

Supporting Information

Mechanistic Studies on the NNN Pincer-Ruthenium Catalysed Transformation of Ethanol to Ethyl Acetate

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1. Experimental Section

General Procedure and Materials. All manipulations were carried out under an inert atmosphere of purified argon using either a standard Schlenk line or a glovebox unless otherwise stated. Solvents such as dioxane, THF, mesitylene, *o*-xylene, *p*-xylene, *m*-xylene, hexane, and toluene were purified by double distillation over sodium/benzophenone under argon prior to use. Ethanol was dried and distilled according to a literature procedure.¹ Deuterated solvents ethanol- d_6 and $CDCl_3$, ruthenium precursors such as $RuCl_3 \cdot 3H_2O$, and $[RuCl_2(p\text{-cymene})]_2$, as well as pyridine-2,6-dicarboxylic acid, DMSO, and other reagents were purchased from commercial suppliers Sigma-Aldrich or Merck and used as received without further purification. Catalytic reactions were performed in oven-dried glassware under an argon atmosphere or, when specified, under ambient conditions.

Physical Measurements. NMR spectra, including 1H , 2H , $^{13}C\{^1H\}$, and ^{31}P , were recorded on Bruker instruments operating at various field strengths: Bruker ASCEND 600 (1H at 600 MHz, $^{13}C\{^1H\}$ at 150 MHz, and ^{31}P at 564 MHz), Bruker AVANCE 500 (1H at 500 MHz, $^{13}C\{^1H\}$ at 125 MHz, and ^{31}P at 470 MHz), and Bruker AVANCE 400 (1H at 400 MHz, $^{13}C\{^1H\}$ at 100 MHz, and ^{31}P at 376 MHz). Chemical shifts (δ) are reported in parts per million (ppm) relative to residual solvent peaks, and coupling constants (J) are given in hertz (Hz). High-resolution mass spectrometry (HRMS) was carried out on an Agilent Accurate-Mass Q-TOF 6546 ESI-MS instrument. Gas chromatography (GC) analyses were performed using an Agilent 7820 GC system equipped with a Front SS7 inlet and an HP-PLOT Q column (30 m $\times$ 530 μ m $\times$ 40 μ m, N_2 as the carrier gas). The temperature program consisted of an initial temperature of 40 $^\circ$ C (held for 0 min), followed by a ramp of 40 $^\circ$ C min $^{-1}$ up to 250 $^\circ$ C with a final hold time of 5 min. The inlet temperature was maintained at 40 $^\circ$ C, with a split ratio of 195 and a carrier flow rate of 25 mL min $^{-1}$ (N_2). Detector temperatures were set to 250 $^\circ$ C for both thermal conductivity detector (TCD) and flame ionization detector (FID).

General Procedure for the Pincer- Ruthenium-Catalyzed Transformation of Ethanol to Ethyl Acetate: In an argon-filled glovebox, a 5 mL sealed pressure tube was charged with complex **1** (14.63 mg, 0.020 mmol, 0.08 M), NaOEt (4.08 mg, 0.060 mmol, 0.25 M), absolute ethanol (117 μ L, 2.00 mmol, 8.5 M), and toluene (0.117 mL) as co-solvent. The resulting reaction mixture was sealed and heated at 120 $^\circ$ C for 24 h. After cooling to room temperature, a small aliquot was removed, dissolved in $CDCl_3$, and analyzed by 1H NMR spectroscopy. The yield of ethyl acetate was quantified using DMSO as an internal standard.

General procedure for the kinetic studies performed for the **1 catalyzed transformation of ethanol to ethyl acetate.**

(a) Variation in the loading of catalyst **1:** To each of the five 5 mL pressure tube, varying amounts of **1** (1.46-14.63 mg, 0.002 – 0.02 mmol, 0.0085-0.085 M), NaOEt (4.08 mg, 0.06 mmol, 0.25 M), ethanol (117 μ L, 2 mmol, 8.5 M), and toluene (0.117 mL) were added inside the glove box, and the resulting reaction mixture (total volume = 0.234 mL) was heated at 120 $^\circ$ C for 24 h. At regular intervals (Figure 1h and S1) an aliquot was withdrawn from the reaction mixture to an NMR tube, and the yield of EtOAc was determined by 1H NMR using $CDCl_3$ as a solvent and DMSO as a standard.

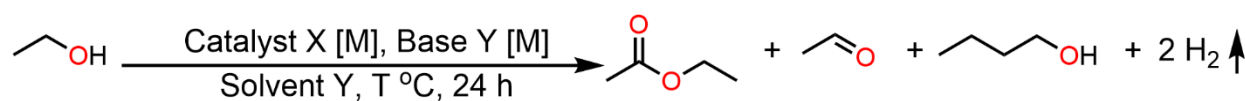
(b) Variation in the loading of NaOEt: To each of the four 5 mL pressure tube **1** (14.63 mg, 0.02 mmol, 0.08 M), varying amounts of NaOEt (1.36- 5.44 mg, 0.02- 0.08 mmol, 0.085- 0.34 M), ethanol (117 μ L, 2 mmol, 8.5 M), and toluene (0.117 mL) were added inside the glove box, and the resulting reaction mixture (total volume = 0.234 mL) was heated at 120 $^\circ$ C for 24 h. At regular intervals (Figure 1g and Figure S2), an aliquot was withdrawn from the reaction mixture

to an NMR tube, and the yield of EtOAc was determined by ^1H NMR using CDCl_3 as a solvent and DMSO as a standard.

(b) Variation in the loading of EtOH: To each of the four 5 mL pressure tube **1** (14.63 mg, 0.02 mmol, 0.08 M), NaOEt (4.08 mg, 0.06 mmol, 0.25 M), varying amounts of ethanol (0.5- 2 mmol, 2.1- 8.5 M), and toluene (0.117 mL or as a makeup solvent at a lower concentration of EtOH) were added inside the glove box, and the resulting reaction mixture (total volume = 0.234 mL) was heated at 120 °C for 24 h. At regular intervals (Figure 1i and Figure S3), an aliquot was withdrawn from the reaction mixture to an NMR tube, and the yield of EtOAc was determined by ^1H NMR using CDCl_3 as a solvent and DMSO as a standard.

2. Optimization of the Reaction Conditions.

Table S1. 1 Catalyzed Dehydrogenative coupling of Ethanol to Ethyl Acetate Under Varying Conditions.

