

intermediate-15

Ru	0.1692910	-0.3867000	0.3437290
O	-2.1741510	-2.6438070	0.6429420
H	-2.2575550	-3.1240530	-0.1905590
C	1.5207590	-2.2333940	0.1959080
C	1.7876720	-1.5692400	1.4103280
C	0.7328910	-1.2827660	2.3373560
C	-0.5994940	-1.6555950	2.1042340
C	-0.9001050	-2.2770200	0.8605940
C	0.1407560	-2.4966430	-0.0943420
H	2.7996680	-1.2640200	1.6492220
H	0.9718800	-0.7413550	3.2465920
H	-1.3881900	-1.4733640	2.8248010
H	-0.1142000	-2.9500900	-1.0505300
C	-3.0126100	0.5516030	-0.0526980
H	-3.1685660	0.7966760	1.0062400
C	-3.9652000	1.4112060	-0.9043690
H	-3.6600800	2.4629580	-0.8244670
C	-5.4400750	1.2873360	-0.5078100
H	-5.5586330	1.5682460	0.5484920

C	-6.0569100	-0.0938450	-0.7393610
H	-5.5393420	-0.8449910	-0.1277510
C	-7.5499150	-0.1345380	-0.4200390
H	-7.7392590	0.1273020	0.6267830
H	-7.9691070	-1.1302630	-0.5935140
H	-8.1072610	0.5732870	-1.0429650
C	-1.5738890	0.7907090	-0.4210790
H	-3.2571610	-0.5091550	-0.1637530
H	-1.2036420	1.7966810	-0.2191150
C	-0.9182500	0.0813030	-1.4486810
H	-1.4111750	-0.7866280	-1.8878580
C	0.4686700	0.3246420	-1.7057760
H	0.9329690	-0.4335880	-2.3391920
C	1.0362760	1.7212070	-1.9550170
H	0.3087460	2.2401950	-2.5939330
H	1.0867690	2.3126800	-1.0358470
C	2.3969300	1.7485320	-2.6754930
H	2.4551180	2.6813240	-3.2481650
C	2.4216280	0.9488700	-3.4276320
H	3.6398710	1.6823220	-1.7798910
H	3.6499170	2.5769030	-1.1416970
H	4.5340330	1.7659650	-2.4114550
C	3.7559370	0.4380890	-0.8954650
H	4.5417090	0.6016710	-0.1446690
H	2.8181660	0.3081190	-0.3417690
C	4.0797580	-0.8492700	-1.6558320
H	3.4340350	-0.9441350	-2.5390160
H	5.1014180	-0.7715430	-2.0473910
C	3.9676730	-2.1347620	-0.8243850
H	4.3783780	-1.9779150	0.1818370
H	4.6113930	-2.8966790	-1.2774330
C	2.5689720	-2.7645020	-0.7521460
H	2.1397280	-2.7952000	-1.7614080
H	2.6825880	-3.8191350	-0.4586700
H	-6.0117650	2.0288840	-1.0806080
H	-3.8437300	1.1387470	-1.9618040
H	-5.8977850	-0.3871120	-1.7866170
C	2.3115540	1.9836910	2.9889520
H	1.5665260	2.1329010	3.7795420
H	3.1927510	2.5740370	3.2569280
H	2.6097490	0.9328600	2.9762500
C	1.7807090	2.4328170	1.6382460
H	2.5086330	2.2049270	0.8570990
C	1.4241550	3.9102430	1.6053320
H	0.6699020	4.1520550	2.3638990
H	1.0382250	4.2033730	0.6257220
H	2.3086250	4.5169680	1.8198980
O	0.6044430	1.6616200	1.2426840
H	-0.1030210	1.8431280	1.8740230

intermediate-15"

Ru	-1.3680070	-0.3157810	0.0701750
O	-3.3994680	-1.1845970	2.5606050
H	-3.3438800	-0.5073680	3.2466940
C	-2.8324290	1.2614870	-0.2089610
C	-3.0512090	0.3936230	-1.3267620
C	-3.1763460	-0.9835310	-1.0889740
C	-3.2325160	-1.5282020	0.2340730
C	-3.2334240	-0.6519780	1.3435390
C	-2.9488130	0.7257130	1.1173710
H	-3.0059190	0.7728460	-2.3406460
H	-3.2037820	-1.6691600	-1.9299200
H	-3.3445280	-2.5928620	0.4006120
H	-2.8224490	1.3936330	1.9663120
C	3.2362520	-1.1235590	1.5149200
H	3.9439400	-1.3321040	2.3301590
C	3.9404950	-1.4346790	0.1825870
H	4.0780270	-2.5213850	0.1052260
C	5.3004530	-0.7503260	0.0134620
H	5.9631800	-1.0567830	0.8346460
C	5.2511710	0.7777550	-0.0551430
H	4.8471210	1.1824530	0.8825080
C	6.6198020	1.4024210	-0.3181710
H	7.3321860	1.1411460	0.4716640
H	6.5602330	2.4941510	-0.3622550
H	7.0383190	1.0536320	-1.2684110
C	2.0246400	-1.9731330	1.7683010
H	3.0012530	-0.0587690	1.5917760
H	0.6493770	-2.0238420	-0.2200050
C	0.7206480	-1.6342750	1.8700440
H	0.0489740	-2.4279090	2.2031540

C	0.0163180	-0.3492380	1.6479870
H	-0.4951730	-0.0111700	2.5547750
C	0.5521610	0.7536860	0.8035840
H	1.4993820	0.4948140	0.3210360
H	-0.0753970	0.8598460	-0.2329320
C	0.5507700	2.1689880	1.3863370
H	1.0631390	2.1213730	2.3550530
H	-0.4810510	2.4606230	1.6121700
C	1.2571670	3.2300490	0.5340930
H	2.3286450	2.9905710	0.5364840
H	1.1731840	4.1923450	1.0549110
C	0.8413660	3.4244180	-0.9324460
H	1.6225960	4.0530920	-1.3747420
H	0.9113540	2.4725340	-1.4788020
C	-0.5161550	4.0926820	-1.2469800
H	-0.7965650	4.7831560	-0.4400730
H	-0.3630670	4.7277560	-2.1259180
C	-1.6935220	3.1532290	-1.5753350
H	-1.2883420	2.2612470	-2.0694090
H	-2.3304420	3.6406800	-2.3200850
C	-2.5737890	2.7391470	-0.3760990
H	-2.1443100	3.1176180	0.5569830
H	-3.5574230	3.2220270	-0.4527330
H	5.7661750	-1.1297110	-0.9052740
H	3.2809760	-1.1507240	-0.6503540
H	4.5522640	1.0795920	-0.8489790
C	-0.6595380	-3.8589170	-1.5384370
H	0.0792310	-4.3817740	-0.9209380
H	-0.8938010	-4.5048780	-2.3895470
H	-1.5692510	-3.7274340	-0.9469560
C	-0.1167440	-2.5249670	-2.0228440
H	-0.8592310	-2.0145960	-2.6432850
C	1.1855010	-2.6511580	-2.7956630
H	1.9598100	-3.1327520	-2.1891270
H	1.5484770	-1.6704600	-3.1131250
H	1.0325010	-3.2657600	-3.6877500
O	0.0818960	-1.6124870	-0.9054240
H	2.2536160	-3.0200520	1.9750610

intermediate-16

Ru	0.9751010	-0.9233350	-0.1456300
O	-0.0922050	-2.4518430	-2.9450470
H	-0.2771580	-1.8299420	-3.6608000
C	2.6227610	-0.3682590	-1.4789860
C	3.1149870	-1.3086250	-0.5080560
C	2.4624040	-2.5398630	-0.3178530
C	1.2948110	-2.8536430	-1.0832720
C	0.9386260	-2.0362780	-2.1943930
C	1.5769860	-0.7907580	-2.3535620
H	3.9308070	-1.0236760	0.1488440
H	2.7743000	-3.2064940	0.4794900
H	0.7240840	-3.7568330	-0.8953180
H	1.2122280	-0.0936140	-3.1031740
C	-3.6160710	-0.6002080	0.9511910
H	-4.0719110	-0.9093360	1.9003480
C	-4.1609580	0.7745350	0.5598430
H	-3.8206280	1.5088880	1.3030540
C	-5.6897400	0.8405960	0.4671180
H	-6.1245380	0.5159690	1.4230080
C	-6.3033120	0.0246520	-0.6731550
H	-6.0620970	-1.0391030	-0.5492580
C	-7.8193700	0.1853960	-0.7633470
H	-8.3083410	-0.1453560	0.1594650
H	-8.2358560	-0.4018170	-1.5873950
H	-8.0980610	1.2322170	-0.9267580
C	-2.0850070	-0.6570980	1.1342470
H	-3.9177350	-1.3535840	0.2121510
H	-1.7561560	0.0899480	1.8611730
C	-1.3795710	-0.4648580	-0.1791990
H	-1.6637780	-1.1792200	-0.9550080
C	-0.7263230	0.6745010	-0.6072200
H	-0.5874870	0.7642880	-1.6842500
C	-0.4961710	1.9700150	0.1460620
H	-1.4543940	2.3081750	0.5625610
H	0.1507340	1.8037430	1.0132550
C	0.0717360	3.0514910	-0.7880060
H	-0.7453000	3.4145800	-1.4240840
H	0.7880010	2.5876130	-1.4796450
C	0.7409130	4.2570630	-0.1177450
H	0.0655340	4.6802740	0.6368670
H	0.8532060	5.0346490	-0.8839550

C	2.1230110	4.0273330	0.5196080
H	2.5030290	5.0073030	0.8288070
H	2.0301960	3.4467870	1.4478180
C	3.1523650	3.3444460	-0.4029260
H	2.9556410	3.6384530	-1.4429230
H	4.1563240	3.7187100	-0.1784150
C	3.1322570	1.8073760	-0.2689810
H	2.2016290	1.5161610	0.2294410
H	3.9359770	1.4853700	0.4038610
C	3.2093760	1.0194470	-1.5910790
H	2.6636930	1.5599250	-2.3722470
H	4.2465480	0.9393490	-1.9412070
H	-5.9859220	1.8907800	0.3456970
H	-3.7308570	1.0871790	-0.4029670
H	-5.8445170	0.3333870	-1.6233020
C	1.0007140	-2.3568690	3.3544990
H	0.0075220	-2.1574890	3.7675490
H	1.6385450	-2.7343320	4.1594620
H	0.9050280	-3.1383270	2.5936420
C	1.5951720	-1.0864400	2.7563520
H	2.5956980	-1.3100800	2.3554600
C	1.7083250	0.0416590	3.7744880
H	0.7232920	0.2890010	4.1811440
H	2.1314130	0.9405690	3.3176000
H	2.3572640	-0.2592340	4.6025000
O	0.7477330	-0.6388490	1.6980050
H	-1.8221190	-1.6362990	1.5477540

intermediate-17

Ru	3.2370660	-0.3077260	-0.2580200
O	1.5451800	-2.4822760	-2.1219870
H	0.5953710	-2.3032300	-2.0929070
C	2.4496200	1.0943360	-1.7684490
C	3.8661300	0.9698920	-1.9014020
C	4.4719160	-0.3074650	-2.0316740
C	3.6705090	-1.4760580	-2.0741340
C	2.2494360	-1.3458680	-2.0517120
C	1.6466400	-0.0836040	-1.8434530
H	4.4885870	1.8543990	-1.8220300
H	5.5532730	-0.3979060	-2.0257570
H	4.1107200	-2.4640240	-2.1383560
H	0.5706510	-0.0134620	-1.7241450
C	-7.3865840	-0.0703890	1.1775430
H	-8.3907520	0.3615480	1.2798690
C	-7.0265630	-0.1653970	-0.3059850
H	-6.9299250	0.8538480	-0.7062390
C	-8.0385160	-0.9361450	-1.1602550
H	-9.0288650	-0.4692420	-1.0597770
C	-8.1508730	-2.4281310	-0.8384840
H	-8.4804400	-2.5637220	0.1992670
C	-9.1119530	-3.1649480	-1.7689490
H	-10.1234020	-2.7488500	-1.7032230
H	-9.1757500	-4.2290930	-1.5203300
H	-8.7922400	-3.0860980	-2.8142950
C	-6.3998030	0.7783560	1.9966730
H	-7.4409580	-1.0744790	1.6179720
H	-6.3572730	1.7917740	1.5814060
C	-5.0300310	0.1700310	2.0819150
H	-5.0164190	-0.8584770	2.4484760
C	-3.8500950	0.7258080	1.7806860
H	-2.9572960	0.1121390	1.9224680
C	-3.5834610	2.1097820	1.2632280
H	-4.5078030	2.6950140	1.2132350
H	-2.9313400	2.6351620	1.9768780
C	-2.9196360	2.1022480	-0.1225690
H	-3.6141120	1.6375960	-0.8332410
H	-2.0368340	1.4472360	-0.0898990
C	-2.5285400	3.4970590	-0.6324630
H	-3.3984580	4.1548990	-0.5160330
H	-2.3441160	3.4517140	-1.7148530
C	-1.3100880	4.1397290	0.0593640
H	-1.4846650	5.2145660	0.1808210
H	-1.2048800	3.7436990	1.0786340
C	0.0204490	3.9796380	-0.6863960
H	-0.0664040	4.4494990	-1.6761160
H	0.7968940	4.5429650	-0.1507840
C	0.4923920	2.5342750	-0.8654130
H	-0.2662280	1.9812690	-1.4320050
H	0.5720240	2.0473430	0.1163090
C	1.8376540	2.4620180	-1.5897470
H	1.7286420	2.8837500	-2.6001630

H	2.5687260	3.1020980	-1.0818570
H	-7.7630850	-0.8258210	-2.2182550
H	-6.0334270	-0.6249990	-0.4091980
H	-7.1534730	-2.8863020	-0.9019740
C	4.6190580	2.1619640	1.4773520
H	5.4695430	2.2554190	2.1600660
H	3.9169890	2.9709460	1.6974370
H	4.9936520	2.2689230	0.4585630
C	3.9907960	0.7885970	1.6901520
H	2.8958850	0.8347100	1.1023000
C	3.5401110	0.5633000	3.1328810
H	4.4381330	0.4507970	3.7490250
H	2.9281700	-0.3339360	3.2367050
H	2.9709100	1.4184400	3.5068170
O	4.7063110	-0.2431540	1.1442370
H	-6.7967530	0.8820850	3.0168480
C	1.4943240	-3.5633960	2.3271030
H	2.1187570	-3.5389020	3.2262130
H	1.0956520	-4.5771130	2.2241340
H	0.6553870	-2.8768040	2.4664040
C	2.2999150	-3.1949030	1.0934940
H	1.6583670	-3.2017950	0.2092040
C	3.5053520	-4.0893060	0.8651900
H	4.1630220	-4.0970240	1.7421450
H	4.0874560	-3.7636970	-0.0010890
C	3.1812300	-5.1185970	0.6881810
O	2.7241840	-1.8006870	1.2253310
H	3.5916030	-1.7479290	1.6784140

intermediate-18

Ru	3.3103480	-0.4870630	-0.2005800
O	1.6395260	-2.4762520	-2.4106180
H	0.6997720	-2.2573470	-2.3636860
C	2.6314560	1.0321210	-1.6673600
C	4.0416880	0.8724380	-1.7658590
C	4.5972400	-0.4178940	-1.9887890
C	3.7914670	-1.5530860	-2.2630580
C	2.3970240	-1.4009790	-2.1923770
C	1.8316000	-0.1470850	-1.7731140
H	4.6927560	1.7269610	-1.6189720
H	5.6759790	-0.5374450	-1.9799610
H	4.2222180	-2.5216160	-2.4870700
H	0.7561870	-0.0704750	-1.6446230
C	-7.4005270	0.0697360	1.0999740
H	-8.3834010	0.5413540	1.2295730
C	-7.0726450	-0.0122410	-0.3917770
H	-6.9478090	1.0094580	-0.7774530
C	-8.1276170	-0.7327240	-1.2379120
H	-9.0999010	-0.2364960	-1.1062640
C	-8.2811450	-2.2266350	-0.9432170
H	-8.5915100	-2.3731190	0.0990100
C	-9.2863770	-2.9129190	-1.8656420
H	-10.2821090	-2.4662800	-1.7681150
H	-9.3788710	-3.9794280	-1.6370450
H	-8.9878460	-2.8225750	-2.9162770
C	-6.3636640	0.8600780	1.9151530
H	-7.4893400	-0.9393400	1.5231370
H	-6.2831180	1.8779750	1.5168970
C	-5.0209430	0.1909110	1.9657100
H	-5.0487410	-0.8481820	2.3004100
C	-3.8209940	0.7046100	1.6691110
H	-2.9547030	0.0481640	1.7827260
C	-3.4961230	2.0907840	1.1930750
H	-4.4001570	2.7059200	1.1313690
H	-2.8495640	2.5790680	1.9376570
C	-2.7916700	2.0956490	-0.1724280
H	-3.4752030	1.6636130	-0.9136810
H	-1.9251550	1.4196940	-0.1290460
C	-2.3515100	3.4909370	-0.6388000
H	-3.2104220	4.1659630	-0.5397110
H	-2.1296950	3.4623370	-1.7146230
C	-1.1442340	4.0908070	0.1089170
H	-1.3028550	5.1653130	0.2533310
H	-1.0801300	3.6669070	1.1203150
C	0.2072990	3.9239130	-0.5963290
H	0.1619410	4.4202570	-1.5758560
H	0.9743890	4.4592930	-0.0202920
C	0.6622590	2.4755290	-0.7952660
H	-0.0820150	1.9492570	-1.4054320
H	0.7029730	1.9630080	0.1751950
C	2.0329050	2.4010250	-1.4676080

H	1.9692160	2.8533460	-2.4686580
H	2.7530530	3.0109990	-0.9103840
H	-7.8717370	-0.6099120	-2.2993560
H	-6.0985150	-0.5042780	-0.5227570
H	-7.3008590	-2.7150200	-1.0392350
C	6.1029130	0.7862630	0.9720930
H	6.9309810	0.7173440	1.6904270
H	5.8061230	1.8367770	0.9287780
H	6.4727440	0.4527220	0.0031770
C	4.9873500	-0.0936700	1.4797100
H	2.7944480	0.5554100	0.8639050
C	4.4591850	0.2556000	2.8485510
H	5.2595580	0.0412320	3.5700150
H	3.5887690	-0.3415500	3.1148520
H	4.2179390	1.3172340	2.9346560
O	4.8523550	-1.2803180	1.0227240
H	-6.7375900	0.9631860	2.9441300
C	0.8858470	-1.1727850	2.7777150
H	1.5113840	-1.5569940	3.5916210
H	-0.1458330	-1.1560460	3.1410450
H	1.1834630	-0.1455270	2.5508190
C	0.9842340	-2.0546290	1.5473430
H	0.3400340	-1.6575610	0.7570810
C	0.6431320	-3.5110740	1.8133500
H	1.2997070	-3.9343130	2.5819860
H	0.7405550	-4.1108170	0.9051180
H	-0.3850160	-3.5949780	2.1769420
O	2.3143050	-2.0020040	0.9488780
H	2.9942030	-2.3222250	1.5649740

intermediate-19

Ru	3.1958470	-0.3626040	-0.3759090
O	1.4772420	-2.2223090	-2.6057070
H	0.5411450	-2.0300710	-2.4678670
C	2.4543350	1.2419190	-1.6530980
C	3.8693500	1.1149700	-1.8169900
C	4.4240460	-0.1452040	-2.1760490
C	3.6199870	-1.2666100	-2.5120140
C	2.2273100	-1.1424410	-2.3594170
C	1.6588910	0.0762370	-1.8570870
H	4.5160480	1.9646000	-1.6292310
H	5.5046890	-0.2481820	-2.2170710
H	4.0485920	-2.2085570	-2.8318270
H	0.5893350	0.1255840	-1.6781990
C	-7.5179160	-0.1304910	1.1354050
H	-8.5074580	0.3225400	1.2802310
C	-7.1793990	-0.1379430	-0.3561470
H	-7.0668870	0.9020910	-0.6935030
C	-8.2189130	-0.8328190	-1.2419490
H	-9.1973760	-0.3518720	-1.0994540
C	-8.3606050	-2.3391510	-1.0114040
H	-8.6830740	-2.5317490	0.0195390
C	-9.3468180	-2.9963120	-1.9747090
H	-10.3480130	-2.5629480	-1.8728670
H	-9.4321670	-4.0720780	-1.7910010
H	-9.0350710	-2.8604210	-3.0165760
C	-6.4961850	0.6308520	1.9955560
H	-7.5972080	-1.1597160	1.5091930
H	-6.4275120	1.6688630	1.6505030
C	-5.1440340	-0.0214500	2.0172280
H	-5.1608270	-1.0841230	2.2681960
C	-3.9478250	0.5323730	1.7843160
H	-3.0730560	-0.1180450	1.8593630
C	-3.6407740	1.9583710	1.4294950
H	-4.5514980	2.5667670	1.4319830
H	-2.9919750	2.3846570	2.2092240
C	-2.9500790	2.0970930	0.0640490
H	-3.6403320	1.7372230	-0.7088360
H	-2.0809370	1.4240330	0.0311730
C	-2.5188060	3.5336530	-0.2647820
H	-3.3769080	4.1928750	-0.0843490
H	-2.3135560	3.6156150	-1.3410370
C	-1.3001020	4.0561390	0.5221020
H	-1.4627620	5.1060920	0.7903200
H	-1.2123990	3.5211230	1.4777250
C	0.0371850	3.9798230	-0.2241050
H	-0.0335550	4.5805230	-1.1420260
H	0.8123290	4.4566630	0.3912700
C	0.4990210	2.5669280	-0.5893260
H	-0.2554350	2.1001860	-1.2345210
H	0.5699660	1.9538500	0.3193070