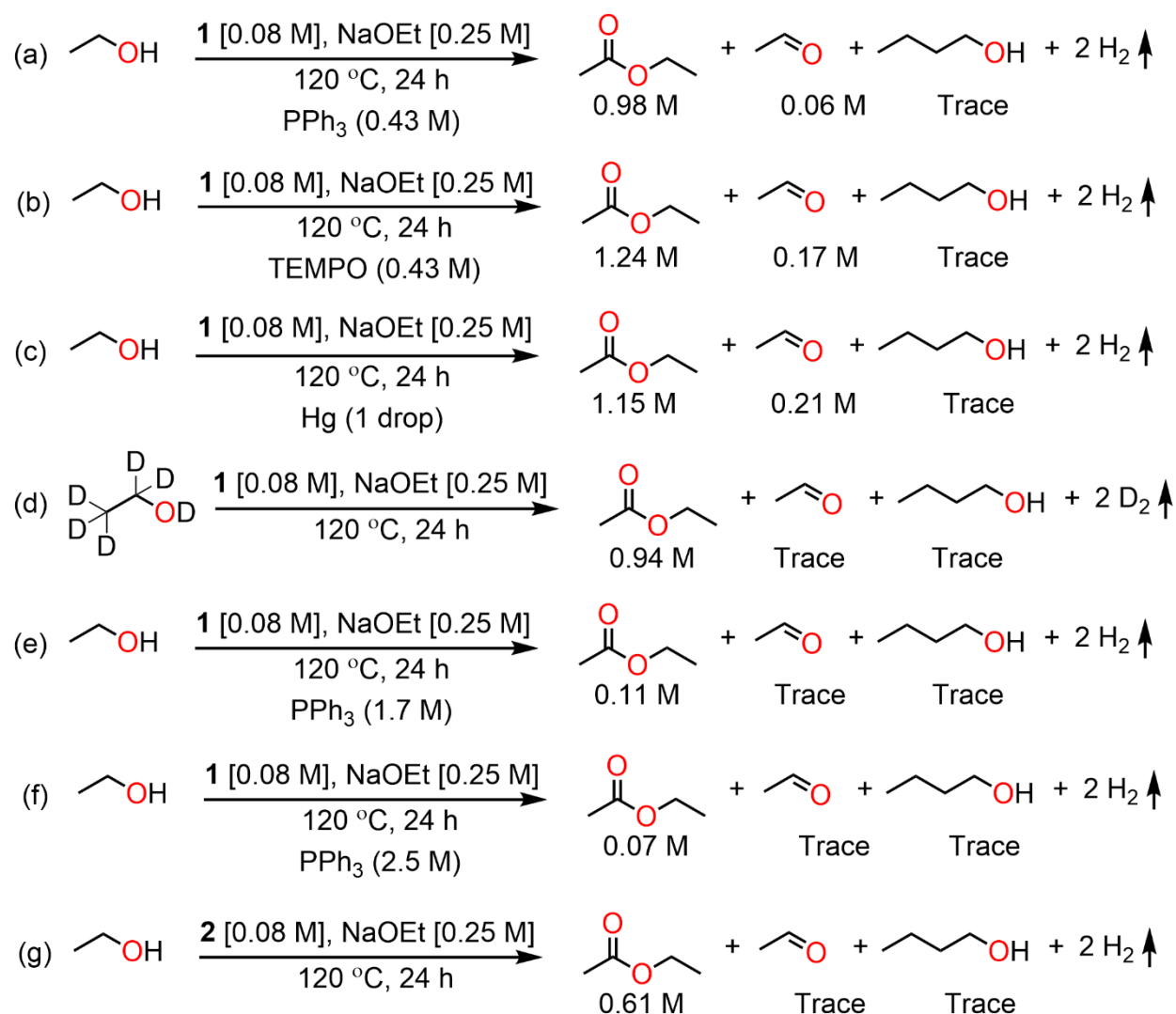


Entry	Catalyst X [M]	Base Y [M]	Temperature (°C)	Solvent (mL)	EtOAc [M]	Benzaldehyde [M]	Butanol [M]
1	1 (0.08 M)	KOtBu (0.25)	140	-	0.43	0.04	0.04
2	1 (0.08 M)	NaOtBu (0.25)	140	-	0.27	0	0.34
3	1 (0.08 M)	NaOH (0.25)	140	-	0.21	0	0
4	1 (0.08 M)	KOH (0.25)	140	-	0.60	Trace	0.13
5	1 (0.08 M)	NaOEt (0.25)	140	-	0.94	Trace	0.21
6	1 (0.08 M)	Na_2CO_3 (0.25)	140	-	0.38	0	0.13
7	1 (0.08 M)	K_2CO_3 (0.25)	140	-	0.21	0	0.13
8	1 (0.08 M)	Cs_2CO_3 (0.25)	140	-	0.47	0.04	0.08
9	1 (0.08 M)	NaHCO_3 (0.25)	140	-	0.64	0	0.34
10	1 (0.08 M)	Na (0.25)	140	-	0.21	0	0.27
11	1 (0.08 M)	NaOEt (0.25)	140	Toluene (0.117)	1.32	Trace	0
12	No Catalyst	NaOEt (0.25)	140	Toluene (0.117)	0	0	0
13	1 (0.08 M)	No Base	140	Toluene (0.117)	0	0	0
14	1 (0.004 M)	NaOEt (0.25)	140	Toluene (0.117)	0.08	0.17	0.17
15	1 (0.008 M)	NaOEt (0.25)	140	Toluene (0.117)	0.17	0.38	0.38
16	1 (0.02 M)	NaOEt (0.25)	140	Toluene (0.117)	0.43	0.27	0.27
17	1 (0.04 M)	NaOEt (0.25)	140	Toluene (0.117)	0.64	0.27	0.13
18	1 (0.17 M)	NaOEt (0.25)	140	Toluene (0.117)	1.11	0	0
19	1 (0.08 M)	NaOEt (0.25)	120	Toluene (0.117)	1.32	0	0
20	1 (0.08 M)	NaOEt (0.25)	130	Toluene (0.117)	1.32	0	0
21	1 (0.08 M)	NaOEt (0.25)	150	Toluene (0.117)	1.11	0	0
22	1 (0.08 M)	NaOEt (0.25)	160	Toluene (0.117)	1.11	0	0
20	1 (0.08 M)	NaOEt (0.25)	100	Toluene (0.117)	0.59	0	0
21	1 (0.08 M)	NaOEt (0.25)	80	Toluene (0.117)	0.17	0	0
23	1 (0.08 M)	NaOEt (0.17)	120	Toluene (0.117)	0.51	0	0
24	1 (0.08 M)	NaOEt (0.08)	120	Toluene (0.117)	0.27	0	0
25	1 (0.08 M)	NaOEt (0.34)	120	Toluene (0.117)	1.28	0	0
26	1 (1 mol%)	NaOEt (3)	120	<i>o</i> -Xylene (0.117)	0.78	0	0
27	1 (1 mol%)	NaOEt (3)	120	<i>p</i> -Xylene (0.117)	0.85	0	0
28	1 (1 mol%)	NaOEt (3)	120	<i>m</i> -Xylene (0.117)	0.94	0	0
29	1 (1 mol%)	NaOEt (3)	120	Mesitylene (0.117)	0.78	0	0
30	1 (1 mol%)	NaOEt (3)	120	Benzene (0.117)	0.94	0	0
31	1 (1 mol%)	NaOEt (3)	120	THF (0.117)	0.73	0	0
32	1 (1 mol%)	NaOEt (3)	120	Dioxane (0.117)	0.08	0	0
33	$\text{RuCl}_3 \cdot 3\text{H}_2\text{O}$	NaOEt (3)	120	Toluene (0.117)	0.60	0.27	0.27
34	$\text{RuCl}_2(\text{PPh}_3)_3$	NaOEt (3)	120	Toluene (0.117)	0.68	0	0
35	$[\text{Ru}(\text{p-cmene})\text{Cl}_2]_2$	NaOEt (3)	120	Toluene (0.117)	0.21	0	0
36	$[\text{Ru}_2(\text{C}_6\text{H}_6)_2\text{Cl}_4]$	NaOEt (3)	120	Toluene (0.117)	0	0.30	0

Reaction conditions: Anhydrous ethanol (0.117 mL, 2.0 mmol, 8.5 M), base (3 mol %, 0.06 mmol, 0.25 M), and **1** (1 mol %, 0.02 mmol, 0.08 M) at T °C. ^bYield of EtOAc, Benzaldehyde and Butanol was calculated by ^1H NMR spectroscopy using DMSO as an internal standard.

3. Control Experiments

Scheme S1. Control Experiments and Mechanistic Insights



4. Kinetics Study

Reaction Profile Diagrams: Kinetic studies were performed by varying the concentrations of catalyst, base and ethanol to determine the rate order dependence. Reactions were conducted in a 5 mL sealed pressure tube, and the concentration of compound EtOAc was monitored over time. The resulting data were plotted as a function of reaction time to assess the reaction kinetics.

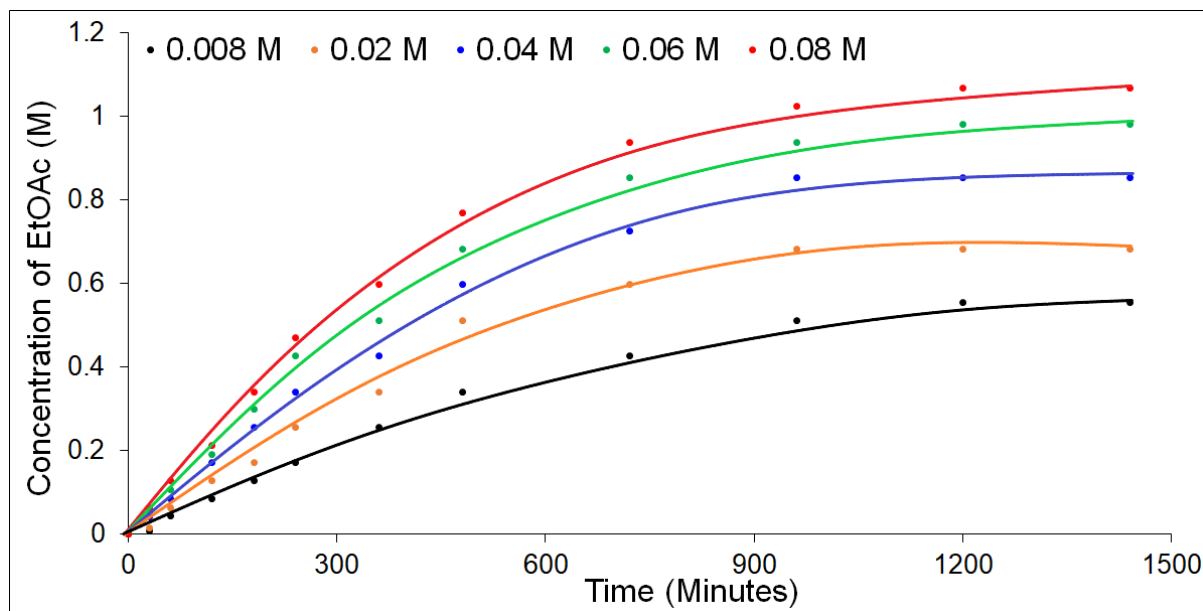


Figure S1: Time-profile of the transformation of ethanol to ethyl acetate of reaction conditions: 8.5 M of EtOH, 0.25 M of NaOEt, 0.117 mL toluene, and 0.1–1 mol %, 0.008 M- 0.08 M of **1** at 120 °C for 24 h in a 5 mL pressure tube.