C	1.8528990	2.5785950	-1.2979140
H	1.7626350	3.1381010	-2.2408910
H	2.5811530	3.1281080	-0.6903300
H	-7.9540210	-0.6632980	-2.2947310
H	-6.1974910	-0.6094510	-0.5032360
H	-7.3743100	-2.8137530	-1.1143300
C	6.1520090	0.8034170	1.1869080
H	6.6091240	1.2064910	2.0946690
H	5.2798720	1.3908810	0.8932370
H	6.9098480	0.8699180	0.3954740
C	5.7707560	-0.6285530	1.3682360
H	2.8929600	0.6203590	0.8320890
C	6.6422240	-1.5071180	2.2080290
H	7.6911130	-1.3992930	1.9118070
H	6.3374150	-2.5513230	2.1355740
H	6.5809240	-1.1802540	3.2534880
O	4.7567850	-1.1140710	0.8454770
H	-6.8769110	0.6755940	3.0263680
C	1.7057960	-1.1700350	3.0654250
H	2.3568970	-1.9204860	3.5299620
H	0.9040580	-0.9487710	3.7759930
H	2.2786770	-0.2544970	2.8974180
C	1.1184410	-1.6884470	1.7657960
H	0.4873580	-0.9214780	1.3090040
C	0.3420960	-2.9841600	1.9258250
H	0.9710460	-3.7715400	2.3567390
H	-0.0419820	-3.3357480	0.9649880
H	-0.5048990	-2.8327290	2.6013530
O	2.1642400	-1.8991760	0.7632690
H	2.8517000	-2.4611450	1.1511040

intermediate-20

Ru	-1.2674510	-0.6546660	-0.6916860
O	-0.2139010	-3.2548980	1.4226110
H	-0.0968750	-2.9950990	2.3470390
C	-2.9146450	-0.8142200	0.7194120
C	-3.3615890	-1.3278010	-0.5356200
C	-2.5635100	-2.2872520	-1.2026880
C	-1.3795990	-2.7872530	-0.5709770
C	-1.1736890	-2.5438180	0.8355110
C	-1.8821310	-1.5022570	1.4480810
H	-4.1935260	-0.8592790	-1.0495180
H	-2.7969050	-2.5904490	-2.2169440
H	-0.7390840	-3.5002820	-1.0781130
H	-1.6329580	-1.1824600	2.4558480
H	-1.4123120	-0.2910590	-2.2161400
C	1.0177560	-0.5331500	-0.5118560
C	0.5752480	0.4411960	-1.4045510
H	0.6817190	0.1916410	-2.4580260
C	3.0581760	0.0269280	0.8824440
H	3.3560110	0.2042250	1.9244320
C	3.9858420	-1.0268840	0.2722770
H	3.7726530	-1.9984040	0.7403060
C	5.4774860	-0.7154180	0.4398660
H	5.7063410	-0.6027320	1.5091940
C	5.9666460	0.5215480	-0.3170920
H	5.4450530	1.4165090	0.0465960
C	7.4732420	0.7349270	-0.1871480
H	7.7665020	0.8667230	0.8601350
H	7.7999130	1.6228480	-0.7367780
H	8.0301190	-0.1226000	-0.5801670
C	1.5629110	-0.3581130	0.8876560
H	3.1767520	0.9843900	0.3611690
H	1.4584630	-1.3101840	1.4213210
H	1.3538010	-1.4517900	-0.9926850
C	0.3147390	1.9257810	-1.1990360
H	1.1409720	2.4442440	-1.7086030
H	-0.5688540	2.1843050	-1.7992410
C	0.1755530	2.5003870	0.2201740
H	1.1711380	2.5768320	0.6704650
H	-0.3852380	1.8141880	0.8668210
C	-0.4925620	3.8829900	0.2772480
H	0.0061390	4.5580700	-0.4300350
H	-0.3008080	4.3014850	1.2731170
C	-2.0111750	3.9362370	0.0289190
H	-2.3284970	4.9732850	0.1804930
H	-2.2422880	3.7151960	-1.0222400
C	-2.8405110	3.0092300	0.9385410
H	-2.3243450	2.8813010	1.8998520
H	-3.8076040	3.4685290	1.1741920
C	-3.0878500	1.6419660	0.2944120

H	-2.1482900	1.3604980	-0.2293770
H	-3.8229900	1.7359640	-0.5124350
C	-3.4793060	0.4875200	1.2471510
H	-3.0701990	0.6733590	2.2453260
H	-4.5667770	0.4185300	1.3568250
H	6.0532460	-1.5860940	0.1003160
H	3.7669490	-1.1468870	-0.7978940
H	5.6999420	0.4224660	-1.3788280
H	1.0046810	0.3919500	1.4505320

intermediate-21

Ru	-1.2680210	-1.0311600	-0.5545630
O	-1.6613850	-1.9828950	2.4682540
H	-1.4750540	-1.2172710	3.0270050
C	-3.2031550	0.0891960	-0.2184910
C	-3.3726890	-0.9766900	-1.1507280
C	-3.1190550	-2.3467240	-0.8362100
C	-2.5490320	-2.6667850	0.3984460
C	-2.2463160	-1.6145500	1.3170260
C	-2.5575400	-0.2506260	1.0052370
H	-3.7252910	-0.7343700	-2.1496070
H	-3.2885000	-3.1158670	-1.5812600
H	-2.2658410	-3.6817500	0.6552520
H	-2.3437290	0.5207180	1.7395160
H	0.2625110	-2.0157660	-0.2670580
C	1.0712850	-1.1474520	-0.3762410
C	0.3579230	0.0864570	-0.8731260
H	0.1270570	-0.0661230	-1.9688900
C	3.2669770	-0.5927370	0.8488880
H	3.6579540	-0.5053240	1.8708000
C	4.2195490	-1.4752300	0.0361080
H	4.1586350	-2.5034340	0.4181420
C	5.6816180	-1.0158770	0.0794130
H	6.0185420	-0.9793190	1.1249940
C	5.9547420	0.3329830	-0.5904910
H	5.3930190	1.1280180	-0.0823940
C	7.4376110	0.6982890	-0.5969840
H	7.8344380	0.7630010	0.4220850
H	7.6095110	1.6643170	-1.0812420
H	8.0280070	-0.0522050	-1.1336020
C	1.8318010	-1.1300900	0.9526650
H	3.2584190	0.4254140	0.4436320
H	1.8722690	-2.1546400	1.3430750
H	1.6526770	-1.6291890	-1.1699310
C	0.7930090	1.5102460	-0.6021170
H	1.8519820	1.6241460	-0.8721950
H	0.2492900	2.1502090	-1.3033130
C	0.5661360	2.0213840	0.8320940
H	1.4117720	1.7337900	1.4661110
H	-0.3100590	1.5112990	1.2477040
C	0.3619670	3.5359700	0.9555450
H	1.2588980	4.0613540	0.6042410
H	0.2833190	3.7658620	2.0260250
C	-0.8671100	4.1221630	0.2377960
H	-0.9748280	5.1596880	0.5707660
H	-0.6760520	4.1896970	-0.8414460
C	-2.1875530	3.3563010	0.4657670
H	-2.0852610	2.6979020	1.3384830
H	-2.9917330	4.0540400	0.7259560
C	-2.6233900	2.5586610	-0.7721800
H	-1.7575350	2.0769300	-1.2366630
H	-3.0032900	3.2701040	-1.5142620
C	-3.6985050	1.4802420	-0.5479510
H	-4.3813610	1.7880100	0.2548670
H	-4.3165490	1.3961120	-1.4469300
H	6.2991420	-1.7814880	-0.4075480
H	3.8982360	-1.5195140	-1.0146310
H	5.5795900	0.3043890	-1.6233630
H	1.2642020	-0.5453260	1.6836440

intermediate-22

Ru	-0.5157550	-0.9189690	-0.0210150
O	0.2196750	-2.2084890	3.0731270
H	0.1445010	-1.5076570	3.7329070
C	-2.5118320	-0.6988080	1.0159060
C	-2.5475580	-1.6630740	-0.0353270
C	-1.6279560	-2.7501980	-0.0243790
C	-0.7537190	-2.9956760	1.0775710
C	-0.6635860	-2.0288950	2.0789820
C	-1.4385510	-0.8221790	1.9452590

H	-3.2611190	-1.5723740	-0.8456760
H	-1.6197350	-3.4401540	-0.8619970
H	-0.1170900	-3.8711400	1.1113330
H	-1.3067000	-0.0335390	2.6847540
H	1.6378620	0.7749990	-1.7107570
C	0.8660330	1.2734440	-1.1147720
C	-0.5237090	0.6817600	-1.4175940
H	-0.5100770	0.1572330	-2.3890580
C	2.5754450	1.5709230	0.8336060
H	2.6183670	1.5312240	1.9297830
C	3.7734000	0.8115030	0.2642350
H	3.6632660	-0.2546010	0.5109320
C	5.1278180	1.2971400	0.7958240
H	5.1301840	1.2338200	1.8932520
C	5.5175400	2.7136310	0.3660710
H	4.7864810	3.4387010	0.7463580
C	6.9111620	3.1113990	0.8475010
H	6.9772610	3.0821420	1.9406240
H	7.1686170	4.1253110	0.5273290
H	7.6758780	2.4339130	0.4521880
C	1.1896500	1.0945670	0.3742130
H	2.6413720	2.6337090	0.5656190
H	1.1435630	-0.0073640	0.6595030
H	0.9284600	2.3393990	-1.3766980
C	-1.6256410	1.7281360	-1.5648490
H	-1.3897550	2.3234870	-2.4632880
H	-2.5623010	1.2172870	-1.8049180
C	-1.8291090	2.6956990	-0.3993880
H	-0.9272000	3.3100090	-0.2769330
H	-1.9191730	2.1277490	0.5304780
C	-3.0177410	3.6569630	-0.5526340
H	-2.7724990	4.3792250	-1.3425360
H	-3.0984110	4.2481510	0.3693530
C	-4.4001550	3.0781730	-0.8903130
H	-5.0701610	3.9377160	-1.0137540
H	-4.3740480	2.5956830	-1.8769170
C	-5.0698660	2.1165800	0.1061880
H	-5.0237620	2.5337210	1.1216950
H	-6.1354250	2.0865880	-0.1458330
C	-4.5381930	0.6668010	0.1030720
H	-4.0612020	0.4762700	-0.8628000
H	-5.3806730	-0.0314230	0.1572640
C	-3.5735140	0.3453180	1.2535870
H	-3.0973870	1.2539950	1.6324320
H	-4.1567420	-0.0362710	2.1047110
H	5.9042970	0.6004060	0.4541680
H	3.7782680	0.8836870	-0.8322300
H	5.4739540	2.7823540	-0.7298240
H	0.4302940	1.6065360	0.9710140
C	2.4902700	-2.6990640	-3.0433060
H	1.9040590	-3.5913160	-3.2833220
H	3.5507460	-2.9608140	-3.0968390
H	2.3059660	-1.9394410	-3.8117100
C	2.1560780	-2.1861150	-1.6534230
C	2.3918710	-3.2111730	-0.5663400
H	2.1269490	-2.8177450	0.4185560
H	3.4518220	-3.4792170	-0.5455180
H	1.8148180	-4.1214330	-0.7562370
O	0.7378230	-1.8086840	-1.6327250
H	0.5537000	-1.3166240	-2.4456050
H	2.7371910	-1.2813260	-1.4384920
TS1-2			
Ru	-1.8176810	0.1162580	-0.0431730
H	-2.7659580	3.6227640	-0.6997700
C	-0.0676530	-1.4454050	0.0217710
C	-0.3554780	-0.9841520	1.3487000
C	-1.6590860	-1.0735250	1.8741240
C	-2.7006670	-1.6116640	1.0779810
C	-2.4221090	-2.0921700	-0.2304460
C	-1.1068950	-1.9839230	-0.7672050
H	0.4422110	-0.5648100	1.9508950
H	-1.8741070	-0.7229700	2.8779450
H	-3.7163340	-1.6808320	1.4517770
H	-0.8943790	-2.3422180	-1.7701910
C	-0.0581200	1.5409250	-0.6497620
H	0.5017130	0.9932820	-1.4064840
C	-1.2609000	2.0835610	-1.0715100
H	-1.5368980	1.9930050	-2.1192490
C	-2.0899870	2.9596350	-0.1490400
H	-1.4647040	3.5883660	0.4879010
C	-2.8312870	1.8928000	0.6321920
H	-2.9601480	1.9726300	1.7081460
C	-3.7714560	1.1482870	-0.1520720
H	-2.9603750	0.3254300	-1.1693800
H	-4.5083260	0.5258080	0.3475380
H	-4.1643360	1.6098580	-1.0603830
C	0.8023870	2.0690810	0.4807280
H	1.2801610	1.2488520	1.0178480
H	0.1978990	2.6105000	1.2155180
C	1.8607310	2.9692760	-0.1118410
H	1.4841040	3.8647980	-0.6048120
C	3.1840920	2.7586860	-0.1048400
H	3.8030330	3.5095560	-0.5968410
C	3.9387620	1.6126250	0.5019780
H	4.7201270	2.0165920	1.1603140
C	3.2850480	1.0177950	1.1499520
H	4.6102460	0.7052730	-0.5463240
H	5.3398020	1.2985990	-1.1105570
H	3.8599270	0.3841890	-1.2821880
C	5.3121350	-0.5166750	0.0622280
H	5.9810940	-0.1773890	0.8634250
H	5.9605660	-0.9743630	-0.6953740
C	4.3618320	-1.5873710	0.6166090
H	4.9220990	-2.2549580	1.2804070
H	3.6180370	-1.1051280	1.2666190
C	3.6472580	-2.4358570	-0.4579980
H	3.7425330	-1.9611350	-1.4440820
H	4.1470550	-3.4057600	-0.5501440
C	2.1573290	-2.6689040	-0.1705150
H	2.0213140	-2.9404560	0.8844010
H	1.7759290	-3.5106560	-0.7602280
C	1.3399970	-1.4047980	-0.5026110
H	1.8543120	-0.5371120	-0.0792360
H	1.3274620	-1.2692940	-1.5900020
O	-3.4488610	-2.6274360	-0.9033300
H	-3.1967800	-2.8450280	-1.8104150
TS2-3			
Ru	-1.8702360	0.0543370	-0.0128850
H	-1.5742580	3.3191260	2.0138990
C	-0.5275030	-1.7653740	-0.0781690
C	-0.8863660	-1.4332420	1.2752760
C	-2.2359980	-1.2903040	1.6612690
C	-3.2479740	-1.4072940	0.6627310
C	-2.9007270	-1.8294800	-0.6670210
C	-1.5400850	-2.0180240	-1.0299300
H	-0.0959260	-1.2298880	1.9907460
H	-2.4975330	-1.0128380	2.6767700
H	-4.2948240	-1.2367270	0.8928430
H	-1.2745840	-2.2887390	-2.0475060
C	0.5148380	3.7618340	-0.3185810
H	0.6975000	4.5270190	-1.0736520
C	-0.7557900	3.6025680	0.0743130
H	-1.4945260	4.2682950	-0.3716370
C	-1.2736990	2.6974630	1.1561730
H	-0.4612840	2.0718240	1.5524680
C	-2.4975730	1.8212210	0.8122310
H	-3.2019120	1.7229060	1.6378410
C	-3.1174340	1.9111120	-0.5346550
H	-2.7491240	1.0197350	-1.2641020
H	-4.2011850	1.7994450	-0.5623000
H	-2.7753790	2.7376220	-1.1608170
C	1.7586380	3.0873330	0.1943010
H	1.5361100	2.1148950	0.6515200
H	2.1515070	3.7077560	1.0178960
C	2.8318340	2.9648610	-0.8602980
H	2.7767170	3.7021050	-1.6612010
C	3.8592880	2.1088330	-0.8799740
H	4.5677860	2.2065870	-1.7033430
C	4.1873830	1.0363240	0.1188640
H	4.9071750	1.4330430	0.8513550
H	3.2950950	0.7727410	0.7018220
C	4.8002290	-0.2105110	-0.5356660
H	5.7398990	0.0814810	-1.0205090
H	4.1444390	-0.5514350	-1.3485540
C	5.0770640	-1.3629980	0.4383700
H	5.6331630	-0.9745790	1.3011470
H	5.7406490	-2.0926210	-0.0429080
C	3.8167890	-2.0859910	0.9307570
H	4.0613390	-2.6960270	1.8082720
H	3.0992200	-1.3357780	1.2934100
C	3.1550440	-2.9827860	-0.1295720

H	3.3703290	-2.6044840	-1.1377290
H	3.6007630	-3.9826850	-0.0882180
C	1.6345630	-3.1026610	0.0311210
H	1.3882470	-3.2942020	1.0840150
H	1.2519420	-3.9581440	-0.5375420
C	0.9270100	-1.8217480	-0.4530360
H	1.4311060	-0.9503720	-0.0178680
H	1.0338830	-1.7327790	-1.5392670
O	-3.9227640	-1.9811360	-1.5161940
H	-3.6110430	-2.1718450	-2.4113730

TS3-4

Ru	-1.2297280	-0.4890440	0.1600020
H	0.1386970	-2.9278750	-0.1895250
C	-1.9873540	1.5712610	-0.4951600
C	-1.1188460	1.0830990	-1.4874790
C	-1.2848600	-0.2434110	-1.9880660
C	-2.4004970	-1.0416330	-1.6107360
C	-3.3898290	-0.4895640	-0.7450870
C	-3.1064040	0.7402400	-0.1116340
H	-0.2538150	1.6593090	-1.7919240
H	-0.5509660	-0.6505980	-2.6752440
H	-2.5462100	-2.0354000	-2.0202950
H	-3.7802210	1.1083440	0.6593110
C	2.6630070	-2.4546530	0.8183750
H	3.5204000	-2.4229900	1.4888920
C	1.4650580	-2.1735590	1.3571660
H	1.4359150	-1.8976160	2.4081850
C	0.1527220	-2.2528070	0.6648310
H	0.3630530	-0.7781070	0.1224580
C	-1.1069590	-2.1536560	1.3704270
H	-1.8775430	-2.9111210	1.2722950
C	-1.1788080	-1.1183400	2.4307500
H	-0.9845990	-0.0420580	1.9544960
H	-2.1372810	-1.0660150	2.9449260
H	-0.3539230	-1.0996010	3.1496560
C	2.9690780	-2.8528960	-0.5894850
H	2.0465030	-3.0239340	-1.1604240
H	3.4642910	-3.8356920	-0.5507930
C	3.8612480	-1.9470850	-1.4133500
H	4.1415990	-2.4137350	-2.3576740
C	4.3443900	-0.7172930	-1.1958600
H	4.9617660	-0.3138530	-2.0001260
C	4.1633230	0.2277530	-0.0426730
H	3.7228100	-0.2703010	0.8249820
H	5.1526520	0.5880180	0.2724170
C	3.2887480	1.4342050	-0.4173630
H	2.2894730	1.0565220	-0.6757420
H	3.6783020	1.9046730	-1.3302710
C	3.1821100	2.4936100	0.6854310
H	4.1418180	3.0164180	0.7745590
H	3.0131240	2.0060800	1.6566260
C	2.0569400	3.5057580	0.4268560
H	2.2171140	4.4119310	1.0224600
H	2.1033950	3.8255360	-0.6240300
C	0.6685790	2.9254390	0.7299550
H	0.6643920	1.8619850	0.4627730
H	0.4880880	2.9590000	1.8136310
C	-0.4814940	3.6283860	0.0038260
H	-0.2353920	3.7439940	-1.0603030
H	-0.5902390	4.6511450	0.3831000
C	-1.8424340	2.9371980	0.1425350
H	-2.1136210	2.8545320	1.2026740
H	-2.6164360	3.5725310	-0.3111640
O	-4.4771900	-1.2312050	-0.5004280
H	-5.0839140	-0.7758450	0.0978630

TS4'-4

Ru	-1.6103750	-0.4520360	0.2784830
H	-0.2820690	-2.8703440	0.1393410
C	-1.4962820	1.6846890	-0.5096890
C	-0.5363660	0.9107000	-1.2075250
C	-0.9163230	-0.3279370	-1.7786420
C	-2.2763980	-0.7479460	-1.7412700
C	-3.2859450	0.1453170	-1.2436010
C	-2.8822360	1.3044340	-0.5570890
H	0.5054680	1.2004680	-1.2086300
H	-0.1658220	-0.9752330	-2.2190480
H	-2.5841690	-1.6941200	-2.1720870
H	-3.6205960	1.9381950	-0.0735250
C	2.2266270	-2.0533490	0.9318450
H	3.0811390	-1.6706220	1.4826310