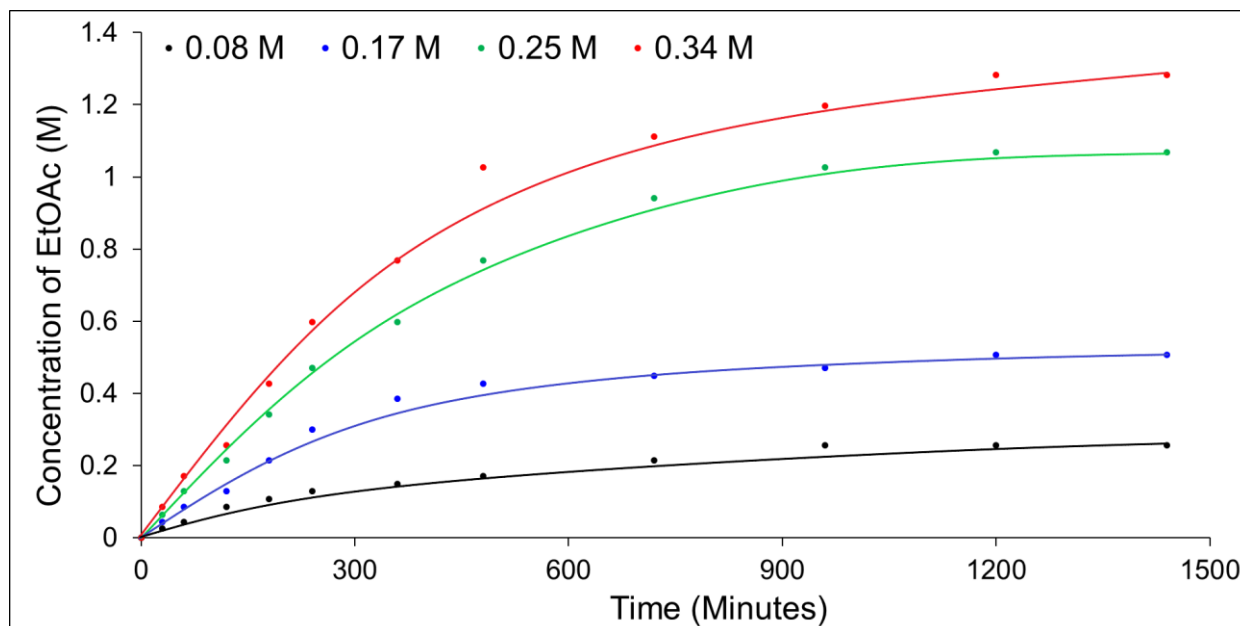


Figure S2: Time-profile of the transformation of ethanol to ethyl acetate of reaction conditions: 2 mmol of Ethanol, 0.08 M **1**, 0.117 mL toluene, and (1-4 mol%, 0.08- 0.34 M) of NaOEt at 120 °C for 24 h in a 5 mL pressure tube.

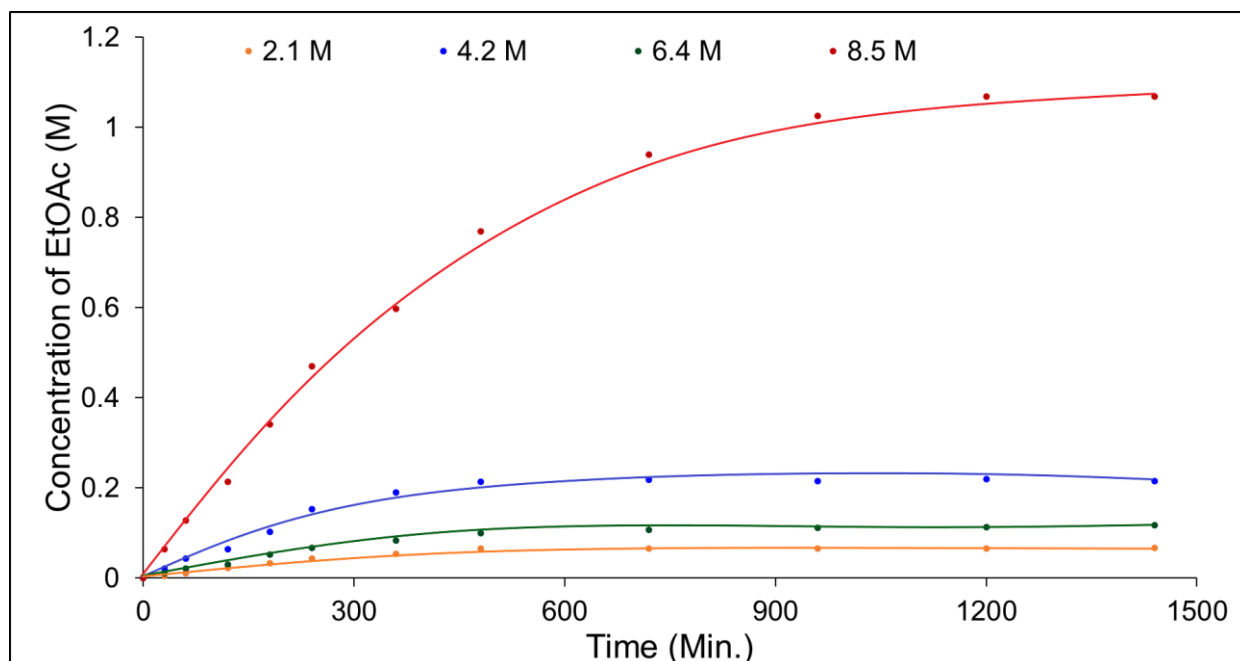


Figure S3: Time-profile of the transformation of ethanol to ethyl acetate of reaction conditions: varying amounts of ethanol (0.5- 2 mmol, 2.1- 8.5 M), 0.08 M **1**, 0.117 mL toluene, and (3 mol%, 0.25 M) of NaOEt at 120 °C for 24 h in a 5 mL pressure tube.

5. GC Analysis:

GC analysis (TCD detection) was performed on a Agilent 7820-GC instrument fitted with Agilent Front SS7 inlet N₂ HP-PLOT Q column (30 m length x 530 µm x 40 µm ID) using the following method:

Agilent 7820-GC Detector

TCD starting temperature 40 °C

Oven temperature 70 °C

Time at starting temp: 0 min

Hold time = 5 min

Ramp : 40 °C/min up to 250 °C

Flow rate (carrier): 25 mL/min (N₂)

Split ratio: 195

Inlet temperature: 40 °C

Detector temperature: TCD: 250

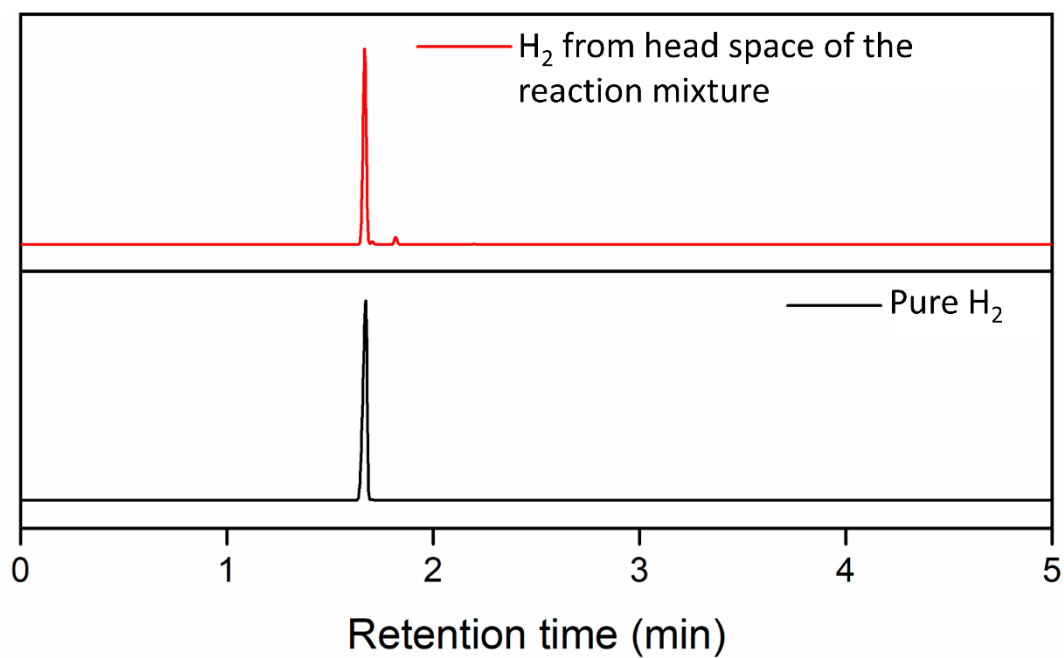


Figure S4. GC-TCD analysis of H₂ gas evolved from transformation of ethanol to ethyl acetate containing 8.5 M of EtOH, 0.25 M of NaOEt, 0.117 mL toluene, and 0.08 M **1** at 120 °C for 24 h in a 5 mL pressure tube