C	1.0187860	-1.6486240	1.3714580
H	1.0227640	-0.9582050	2.2121900
C	-0.2930490	-2.0667590	0.8736770
H	-1.3451340	0.0938320	2.2628980
C	-1.4910510	-2.0169630	1.6957150
H	-2.0677740	-2.9224090	1.8907470
C	-1.5209870	-0.9245190	2.7409250
H	-2.6330860	-1.5902680	0.8488570
H	-2.4748580	-0.8637680	3.2640480
H	-0.6976040	-1.0005910	3.4564500
C	2.5432360	-2.9954510	-0.1897780
H	1.6309990	-3.4937060	-0.5375510
H	3.1707930	-3.8067910	0.2131160
C	3.2498930	-2.4321800	-1.4111940
H	3.1029030	-3.0522810	-2.2959090
C	4.0426740	-1.3630850	-1.5647930
H	4.4281940	-1.2059490	-2.5724770
C	4.4624370	-0.3205400	-0.5622290
H	4.5362950	-0.7436340	0.4438970
H	5.4720700	0.0267860	-0.8135070
C	3.5036790	0.8807920	-0.5460230
H	2.4898810	0.4812670	-0.4194440
H	3.5265210	1.3725530	-1.5287090
C	3.7891420	1.9138010	0.5461530
H	4.8077590	2.3024970	0.4244210
H	3.7662810	1.4253950	1.5308850
C	2.8005130	3.0874550	0.5242390
H	3.1571840	3.8828600	1.1879970
H	2.8087370	3.5202340	-0.4858900
C	1.3545310	2.7053420	0.9037090
H	1.2156520	1.6250310	0.7739900
H	1.1858630	2.8931480	1.9721920
C	0.3022730	3.4663020	0.0871210
H	0.5817180	3.4623170	-0.9750430
H	0.3166300	4.5220790	0.3813740
C	-1.1398910	2.9672830	0.2212280
H	-1.4102790	2.8573760	1.2801330
H	-1.8195640	3.7351210	-0.1719180
O	-4.5523500	-0.2472200	-1.3873140
H	-5.1621780	0.3634990	-0.9516010

TS6-7

Ru	0.6055540	-0.5646660	-0.4663710
H	3.8326800	2.7599780	-1.4368670
C	-0.7098670	-2.3495920	-0.8961960
C	-0.9037970	-1.3839870	-1.9072780
C	0.2171440	-0.8115780	-2.5680690
C	1.5337210	-1.2767520	-2.3017600
C	1.7108810	-2.3913410	-1.4274600
C	0.6242080	-2.8237020	-0.6410600
H	-1.8975220	-1.0092570	-2.1160180
H	0.0743650	-0.0071480	-3.2802380
H	2.3907060	-0.8594460	-2.8169300
H	0.7764810	-3.5840280	0.1209960
C	-0.1096110	1.5948980	-0.5731430
H	-0.3369640	1.8001460	0.4783500
C	1.1202390	2.1761490	-0.9751160
H	1.3288610	2.1786550	-2.0495730
C	2.1368980	2.6278570	-0.1101660
H	1.7705020	3.0130010	0.8481400
C	3.3405780	3.3736700	-0.6709660
H	2.9971270	4.2798130	-1.1875520
C	4.3518300	3.7789730	0.3988560
H	3.8890650	4.4248710	1.1528610
H	5.1869000	4.3319230	-0.0401770
H	4.7678180	2.9102120	0.9198820
C	-1.3238770	1.8446610	-1.4726140
H	-2.0588610	1.0442470	-1.3701360
H	-1.0012740	1.8488780	-2.5239050
C	-1.9716050	3.1646620	-1.1412900
H	-1.3141960	4.0330590	-1.1843490
C	-3.2500590	3.3501080	-0.7870950
H	-3.5621960	4.3664990	-0.5485290
C	-4.3093480	2.2897410	-0.6647000
H	-5.2689970	2.6930930	-1.0115340
H	-4.0825350	1.4503280	-1.3310360
C	-4.4757960	1.7749200	0.7755880
H	-4.8372750	2.5913310	1.4124290
H	-3.4839750	1.5162700	1.1723900
C	-5.4195410	0.5745100	0.9167530
H	-6.4323780	0.8721960	0.6178560
H	-5.4857990	0.3117040	1.9807690

C	-5.0234370	-0.6770250	0.1194500
H	-5.7270410	-1.4822900	0.3667230
H	-5.1516850	-0.4957190	-0.9560030
C	-3.5963710	-1.1651120	0.3779050
H	-2.8864300	-0.3921610	0.0546420
H	-3.4427120	-1.2951230	1.4585930
C	-3.2664640	-2.4807070	-0.3297150
H	-3.4859310	-2.4010280	-1.4027930
C	-3.9465170	-3.2558430	0.0430030
H	-1.8375390	-2.9935570	-0.1197570
H	-1.5816410	-2.9583510	0.9463390
H	-1.8031670	-4.0563900	-0.3980800
O	2.9460770	-2.8901720	-1.3170680
H	2.9711790	-3.6138340	-0.6771650
C	3.4309700	-0.5336810	0.8728050
C	3.9384640	-0.1397120	2.2573930
H	3.2173580	-0.3966050	3.0366890
H	4.1291580	0.9368340	2.3072010
H	4.8770870	-0.6568810	2.4802470
C	4.4778640	-0.2479240	-0.1995900
H	5.3786050	-0.8420870	-0.0166750
H	4.7685940	0.8066950	-0.1867810
H	4.1165290	-0.4956420	-1.1990020
O	2.1928110	0.1479190	0.6199300
H	2.3838180	1.4093500	0.2888440
H	3.2100020	-1.6095750	0.8774510
C	0.1315620	-0.2786780	2.8241570
H	0.9818570	0.3933960	2.6791570
C	0.6109930	-1.6272270	3.3229520
H	1.1286160	-1.5106940	4.2795860
H	1.3106430	-2.0795940	2.6147750
H	-0.2314830	-2.3099930	3.4720850
C	-0.9043460	0.3587910	3.7340190
H	-0.4698090	0.5377760	4.7215750
H	-1.7752260	-0.2924090	3.8633790
H	-1.2403020	1.3287440	3.3494460
O	-0.4609370	-0.4933960	1.5011590
H	-1.1942210	0.1253820	1.3946980

TS8-9

Ru	-0.9633110	-1.0696530	0.0676190
H	4.6320240	-1.8035300	-1.5660220
C	-1.1942910	-0.4153790	-2.0693270
C	0.1196240	-0.1306610	-1.6361990
C	0.8988350	-1.1501870	-1.0161040
C	0.3932970	-2.4708200	-0.9060510
C	-0.8670760	-2.8054150	-1.4948640
C	-1.6835920	-1.7681630	-1.9845240
H	0.5055210	0.8789480	-1.6848270
H	1.8719150	-0.9007670	-0.6015290
H	0.9689110	-3.2578120	-0.4331910
H	-2.6903000	-1.9855930	-2.3307580
C	4.3889270	0.8654800	-0.3475050
H	4.8483990	0.5677940	-1.2899910
C	4.2471080	-0.0465190	0.6215410
H	3.8057620	0.2690700	1.5685540
C	4.6968370	-1.4826300	0.5708420
H	5.4082210	-1.6443580	1.3950740
C	5.3324610	-1.9588160	-0.7338260
C	6.2095260	-1.3383760	-0.9558070
H	5.7484730	-3.4271860	-0.6830500
H	6.4776230	-3.6059110	0.1144120
H	6.2056710	-3.7432090	-1.6252630
H	4.8893110	-4.0819500	-0.4959650
C	4.0286420	2.3281980	-0.2666060
H	3.2824700	2.5631430	-1.0375560
H	4.9222220	2.8961040	-0.5739010
C	3.5944890	2.8323470	1.0788360
H	4.2320930	2.5298200	1.9095190
C	2.5797980	3.6632890	1.3509200
H	2.4564120	3.9761970	2.3891070
C	1.6007750	4.2717100	0.3880610
H	1.8837040	5.3198310	0.2053170
H	1.6639130	3.7732720	-0.5855960
C	0.1567580	4.2492910	0.9076940
H	0.1212610	4.7768380	1.8695240
H	-0.1266720	3.2110820	1.1321620
C	-0.8656110	4.8941930	-0.0377790
H	-0.5761310	5.9390340	-0.2072310
H	-1.8409070	4.9340030	0.4663820
C	-1.0358400	4.2096180	-1.4003020
H	-1.7079170	4.8163430	-2.0202880

H	-0.0753820	4.1975200	-1.9325090
C	-1.5841930	2.7834070	-1.3210080
H	-0.9740080	2.1979380	-0.6208790
H	-2.6003890	2.8105170	-0.9016150
C	-1.6250800	2.0815110	-2.6820210
H	-0.6375970	2.1338700	-3.1600100
H	-2.2937360	2.6411060	-3.3467710
C	-2.1124510	0.6297700	-2.6625760
H	-3.0780240	0.5650370	-2.1461750
H	-2.3041410	0.3058330	-3.6951530
O	-1.2318220	-4.0859010	-1.4314710
H	-2.1337420	-4.2131490	-1.7544460
C	-0.5972080	-1.4696260	2.3194430
C	0.7395650	-2.1387180	2.5818200
H	0.9417490	-2.9152300	1.8454160
H	0.6802150	-2.6156940	3.5678890
H	1.5629210	-1.4213770	2.6093430
C	-1.0082570	-0.4821940	3.4005450
H	-0.1892430	0.1898100	3.6680570
H	-1.2725420	-1.0663340	4.2901390
H	-1.8809160	0.1047960	3.1153550
O	-1.5336430	-2.1669790	1.7333080
H	3.8446540	-2.1364380	0.8191970
H	-0.2037990	-0.2741610	1.2670530
C	-3.9513990	-0.3508790	1.2419390
H	-3.6226990	-0.8121600	2.1774770
C	-4.6037130	-1.4050470	0.3749640
H	-5.4915140	-1.7931440	0.8820300
H	-3.9212940	-2.2424580	0.2121550
H	-4.9148900	-0.9875390	-0.5880800
C	-4.8403900	0.8490810	1.5151660
H	-5.7324700	0.5298610	2.0611180
H	-5.1630900	1.3246590	0.5837260
H	-4.3351510	1.5979940	2.1367280
O	-2.7474060	0.1198410	0.5407330
H	-2.4982310	0.9838590	0.8918800

TS9-10

Ru	-1.1330120	-0.8022480	-0.0466800
H	4.0568950	-2.5936050	-1.5308490
C	-1.2956560	0.1671410	-2.0467090
C	0.0567570	0.1390200	-1.6054610
C	0.6497340	-1.0921110	-1.2037490
C	-0.1071650	-2.2879090	-1.2703280
C	-1.4107640	-2.2835490	-1.8680200
C	-2.0151720	-1.0647620	-2.2123950
H	0.6193340	1.0574520	-1.5078870
H	1.6574930	-1.0994790	-0.7998480
H	0.3097810	-3.2309100	-0.9370370
H	-3.0280000	-1.0443900	-2.6053660
C	4.4703530	0.0446820	-0.3015570
H	4.8589060	-0.3654830	-1.2338000
C	4.0562430	-0.7919050	0.6571290
H	3.6833610	-0.3653260	1.5895920
C	4.0943690	-2.2960590	0.6107260
H	4.6868780	-2.6487370	1.4687270
C	4.6435320	-2.9311990	-0.6654110
H	5.6658770	-2.5716170	-0.8346230
C	4.6429380	-4.4571870	-0.6116800
H	5.2570870	-4.8258100	0.2169350
H	5.0412300	-4.8881990	-1.5348750
C	3.6301240	-4.8540300	-0.4721200
H	4.5072440	1.5508430	-0.2141040
H	3.8133790	1.9775510	-0.9509210
H	5.5033780	1.8710220	-0.5599930
C	4.2757510	2.1314870	1.1506610
H	4.8689310	1.6764530	1.9440630
C	3.4942030	3.1668750	1.4819180
H	3.5028460	3.4815770	2.5268430
C	2.6211420	3.9953010	0.5841340
H	3.1044940	4.9703500	0.4175510
H	2.5383530	3.5311580	-0.4049190
C	1.2274850	4.2464260	1.1770810
H	1.3453810	4.7098410	2.1651170
H	0.7391030	3.2796500	1.3629130
C	0.3284300	5.1495620	0.3227070
H	0.8305960	6.1158360	0.1862490
H	-0.5910470	5.3676270	0.8829440
C	-0.0506610	4.5976170	-1.0574830
H	-0.5950910	5.3732960	-1.6110720
H	0.8581590	4.4015700	-1.6420370