6. HRMS Analysis:

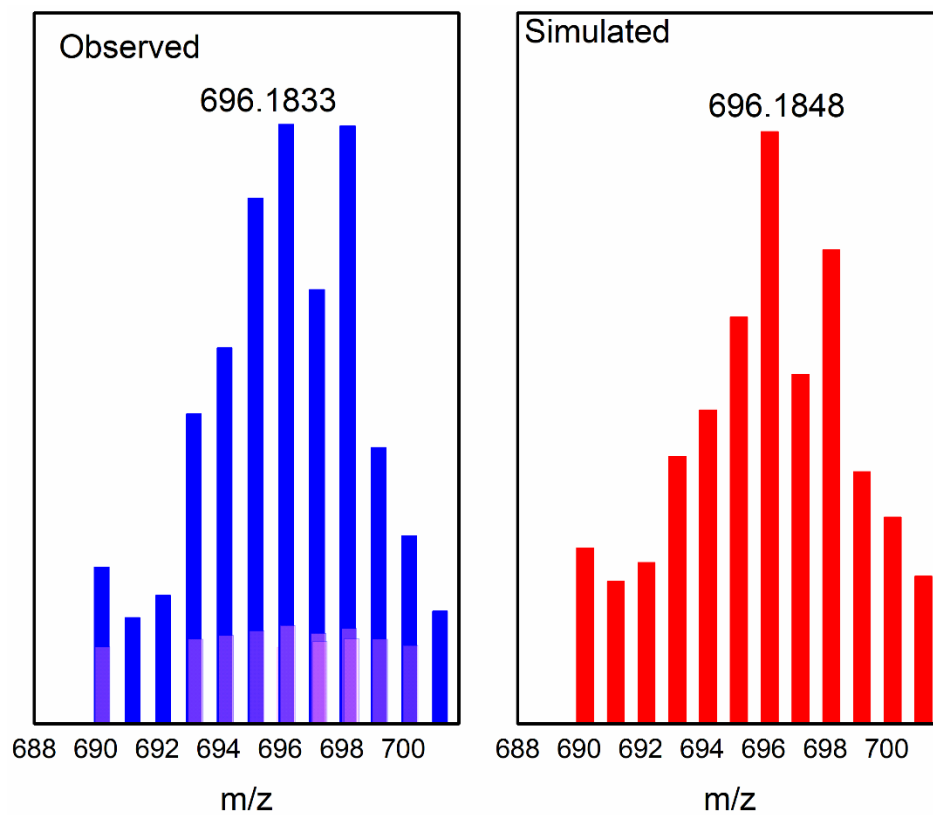


Figure S5: HRMS(ESI) expanded spectrum of m/z 696.1848 of reaction mixture at t = 1h (a) Observed (b) Simulated.

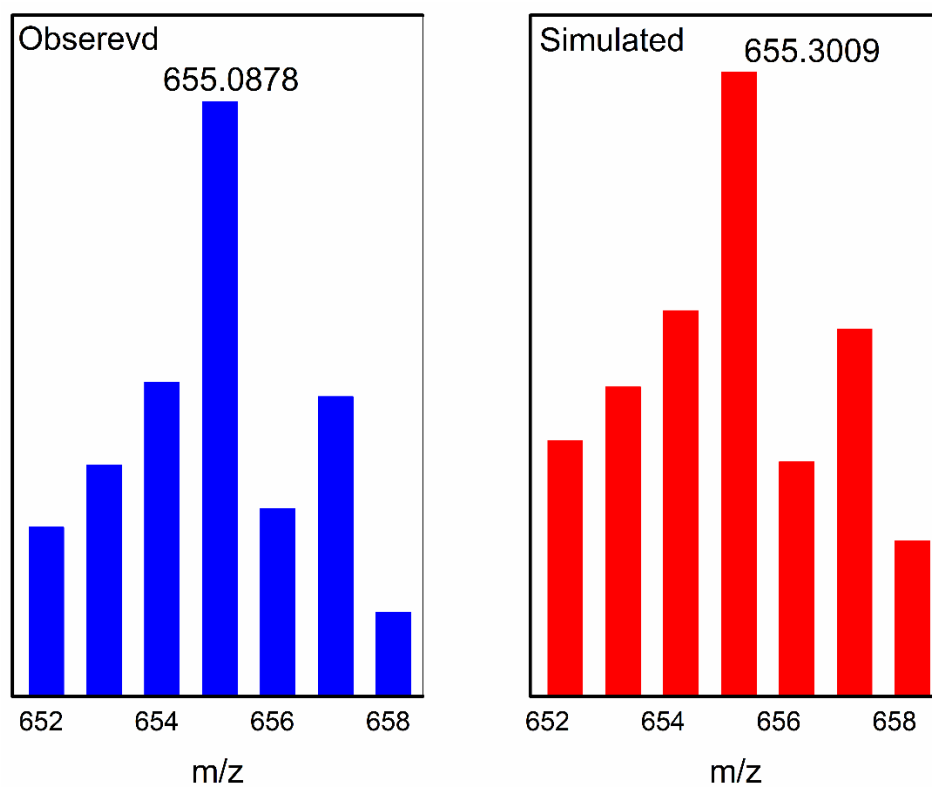


Figure S6: HRMS(ESI) expanded spectrum of m/z 655.3009 of reaction mixture at $t = 1\text{ h}$ (a) Observed (b) Simulated.

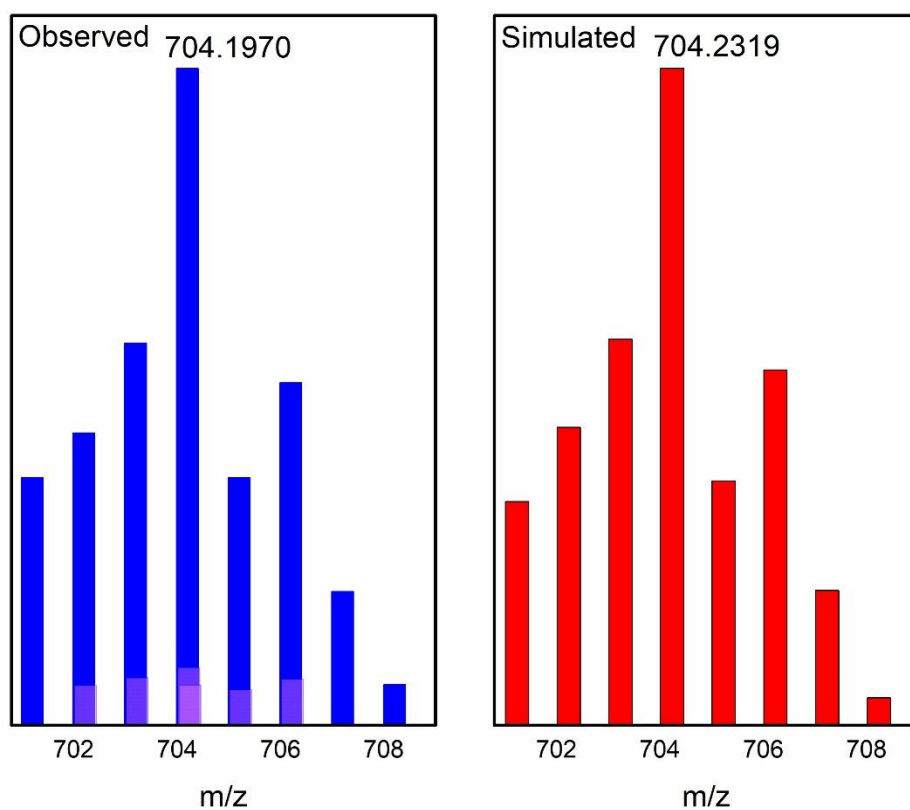


Figure S7: HRMS(ESI) expanded spectrum of m/z 704.2319 of reaction mixture at $t = 1\text{ h}$ (a) Observed (b) Simulated.