C	-0.9050260	3.3288080	-1.0111260
H	-0.4080890	2.5769540	-0.3851100
H	-1.8604920	3.5513990	-0.5156340
C	-1.1868740	2.7508000	-2.4011470
H	-0.2448840	2.6082420	-2.9480790
H	-1.7439750	3.4964560	-2.9809420
C	-1.9991140	1.4520360	-2.4304490
H	-2.8901060	1.5527870	-1.7988220
H	-2.3728110	1.2927040	-3.4509320
O	-2.0126440	-3.4745550	-1.9651090
H	-2.9287620	-3.3775600	-2.2570080
C	-1.3244350	-2.5830550	2.0250820
C	-0.7338110	-3.9362920	1.7545830
H	-1.0966830	-4.3410270	0.8099920
H	-1.0272770	-4.6104110	2.5696030
H	0.3596010	-3.8972430	1.7673670
C	-0.9377040	-1.9099390	3.3110760
H	0.1450450	-1.9146890	3.4586060
H	-1.3744960	-2.4910760	4.1346140
H	-1.3166260	-0.8900130	3.3554310
O	-2.2432650	-2.1356990	1.3028470
H	3.0805400	-2.6861350	0.8032030
H	-0.1701420	-0.3454030	1.1276290
C	-3.6878870	0.5429010	1.5030100
H	-3.4980320	-0.2164790	2.2678250
C	-4.6919970	0.0096650	0.5041170
H	-5.6257230	-0.2373300	1.0168250
H	-4.3153150	-0.9007750	0.0313300
H	-4.9111800	0.7548770	-0.2670480
H	-4.1049670	1.8541390	2.1448640
H	-5.0312920	1.7113430	2.7084820
H	-4.2806530	2.6258070	1.3891470
H	-3.3506240	2.2190340	2.8518680
O	-2.4293490	0.7606760	0.7807200
H	-1.8625790	1.3282820	1.3174930

TS11-12

Ru	-1.0189780	0.1856530	-0.3785380
O	-0.2731560	1.6692580	-3.2983590
H	0.6822190	1.5879580	-3.4107030
C	-0.4629310	-1.6844770	-1.7280320
C	-1.8275850	-1.6318480	-1.3000820
C	-2.6490520	-0.5091100	-1.6054730
C	-2.1356880	0.5932100	-2.3468700
C	-0.7693890	0.5944950	-2.6659100
C	0.0656960	-0.5165560	-2.3108640
H	-2.2579230	-2.4838060	-0.7850840
H	-3.6935720	-0.5148960	-1.3134970
H	-2.7531410	1.4407290	-2.6190530
H	1.1142030	-0.4842520	-2.5899980
C	-0.4939240	-0.7177460	1.5255840
H	-0.7785430	-1.7668300	1.4390670
C	-1.5752850	0.1748230	1.7960670
H	-1.2738760	1.1283120	2.2364650
C	-2.9402440	-0.2440950	2.3264320
H	-2.8226950	-0.2668320	3.4207830
C	-3.5242030	-1.5812140	1.8800750
H	-2.8073750	-2.3889320	2.0746250
C	-4.8401550	-1.8957520	2.5907010
H	-4.7005790	-1.9595830	3.6748220
H	-5.2523900	-2.8510740	2.2537970
H	-5.5920250	-1.1228850	2.3983840
C	0.8801570	-0.6019370	2.1812350
H	1.5966210	-1.1807920	1.5937070
H	0.7912430	-1.1372730	3.1429690
C	1.4489170	0.7597300	2.4732240
H	0.7667320	1.5020690	2.8899820
C	2.7501080	1.0950670	2.3858190
H	3.0294190	2.1073440	2.6788410
C	3.8713710	0.1884050	1.9611390
H	4.7523960	0.4083360	2.5749020
H	3.6028320	-0.8464880	2.1911600
C	4.2546080	0.3053560	0.4676710
H	4.9602360	1.1330220	0.3336400
H	3.3655200	0.5807890	-0.1133190
C	4.8645510	-0.9798140	-0.1114780
H	5.7616460	-1.2447820	0.4618770
H	5.2109980	-0.7722670	-1.1323060
C	3.9186110	-2.1901580	-0.1364650
H	4.4693720	-3.0646630	-0.5032340
H	3.6193520	-2.4491670	0.8884470

C	2.6621790	-1.9865820	-0.9902800
H	2.2488640	-0.9918580	-0.7868080
H	2.9435600	-2.0004950	-2.0536040
C	1.5735290	-3.0247000	-0.7215540
H	1.2469160	-2.9442610	0.3222460
H	1.9934970	-4.0324840	-0.8273920
C	0.3392460	-2.9653430	-1.6382460
H	0.6541990	-3.1968680	-2.6647840
H	-0.3442390	-3.7692900	-1.3470240
H	-3.6674690	0.5539090	2.1290060
H	-2.0902420	1.0035430	0.4611110
C	-0.0635520	3.2456750	0.3576480
H	-0.4806330	3.2179990	1.3739810
C	-1.1181480	3.7416750	-0.6081410
H	-1.3747680	4.7749370	-0.3573500
H	-2.0303300	3.1436240	-0.5493390
H	-0.7465190	3.7170990	-1.6361510
C	1.1922730	4.1024960	0.3411970
H	0.9518490	5.1202750	0.6616070
H	1.6135560	4.1511640	-0.6674690
H	1.9572360	3.7132770	1.0194050
H	-3.6928320	-1.5651420	0.7971630
O	0.3146570	1.8754470	0.0003290
H	1.0031780	1.5945600	0.6386770

TS12-13

Ru	-0.9266250	-0.1599220	-0.3705550
O	-0.9024890	2.1242080	-3.0121150
H	0.0191990	2.2386380	-3.2747470
C	-0.2448430	-1.4362900	-2.0696000
C	-1.5522310	-1.7763380	-1.6118070
C	-2.5718310	-0.7682530	-1.5578380
C	-2.3955580	0.5325140	-2.1311320
C	-1.1181640	0.8851230	-2.5480060
C	-0.0384480	-0.0545430	-2.3582610
H	-1.7719720	-2.7870300	-1.2841510
H	-3.5479160	-1.0331690	-1.1646560
H	-3.2075260	1.2477250	-2.1822030
H	0.9706450	0.2793670	-2.5864840
C	-0.1970760	-0.9925330	1.3338450
H	-0.0794000	-2.0691780	1.4510780
C	-1.4352970	-0.3946490	1.9151890
H	-1.2280340	0.4917250	2.5227810
C	-2.4298910	-1.3206830	2.6217900
H	-1.9348400	-1.6742970	3.5356930
C	-2.9327670	-2.5208940	1.8220400
H	-2.0853740	-3.1302450	1.4837000
C	-3.8930610	-3.3925070	2.6291470
H	-3.4075350	-3.7904790	3.5262410
H	-4.2472470	-4.2427140	2.0394730
H	-4.7708200	-2.8229800	2.9521200
C	1.0899390	-0.1893650	1.3374480
H	1.0150990	0.5759890	0.5149480
H	1.8883780	-0.8472000	0.9912980
C	1.5406270	0.5538910	2.5697180
H	0.7780170	0.9901990	3.2128770
C	2.8333180	0.7211340	2.8875520
H	3.0627090	1.2970390	3.7827450
C	3.9981910	0.1392050	2.1230210
H	4.9114530	0.2368560	2.7181980
H	3.8305680	-0.9413480	2.0231150
C	4.2391590	0.7500380	0.7244790
H	4.7896200	1.6911780	0.8361030
H	3.2796690	1.0301650	0.2726740
C	5.0089950	-0.1701810	-0.2362780
H	5.9714060	-0.4357190	0.2189950
H	5.2542770	0.3958750	-1.1443520
C	4.2820610	-1.4655910	-0.6284150
H	4.9817550	-2.1191430	-1.1627370
H	4.0139580	-2.0211450	0.2807940
C	3.0213560	-1.2772630	-1.4891370
H	2.4959590	-0.3700970	-1.1678370
H	3.3130880	-1.1111260	-2.5354560
C	2.0788390	-2.4807000	-1.3922400
H	1.7593460	-2.6098570	-0.3503160
H	2.6432490	-3.3871940	-1.6443380
C	0.8304900	-2.4794070	-2.2903110
H	1.1437780	-2.3914240	-3.3392390
H	0.3534680	-3.4610780	-2.2024060
H	-3.2882560	-0.7240380	2.9539490
H	-2.0535940	0.1516690	1.0545920

C	-1.1048010	3.7217800	0.8545180
H	-1.3922590	3.7976040	1.9141400
C	-2.3599530	3.7161710	0.0040490
H	-2.9191670	4.6433360	0.1576460
H	-3.0124860	2.8805170	0.2738160
H	-2.1045980	3.6393090	-1.0570630
C	-0.1642500	4.8670230	0.5087160
H	-0.6505560	5.8312190	0.6848190
H	0.1306320	4.8189510	-0.5444310
H	0.7421340	4.8419130	1.1243900
H	-3.4375260	-2.1629380	0.9148350
O	-0.4372530	2.4520360	0.6622550
H	0.3713120	2.4736740	1.1917540