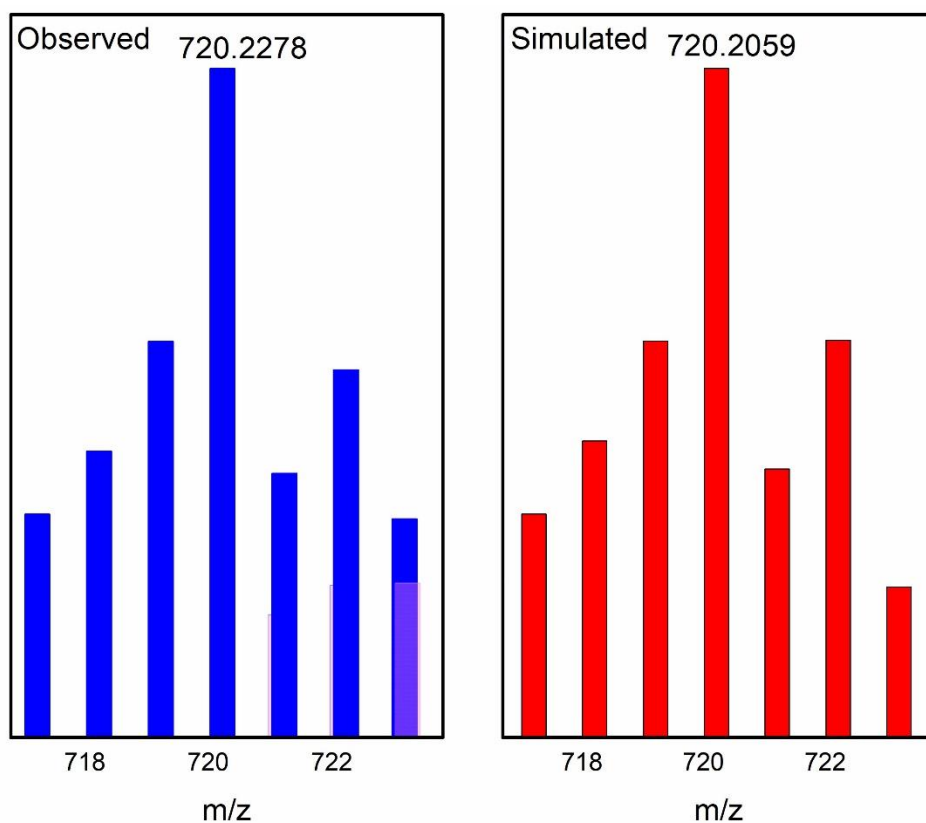


Figure S8: HRMS(ESI) expanded spectrum of m/z 720.2059 of reaction mixture at $t = 1\text{ h}$ (a) Observed (b) Simulated.

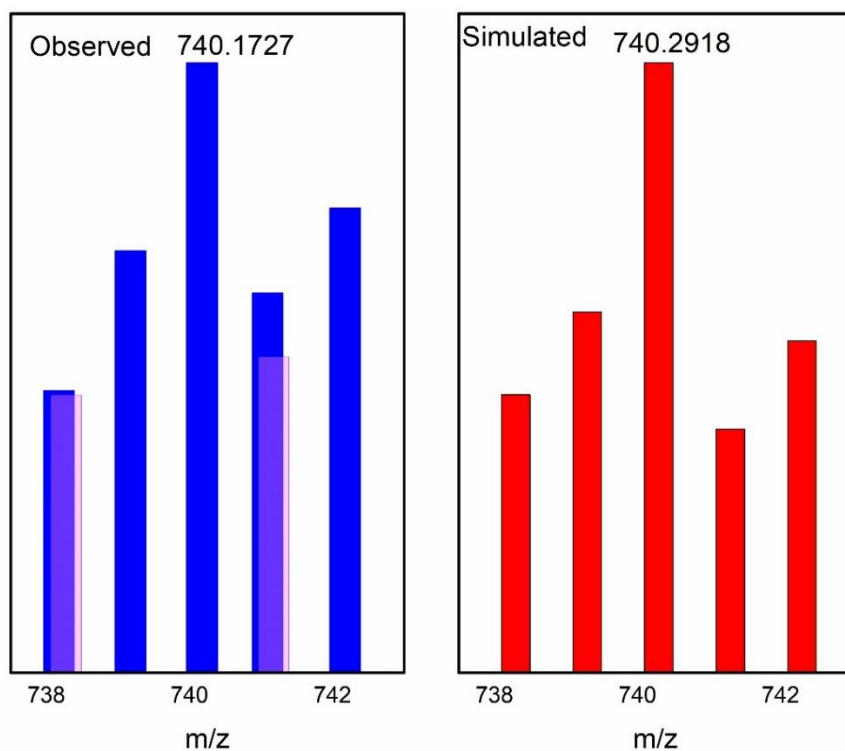


Figure S9: HRMS(ESI) expanded spectrum of m/z 740.2918 of reaction mixture at $t = 1\text{ h}$ (a) Observed (b) Simulated.

7. Representative NMR Spectrum:

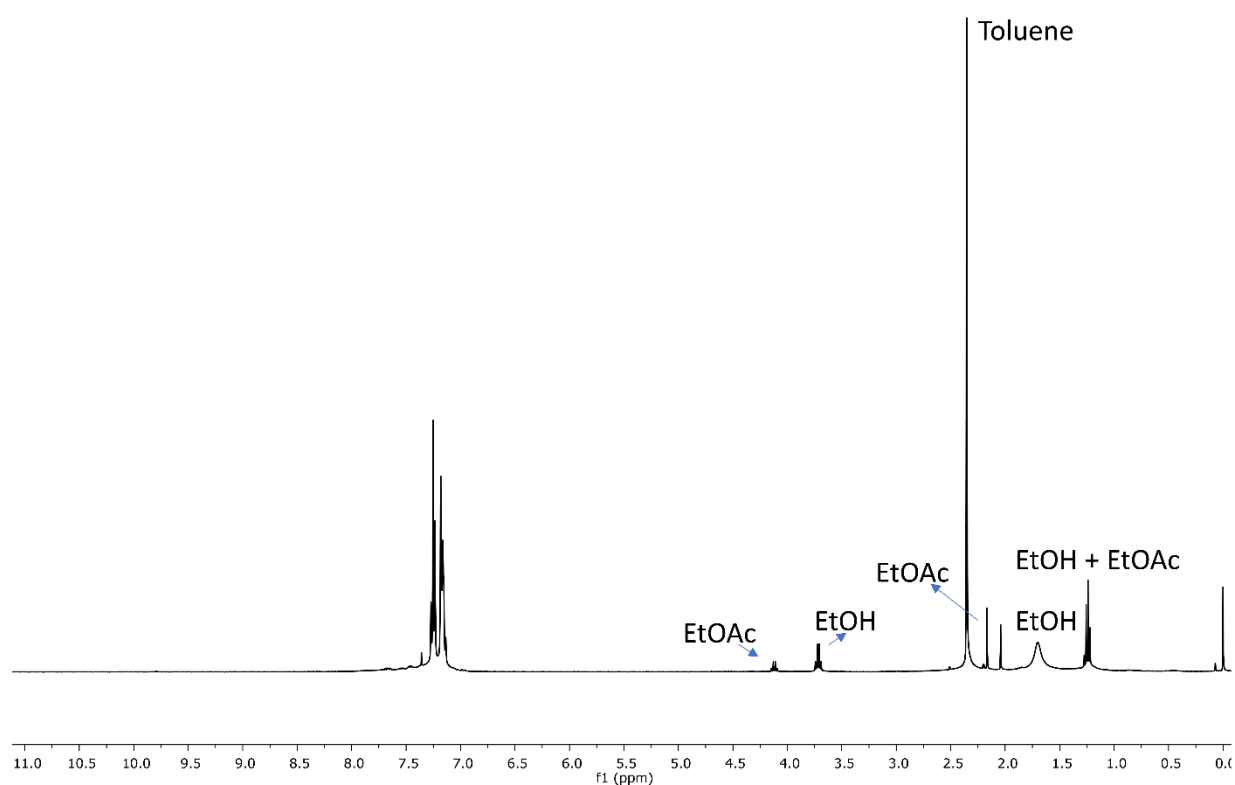
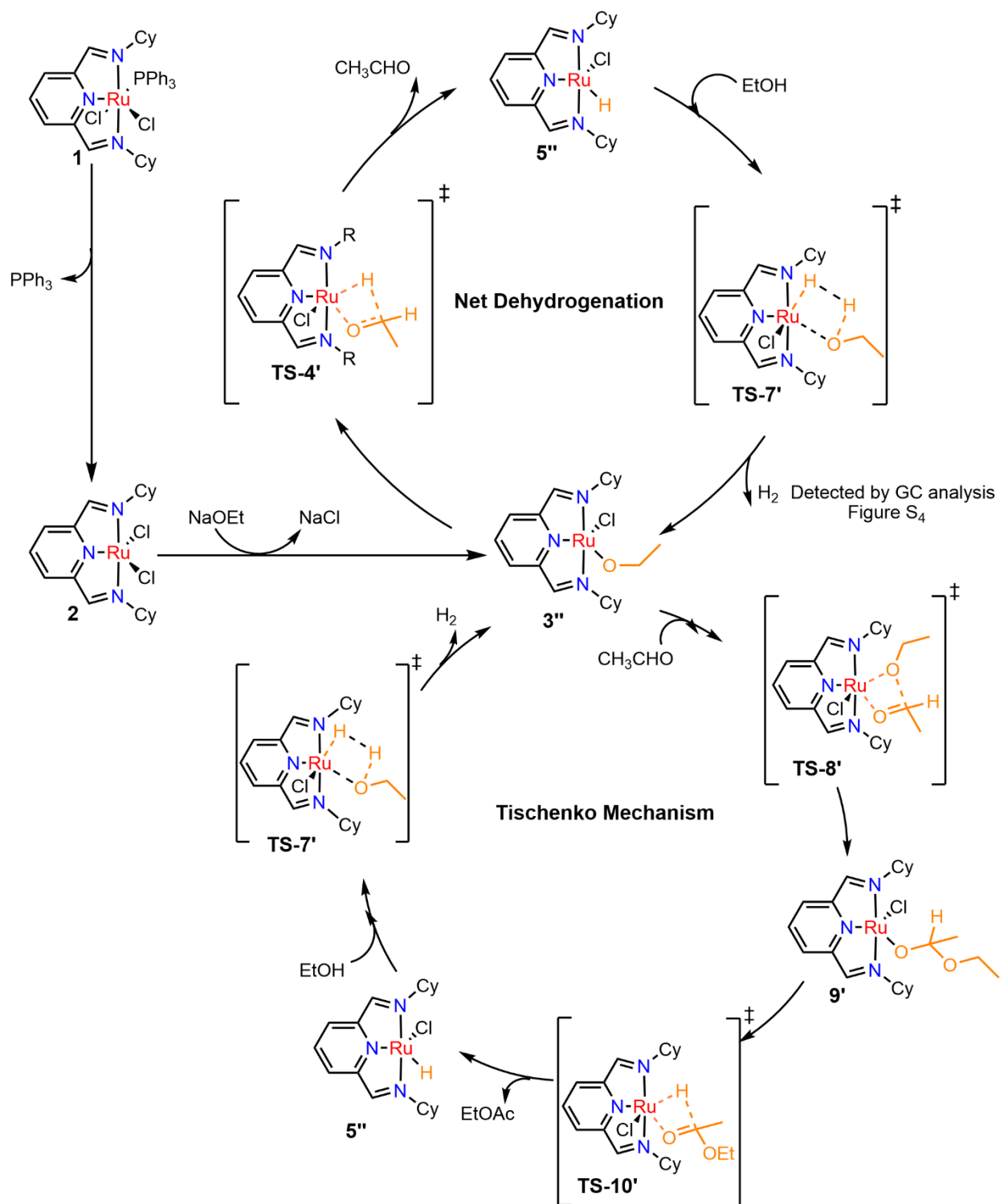