TS13-14

Ru	-1.0753100	-0.6642740	-0.2231270
O	1.5537520	-2.8673800	-0.3782450
H	2.4041120	-2.4196960	-0.1004400
C	-0.5500490	-0.8525750	1.9579740
C	-1.7881930	-1.5288230	1.7583600
C	-1.9021140	-2.4993510	0.7406290
C	-0.7746350	-2.9300230	-0.0248130
C	0.4957320	-2.3866660	0.2484080
C	0.5465100	-1.2454800	1.1226310
H	-2.6582650	-1.2541340	2.3452420
H	-2.8692590	-2.9457070	0.5337030
H	-0.8715530	-3.7032280	-0.7779580
H	1.5021880	-0.7433200	1.2307670
C	-2.0231200	1.1211990	-0.6376880
H	-2.5652200	1.6352310	0.1489760
C	-2.7278240	0.2932200	-1.6453660
H	-2.4408310	0.5535060	-2.6698960
C	-4.2447870	0.1291490	-1.5557210
H	-4.6729950	1.0860890	-1.8832460
C	-4.8338090	-0.2449270	-0.1978670
H	-4.5331710	0.4889900	0.5605300
C	-6.3586360	-0.3328540	-0.2394240
H	-6.8039880	0.6260990	-0.5241330
H	-6.7656680	-0.6096810	0.7371610
H	-6.6942250	-1.0822550	-0.9641100
C	-0.6438030	1.4528020	-0.9401030
H	-0.0215940	0.1067120	-1.2128320
H	-0.1430570	1.9596560	-0.1198600
C	-0.1412320	1.9195250	-2.2660670
H	-0.4704560	1.3874930	-3.1556080
C	0.6941410	2.9623650	-2.3991900
H	0.9984660	3.2257440	-3.4107670
C	1.2353440	3.8105980	-1.2771170
H	1.5361350	4.7856970	-1.6738480
H	0.4274340	4.0213370	-0.5671390
C	2.4298340	3.1774620	-0.5275320
H	3.3443200	3.3371950	-1.1100150
H	2.2944270	2.0895360	-0.4904520
C	2.6336720	3.7210390	0.8947520
H	2.7679400	4.8090860	0.8496590
H	3.5748740	3.3185830	1.2913840
C	1.4962760	3.4059740	1.8784150
H	1.6836930	3.9318220	2.8221520
H	0.5562910	3.8296130	1.4977780
C	1.2930040	1.9111980	2.1631210
H	1.4155500	1.3496930	1.2307450
H	2.0819720	1.5529460	2.8385590
C	-0.0813450	1.6069360	2.7633570
H	-0.8669850	1.9813630	2.0935350
H	-0.1929180	2.1737780	3.6960150
C	-0.3765120	0.1343800	3.0960670
H	0.4226200	-0.2535560	3.7422670
H	-1.2904640	0.1001360	3.6982930
H	-4.5590830	-0.6082110	-2.3041310
H	-2.2187090	-0.8058800	-1.6414850
C	4.8943620	-1.5892280	-0.5452290
H	5.6026130	-0.8793670	-0.0969750
C	4.3012950	-0.9798330	-1.8008420
H	5.0952170	-0.7640980	-2.5208320
H	3.7854260	-0.0425690	-1.5748130
C	3.5931500	-1.6680280	-2.2737270
H	5.5875180	-2.9194710	-0.7915620
H	6.4271130	-2.7885430	-1.4804070
H	4.8954590	-3.6454980	-1.2299640
H	5.9917080	-3.3401700	0.1363120
H	-4.4201030	-1.2087200	0.1234700

O	3.8024190	-1.7538570	0.4024410
H	4.1523350	-2.2093690	1.1789350

TS14-15

Ru	1.3931730	0.1682920	0.3389600
O	-0.7176920	2.8419780	0.4973220
H	-1.6874960	2.6013570	0.4507640
C	0.3480460	-0.2574740	2.2544910
C	1.7072480	0.1222570	2.5076620
C	2.2339220	1.3588640	2.0662120
C	1.4023950	2.1878050	1.2837600
C	0.0024360	1.9184590	1.1193080
C	-0.4900760	0.6658240	1.5448690
H	2.3485790	-0.5734800	3.0390440
H	3.2705950	1.6212020	2.2389580
H	1.7938750	3.0928440	0.8296460
H	-1.5260920	0.4150040	1.3434770
C	2.0461640	-1.1564910	-1.1916640
H	2.6706980	-2.0521120	-1.2328690
C	2.5508150	0.0917040	-1.8836890
H	2.0185960	0.2154680	-2.8331770
C	4.0594970	0.2194600	-2.0983110
H	4.3528540	-0.5809970	-2.7913020
C	4.9435080	0.1623460	-0.8532230
H	4.7955740	-0.7906860	-0.3275790
C	6.4248850	0.3244920	-1.1895820
H	6.7692840	-0.4680590	-1.8620900
H	7.0412600	0.2838070	-0.2871900
H	6.6173870	1.2838610	-1.6813080
C	0.6009260	-1.2672700	-1.1124220
H	2.5742440	-0.9542600	0.1681620
H	0.2458530	-2.1876420	-0.6567280
C	-0.3155350	-0.6651830	-2.0918710
H	-0.0389530	0.3047970	-2.4996190
C	-1.4694990	-1.2012230	-2.5392240
H	-2.0285780	-0.6170760	-3.2703930
C	-2.0888210	-2.5043250	-2.1399970
H	-2.2836130	-3.1022270	-3.0396870
H	-1.3789090	-3.0871610	-1.5474790
C	-3.4097870	-2.3197740	-1.3548460
H	-4.2495750	-2.2537130	-2.0557930
H	-3.3841650	-1.3547160	-0.8346150
C	-3.6914180	-3.4293830	-0.3318640
H	-3.9021280	-4.3718750	-0.8522820
H	-4.6117770	-3.1704640	0.2070670
C	-2.5589110	-3.6723330	0.6769400
H	-2.9112670	-4.3696300	1.4470890
H	-1.7280640	-4.1915870	0.1798420
C	-2.0169420	-2.4063020	1.3469180
H	-1.8061900	-1.6510490	0.5814570
H	-2.7878090	-1.9772050	2.0034370
C	-0.7433350	-2.6688010	2.1467360
H	0.0456010	-3.0388820	1.4787100
H	-0.9297620	-3.4793000	2.8626180
C	-0.2008740	-1.4852870	2.9576390
H	-0.9934630	-1.1241230	3.6282750
H	0.5902880	-1.8616790	3.6144970
H	4.2473070	1.1592770	-2.6311230
H	2.1703350	1.0121570	-1.3008650
C	-4.1569780	2.7211950	-0.5817080
H	-5.0468500	2.0774450	-0.5633630
C	-3.4098000	2.5052410	-1.8834240
H	-4.0638860	2.7298020	-2.7301820
H	-3.0772630	1.4674810	-1.9722150
H	-2.5357400	3.1619090	-1.9464930
C	-4.5660890	4.1676820	-0.3560350
H	-5.2430180	4.4997450	-1.1485510
H	-3.6910200	4.8254230	-0.3555760
H	-5.0959520	4.2921770	0.5954130
H	4.6331490	0.9496450	-0.1530970
O	-3.2827330	2.2677210	0.4880210
H	-3.6907780	2.5131760	1.3280770

TS15-16

Ru	1.2461200	-0.5179420	-0.2143150
O	2.6519470	-0.7602620	-3.1895870
H	2.9701800	0.0943880	-3.5078580
C	3.3787460	0.0537260	0.3842190
C	3.0447310	-1.1928380	0.9622890
C	2.4990430	-2.2300920	0.1518330

C	2.3653220	-2.0777620	-1.2526170
C	2.7766750	-0.8552730	-1.8568080
C	3.1947490	0.2176730	-1.0314770
H	3.1484310	-1.3355430	2.0326130
H	2.1555460	-3.1491030	0.6138630
H	1.9523930	-2.8678460	-1.8690970
H	3.4334210	1.1760470	-1.4853510
C	-3.2504060	-0.5016720	-0.2998500
H	-2.8535120	0.3256780	0.2974210
C	-4.2386630	0.0486050	-1.3375650
H	-3.6879330	0.6923880	-2.0363270
C	-5.4051720	0.8360690	-0.7306610
H	-5.0115780	1.6424250	-0.0941140
C	-6.4018300	-0.0040240	0.0717180
H	-5.8954500	-0.4881540	0.9170040
C	-7.5773330	0.8165070	0.5981940
H	-7.2372450	1.6170130	1.2646600
H	-8.2789350	0.1931980	1.1606490
H	-8.1330060	1.2841280	-0.2219860
C	-2.1387050	-1.3459730	-0.9266690
H	-3.7816540	-1.1448700	0.4105980
H	-1.3162110	-1.5012340	0.0577130
C	-1.1081910	-0.8561100	-1.7671710
H	-0.8056540	-1.5093460	-2.5873410
C	-0.2433650	0.2555490	-1.6135560
H	0.3110260	0.5203230	-2.5145540
C	-0.3175720	1.3164800	-0.5648930
H	-1.2133380	1.2278400	0.0524360
H	0.4956760	1.1364750	0.2672760
C	-0.0747960	2.7478330	-1.0492580
H	-0.8749810	2.9920720	-1.7579060
H	0.8530990	2.7719930	-1.6344310
C	-0.0440530	3.8127200	0.0602180
H	-1.0669930	3.9999460	0.4082390
H	0.2995210	4.7545970	-0.3839010
C	0.8237290	3.4517210	1.2735150
H	0.8275630	4.2918660	1.9766880
H	0.3441720	2.6258650	1.8174990
C	2.2591780	3.0483570	0.9105310
H	2.2442030	2.5634940	-0.0719930
H	2.8837240	3.9404630	0.7807700
C	2.9217620	2.0865200	1.9052710
H	2.1606260	1.4585870	2.3862510
H	3.4142830	2.6414710	2.7106850
C	3.9579250	1.1629190	1.2403460
H	4.6403240	1.7599500	0.6243090
H	4.5724780	0.6888390	2.0128260
H	-5.9451870	1.3361920	-1.5452410
H	-4.6319380	-0.7832190	-1.9375840
H	-6.7771990	-0.8175200	-0.5639510
C	-0.7404260	-3.3919070	1.8400230
H	-1.7985160	-3.4152320	1.5599980
H	-0.6211840	-4.0018590	2.7407040
H	-0.1674120	-3.8597820	1.0332450
C	-0.2784570	-1.9614540	2.0992180
H	0.7666900	-1.9815760	2.4319250
C	-1.1119070	-1.2673640	3.1689350
H	-2.1610090	-1.2069680	2.8625240
H	-0.7463730	-0.2521010	3.3471310
H	-1.0661240	-1.8195880	4.1129750
O	-0.3341180	-1.1803700	0.8923650
H	-2.5197300	-2.3080730	-1.2754520

TS17-18

Ru	3.3553060	-0.5154030	-0.2549000
O	1.5604020	-2.5872870	-2.1732850
H	0.6237220	-2.3550050	-2.1326920
C	2.6060700	0.9495950	-1.7439690
C	4.0156780	0.7648610	-1.8891250
C	4.5602230	-0.5359090	-2.0584430
C	3.7233570	-1.6775670	-2.1905940
C	2.3293220	-1.4967400	-2.0930280
C	1.7819330	-0.2085210	-1.7839060
H	4.6759420	1.6213880	-1.8085780
H	5.6377910	-0.6660060	-2.0726550
H	4.1289040	-2.6732060	-2.3251210
H	0.7130950	-0.1108690	-1.6219620
C	-7.3307590	0.1036590	1.0968810
H	-8.3181550	0.5694230	1.2123560
C	-6.9909450	0.0028200	-0.3910480
H	-6.8709930	1.0199380	-0.7901910