Figure 10: Representative NMR Spectrum of EtOH to EtOAc transformation. Reactions were performed with 8.54 M of EtOH, NaOEt (0.25 M), 0.08 M of **1** and 0.117 mL toluene at 120 °C for 24 h in a 5 mL pressure tube.

8. Proposed Catalytic Pathway Involving Mono-Salt Metathesis:



Scheme S2: Plausible mechanism involving mono salt metathesis in the **1** catalyzed transformation of ethanol to ethyl acetate.

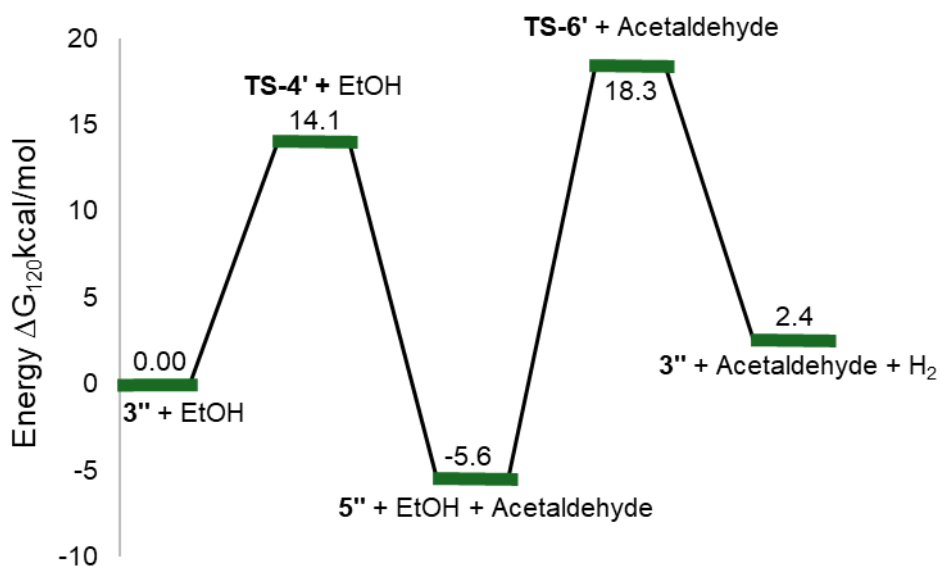


Figure 11. Free energy (ΔG_{120}) profile of **1** catalyzed net dehydrogenation involving mono salt metathesis at 120 °C.

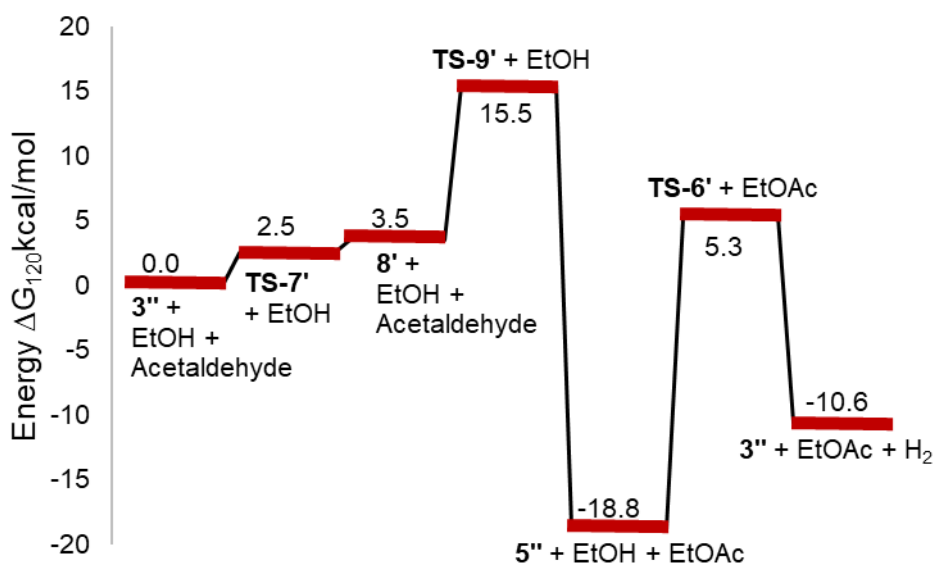


Figure 12. Free energy (ΔG_{120}) profile of **1** catalyzed transformation of ethanol to EtOAc (Tischenko Mechanism) involving mono salt metathesis at 120 °C.

9. Synthesis of $\text{Cy}^2\text{NNNRuCl}_2$ (2**):** In an inert atmosphere glove box, a J. Young NMR tube was charged with $[\text{Ru}(\text{benzene})\text{Cl}_2]_2$ (0.020 g, 0.040 mmol) and the ligand⁵ Cy^2NNN (0.024 g, 0.080 mmol) in dry toluene (0.468 mL). The tube was sealed, removed from the glove box, and subsequently heated at 60 °C for 16 h. HRMS (ESI): m/z calculated for $[\mathbf{2} - \text{Cl} + \text{NCCH}_3]^+ = 475.1203$, found 475.1196; m/z calculated for $[\mathbf{2} - \text{Cl} + 2\text{NCCH}_3]^+ = 516.1468$, found 516.1447.

The resulting solution of $\text{Cy}^2\text{NNNRuCl}_2$ in toluene was employed for the control experiment (Scheme S1g and Figure S16).

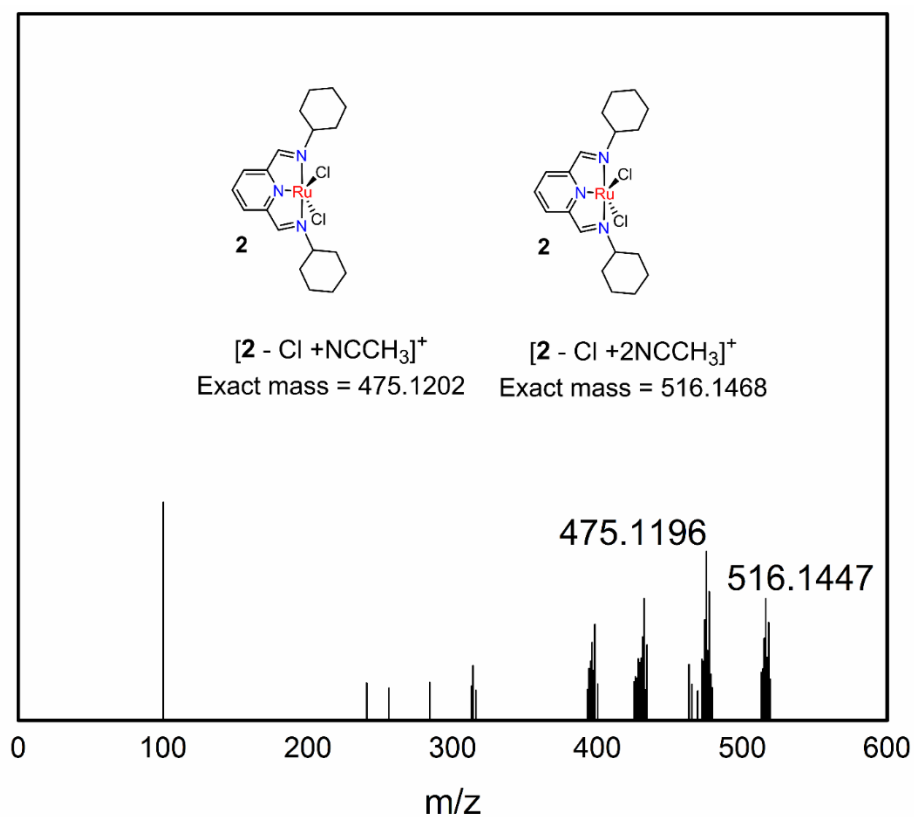


Figure S13: HRMS(ESI) spectrum of **2**

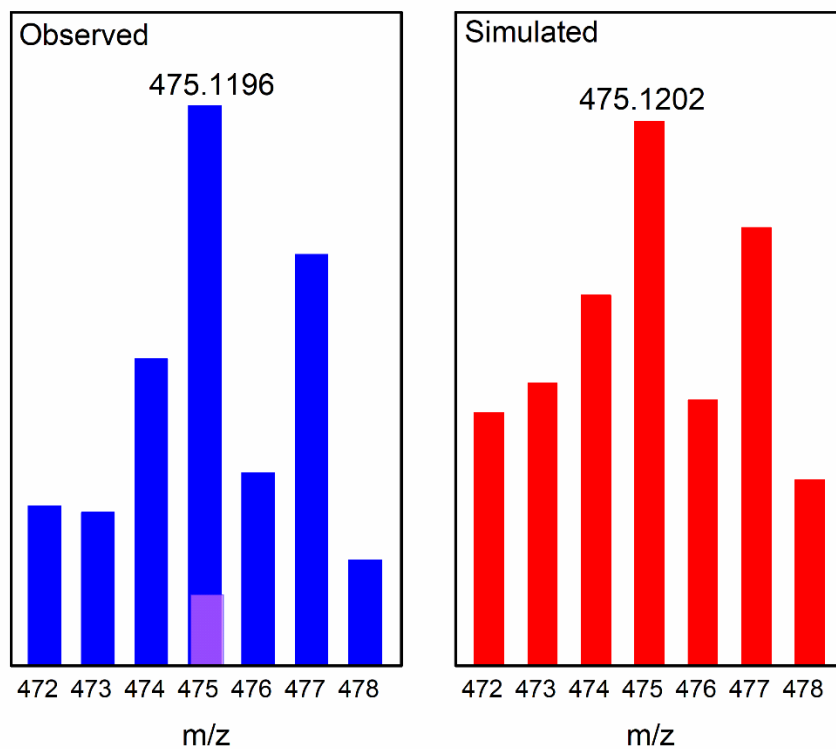


Figure S14: HRMS(ESI) expanded spectrum of m/z 475.1196 of **2** (a) Observed (b) Simulated.

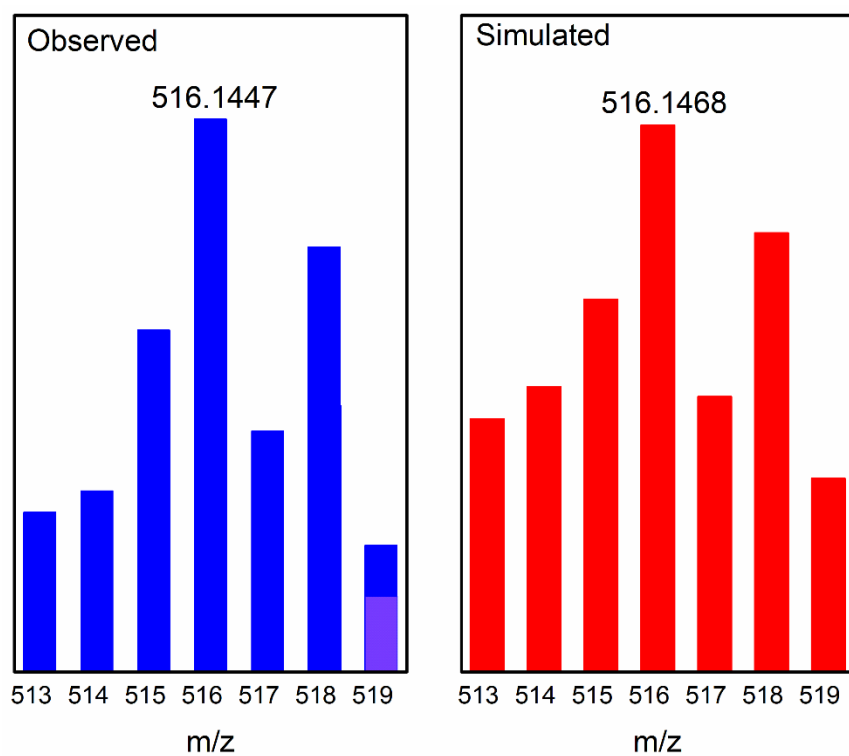


Figure S15: HRMS(ESI) expanded spectrum of m/z 516.1447 of **2** (a) Observed (b) Simulated.

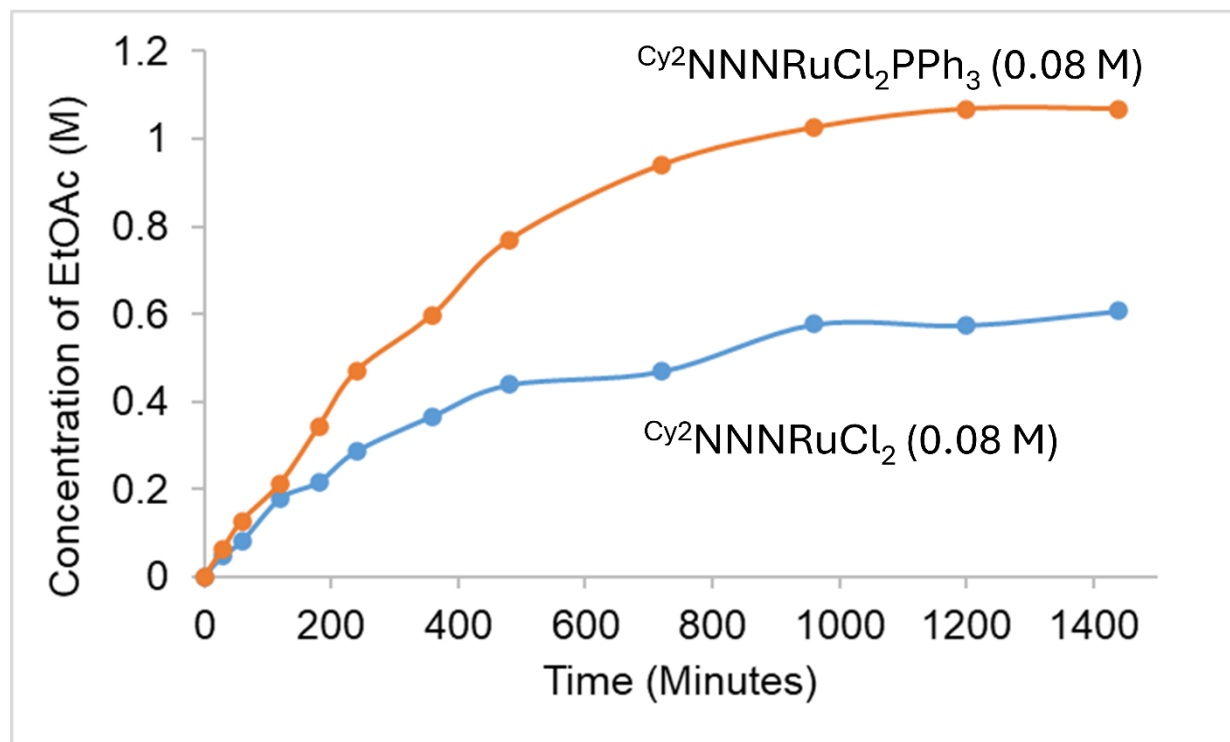


Figure S16: Reactivity of catalyst $\text{Cy}^2(\text{NNN})\text{Ru}(\text{PPh}_3)\text{Cl}_2$ (**1**) versus $\text{Cy}^2(\text{NNN})\text{RuCl}_2$ (**2**)