C	-8.0336710	-0.7380430	-1.2347350
H	-9.0110520	-0.2485480	-1.1165080
C	-8.1763910	-2.2291270	-0.9208440
H	-8.4918060	-2.3642730	0.1214030
C	-9.1700460	-2.9364210	-1.8399290
H	-10.1702370	-2.4974450	-1.7540750
H	-9.2544690	-4.0006000	-1.5977470
H	-8.8661560	-2.8573120	-2.8899310
C	-6.3061400	0.9139350	1.9082020
H	-7.4149330	-0.8998580	1.5339960
H	-6.2308800	1.9267030	1.4960720
C	-4.9587370	0.2560610	1.9775040
H	-4.9807100	-0.7771790	2.3303250
C	-3.7610590	0.7729910	1.6774040
H	-2.8907060	0.1247710	1.8061530
C	-3.4429280	2.1524650	1.1778280
H	-4.3478060	2.7663790	1.1170590
H	-2.7883240	2.6515980	1.9080300
C	-2.7536960	2.1371120	-0.1955060
H	-3.4495160	1.7039500	-0.9244890
H	-1.8935890	1.4530440	-0.1544600
C	-2.3046560	3.5231850	-0.6809490
H	-3.1523730	4.2104140	-0.5701950
H	-2.1039900	3.4843130	-1.7605660
C	-1.0753480	4.1121100	0.0388790
H	-1.2127600	5.1912050	0.1701850
H	-1.0029660	3.7012200	1.0551870
C	0.2618460	3.9111860	-0.6851030
H	0.2101950	4.3951870	-1.6704260
H	1.0478130	4.4399660	-0.1285930
C	0.6856550	2.4519690	-0.8720680
H	-0.0796860	1.9327070	-1.4615870
H	0.7318270	1.9516040	0.1047530
C	2.0417100	2.3370950	-1.5681710
H	1.9696180	2.7697450	-2.5771080
H	2.7842820	2.9447300	-1.0380740
H	-7.7714300	-0.6273310	-2.2959560
H	-6.0120690	-0.4834850	-0.5074480
H	-7.1913950	-2.7103500	-1.0043980
C	5.5422800	1.3298990	1.1932320
H	6.3670530	1.3464890	1.9162300
H	5.0357390	2.2963170	1.2498410
H	5.9684100	1.1859970	0.2007300
C	4.6287420	0.1782250	1.5721000
H	3.1912380	0.5880440	0.9525310
C	4.1324680	0.2306920	3.0058290
H	4.9943660	0.0183380	3.6496340
H	3.3680000	-0.5192310	3.2026530
H	3.7474470	1.2183000	3.2704810
O	4.8821360	-1.0005430	1.0618150
H	-6.6883190	1.0283840	2.9329050
C	0.7348250	-1.3396430	2.6986470
H	1.3071690	-1.6331470	3.5856170
H	-0.3252220	-1.4466280	2.9472390
H	0.9272180	-0.2850950	2.4825000
C	1.0748500	-2.2168480	1.5072960
H	0.4620200	-1.9206630	0.6505530
C	0.9049970	-3.7021910	1.7757250
H	1.5409110	-4.0254810	2.6078580
H	1.1593710	-4.2931330	0.8925310
H	-0.1309500	-3.9180250	2.0528160
O	2.4326960	-1.9827630	1.0365170
H	3.1055430	-2.2658860	1.6756620

TS18-19

Ru	3.2542140	-0.4866430	-0.2901730
O	1.6048440	-2.5836040	-2.3537450
H	0.6648790	-2.3662040	-2.3113480
C	2.5799810	0.9657070	-1.7681770
C	3.9931570	0.8094210	-1.8764750
C	4.5516170	-0.4872980	-2.0619290
C	3.7526170	-1.6366890	-2.2862470
C	2.3568530	-1.4892720	-2.2039480
C	1.7835930	-0.2199840	-1.8465910
H	4.6427270	1.6693860	-1.7555500
H	5.6313980	-0.6010560	-2.0494140
H	4.1863690	-2.6119390	-2.4704930
H	0.7087170	-0.1463920	-1.7102710
C	-7.3885710	0.0648870	1.1661920
H	-8.3694350	0.5359170	1.3124070
C	-7.0767490	0.0021410	-0.3299400

H	-6.9531800	1.0286090	-0.7031440
C	-8.1425480	-0.7035960	-1.1749370
H	-9.1118570	-0.2060370	-1.0271680
C	-8.2982370	-2.2008410	-0.8989910
H	-8.6006000	-2.3603130	0.1436850
C	-9.3130540	-2.8714970	-1.8224380
H	-10.3064070	-2.4227070	-1.7113360
H	-9.4075660	-3.9406260	-1.6072700
H	-9.0223060	-2.7682760	-2.8740770
C	-6.3420140	0.8438920	1.9802580
H	-7.4740930	-0.9495280	1.5771040
H	-6.2629340	1.8657170	1.5920170
C	-5.0003680	0.1713750	2.0106030
H	-5.0251640	-0.8664560	2.3494320
C	-3.8046650	0.6803550	1.6895420
H	-2.9385360	0.0214220	1.7891330
C	-3.4851300	2.0626160	1.1987170
H	-4.3874420	2.6820310	1.1577450
H	-2.8164170	2.5511670	1.9232670
C	-2.8173140	2.0563580	-0.1851080
H	-3.5214720	1.6203990	-0.9044180
H	-1.9512570	1.3791390	-0.1603590
C	-2.3873960	3.4470410	-0.6739420
H	-3.2423970	4.1244030	-0.5576320
H	-2.1940770	3.4087770	-1.7548570
C	-1.1594670	4.0510450	0.0357870
H	-1.3120350	5.1275260	0.1725760
H	-1.0705660	3.6377620	1.0498330
C	0.1731420	3.8723180	-0.7019540
H	0.1021310	4.3539030	-1.6873680
H	0.9546220	4.4169620	-0.1544540
C	0.6250180	2.4215500	-0.8891750
H	-0.1340610	1.8831570	-1.4699270
H	0.6946300	1.9256520	0.0881410
C	1.9776600	2.3368480	-1.5960820
H	1.8858140	2.7633610	-2.6060630
H	2.7072040	2.9639840	-1.0707810
H	-7.8965960	-0.5673620	-2.2370920
H	-6.1055310	-0.4906950	-0.4779750
H	-7.3203190	-2.6908300	-1.0095630
C	6.2774940	0.7752140	1.0141550
H	7.1628900	0.7869370	1.6627450
H	5.9385280	1.8125290	0.9362400
H	6.5576430	0.3897840	0.0348170
C	5.2286540	-0.0783950	1.6621160
H	2.8333010	0.5910890	0.8016470
C	4.8333410	0.2700160	3.0649640
H	5.6135680	-0.1203060	3.7327660
H	3.8848010	-0.1913770	3.3365590
H	4.7909940	1.3506050	3.2196350
O	4.8209810	-1.1340270	1.1311420
H	-6.7059030	0.9366270	3.0137760
C	1.0105490	-1.0082680	2.8412080
H	1.6492680	-1.4332900	3.6248390
H	0.0050200	-0.9108730	3.2606800
H	1.3726370	-0.0093670	2.5833060
C	0.9788790	-1.9068050	1.6190610
H	0.3282920	-1.4701280	0.8559620
C	0.5453470	-3.3309130	1.9227590
H	1.2063190	-3.7933860	2.6644640
H	0.5555110	-3.9461450	1.0197160
H	-0.4678130	-3.3356250	2.3353160
O	2.2808880	-1.9550480	0.9611130
H	2.9672420	-2.2175520	1.5957140

TS22-23

Ru	0.4544820	-0.8653400	-0.1573790
O	-0.6835210	-1.1261310	-3.2246140
H	-0.5878590	-0.2844330	-3.6892670
C	2.4570320	-0.6468010	-1.3111730
C	2.3782940	-1.8172330	-0.4878030
C	1.3317000	-2.7599010	-0.6779660
C	0.3105120	-2.5359150	-1.6313590
C	0.3385230	-1.3374020	-2.3863150
C	1.3834260	-0.3856410	-2.1944250
H	3.1300250	-2.0010050	0.2710300
H	1.2594600	-3.6152410	-0.0152440
H	-0.5171080	-3.2240270	-1.7543400
H	1.3825840	0.5363930	-2.7706750
H	-1.7307610	1.1006270	1.9015250
C	-0.9577650	1.4240360	1.1976920

C	0.4012350	0.8239840	1.6119760
H	0.2893830	0.5188730	2.6726610
C	-2.8027420	1.3260790	-0.6413260
H	-2.9092620	1.1107080	-1.7121940
C	-3.8994060	0.5838510	0.1240800
H	-3.6900710	-0.4945410	0.0827890
C	-5.3096020	0.8305220	-0.4248100
H	-5.3426620	0.5370710	-1.4839190
C	-5.8169650	2.2674160	-0.2783420
H	-5.1670620	2.9561900	-0.8341080
C	-7.2544880	2.4356870	-0.7650860
H	-7.3494820	2.1694140	-1.8236110
H	-7.5949170	3.4691130	-0.6515420
H	-7.9415660	1.7958520	-0.2008430
C	-1.3602950	1.0096320	-0.2153970
H	-2.9284690	2.4116360	-0.5343100
H	-1.3202340	-0.1359040	-0.3176190
H	-0.9356790	2.5195440	1.2592250
C	1.5947410	1.7772670	1.6524390
H	1.3956920	2.5152120	2.4453290
H	2.4676930	1.2154710	1.9982150
C	1.9172440	2.5333550	0.3681070
H	1.0715660	3.1849830	0.1095650
H	1.9876230	1.8124760	-0.4498620
C	3.1756340	3.4153200	0.4368860
H	2.9470150	4.2748680	1.0804030
H	3.3567510	3.8398920	-0.5599700
C	4.4801680	2.7976180	0.9651420
H	5.1896420	3.6246180	1.0899070
H	4.3224340	2.4066810	1.9790380
C	5.1922460	1.7222040	0.1296390
H	5.4263760	2.1192000	-0.8678200
H	6.1624750	1.5405690	0.6047510
C	4.4610130	0.3719360	-0.0100220
H	3.7989200	0.2280100	0.8503850
H	5.1894410	-0.4451420	0.0318590
C	3.6616230	0.2526860	-1.3167010
H	3.3691370	1.2402890	-1.6845450
H	4.3153220	-0.1583360	-2.1013420
H	-6.0040310	0.1574010	0.0939460
H	-3.8770260	0.8644660	1.1854630
H	-5.7486770	2.5677340	0.7763690
H	-0.6725150	1.4616180	-0.9346010
C	-1.3279000	-2.4694530	3.5172110
H	-0.7366640	-3.3852620	3.6121770
H	-2.3306450	-2.6624090	3.9107980
H	-0.8608650	-1.6958510	4.1331670
C	-1.4011760	-2.0363640	2.0572550
C	-2.0548800	-3.0921750	1.1777210
H	-2.1224760	-2.7567570	0.1374410
H	-3.0707060	-3.3076060	1.5231350
H	-1.4823020	-4.0252080	1.2100230
O	-0.0538170	-1.7794050	1.6371430
H	0.3637180	-0.5028040	1.6733780
H	-1.9917640	-1.1093940	1.9931480