10. Computational Studies:

Computational details: All geometry optimizations for the studied complexes were carried out using density functional theory (DFT) at the PBE² level of theory, as implemented in the Gaussian 09 software package.³ The LANL2DZ⁴ basis set, including effective core potentials, was employed for the ruthenium center, while the 6-311G(d, p) basis set with polarization functions was used for all non-metal atoms. Empirical dispersion corrections (Grimme's D3) were included in all geometry optimizations and energy calculations to account for long-range interactions. Transition states were located via the synchronous transit-guided quasi-Newton (QST2) method. The basis set definitions were specified using the genecp keyword to accommodate effective core potentials appropriately. The chosen computational methodology and basis sets were guided by precedent in the literature for structurally similar pincer-type metal complexes.²⁰ Frequency calculations were performed to verify the nature of the stationary points-either minima or first-order saddle points-on the potential energy surface. Gibbs free energies (ΔG) were computed from the sum of electronic and thermal free energies at 120°C, in alignment with the experimental reaction conditions.

Optimized XYZ coordinates:

EtOH

C	1.22077600	-0.22431500	0.00005200
H	1.28132800	-0.86716500	-0.89098500
H	1.28131700	-0.86698600	0.89121600
H	2.08483500	0.45800700	-0.00003300
C	-0.08440000	0.55318300	-0.00004700
H	-0.13099700	1.20836800	0.89463100
H	-0.13088000	1.20831700	-0.89477900
O	-1.15251200	-0.40153400	-0.00010600
H	-1.98376700	0.09852000	0.00076400

Acetaldehyde

C	-1.17175000	-0.15086700	0.00009100
H	-1.71672400	0.22472000	-0.88298900
H	-1.15796600	-1.24817900	-0.00120400
H	-1.71704800	0.22335800	0.88329400
C	0.23274500	0.39845900	0.00012300
H	0.29404400	1.52223200	-0.00038100
O	1.24146600	-0.27596000	0.00000000

H₂

H	0.00000000	0.00000000	0.37595000
H	0.00000000	0.00000000	-0.37595000

EtOAc

C	2.14351800	-0.88822200	0.00390300
H	1.87585500	-1.76298100	-0.60316900
H	3.07320500	-0.43299700	-0.35627100
H	2.29771000	-1.23210100	1.03884100

C	1.04226300	0.14641700	-0.01257900
O	1.20053700	1.35114400	-0.00180400
O	-0.18078600	-0.45593400	-0.01633500
C	-1.31672900	0.45305200	0.01209300
H	-1.25558700	1.12311100	-0.86039000
H	-1.24492100	1.08165700	0.91432300
C	-2.57221200	-0.39625000	0.00003400
H	-3.46331300	0.24926800	0.02251900
H	-2.61744200	-1.01657500	-0.90709100
H	-2.60454100	-1.06104900	0.87565300

3

Ru	-0.07609300	-0.04209400	-0.01978900
N	1.98513800	0.29704000	-0.19008100
N	-0.07009900	1.77974000	-0.49510300
N	-2.08668700	0.32885900	-0.03185900
C	2.25672900	1.55189900	-0.52150100
H	3.27835800	1.91095200	-0.66882700
C	1.14488200	2.43148100	-0.70719200
C	-2.39203700	1.58492300	-0.34166100
H	-3.41987700	1.95388500	-0.34175100
C	-1.29460000	2.44448300	-0.64044400
C	1.14340100	3.78217000	-1.06981400
H	2.09647100	4.28802000	-1.23618400
C	-1.28733800	3.79619200	-1.00266800
H	-2.24057900	4.31819800	-1.10858500
C	-0.07443400	4.46583300	-1.21672600
H	-0.07693900	5.51951500	-1.49865800
O	-0.19590300	-1.26968800	-1.57561700
C	0.84364600	-1.66682100	-2.44346500
H	1.52386000	-0.81913900	-2.66629500
H	1.46532800	-2.46758000	-1.98330000
C	0.23414200	-2.19473300	-3.74164300
H	-0.35910300	-1.40662500	-4.22918700
H	1.01949500	-2.53052800	-4.43915600
H	-0.43344600	-3.04394100	-3.53102700
C	-3.09641900	-0.64069100	0.39846700
C	-4.44515700	-0.05950600	0.84948000
C	-3.30240300	-1.70594000	-0.69847000
H	-2.63208900	-1.13390800	1.27623500
C	-5.35769700	-1.18397600	1.36726400
H	-4.94417000	0.43736600	-0.00344800
H	-4.28681800	0.70364800	1.62994700
C	-4.22513400	-2.82645500	-0.19926800
H	-3.75298400	-1.20746800	-1.57702800
H	-2.32381200	-2.08923800	-1.02414100
C	-5.56710300	-2.27372800	0.30436600
H	-6.32618100	-0.76451200	1.68607100
H	-4.89912200	-1.63398400	2.26711300
H	-4.38919700	-3.56258400	-1.00347800

H	-3.72231500	-3.36875200	0.62314500
H	-6.19301300	-3.08617100	0.70950900
H	-6.12371100	-1.84273100	-0.54893200
C	3.05915300	-0.69529900	-0.01412700
C	4.46972800	-0.26037400	-0.43721400
C	3.06718400	-1.22898500	1.43184800
H	2.76728400	-1.54234100	-0.66342000
C	5.45269200	-1.43623600	-0.30171700
H	4.81321100	0.57239700	0.20462400
H	4.46128900	0.10816000	-1.47735700
C	4.04651100	-2.40234200	1.57214900
H	3.37129100	-0.40821100	2.10646600
H	2.04416600	-1.51571200	1.72193800
C	5.46116100	-2.00712900	1.12398700
H	6.46477900	-1.11202500	-0.59439500
H	5.16129100	-2.23209000	-1.01188800
H	4.05669400	-2.75692000	2.61562600
H	3.68997000	-3.24939800	0.95682000
H	6.14232500	-2.87188000	1.18417200
H	5.85972700	-1.24305100	1.81726900
C	0.59594700	0.72897400	2.83964700
H	0.70511700	0.18134400	3.79859800
H	1.62113700	0.91849400	2.46150500
C	-0.10283800	2.06868300	3.08780800
H	-1.11723300	1.90372000	3.48187800
H	0.46202400	2.68183500	3.81050000
H	-0.18940100	2.63411100	2.14703200
O	-0.15463400	-0.08840100	1.97111400

TS-4

C	-1.25788900	2.49093200	-0.68401700
C	-1.31427600	3.89204600	-0.79476800
C	-0.14106800	4.62796400	-0.57891800
C	1.06088500	3.98607200	-0.24469500
C	1.07346300	2.58410700	-0.14998300
H	-2.25991700	4.39008200	-1.01498300
H	-0.16606800	5.71674900	-0.65619700
H	1.97145800	4.55873100	-0.06070300
C	2.18479400	1.69945100	0.12426600
H	3.19346100	2.10473000	0.25082800
C	-2.33936200	1.53169900	-0.72552800
H	-3.37408400	1.86680700	-0.84909900
N	1.95721600	0.39539200	0.12460900
N	-0.07147800	1.88771800	-0.39959700
N	-2.04387700	0.26175200	-0.51125700
Ru	-0.03357000	-0.10360200	-0.17799500
H	-1.18759600	-1.90295100	-1.80036600
C	-0.09067700	-1.77593000	-1.66533500
C	0.67265600	-3.08855300	-1.66047800
O	0.46190200	-0.72361000	-2.20119700

H	0.11741500	-1.71419400	0.19342100
H	1.70214100	-2.94922700	-1.30261900
H	0.17086400	-3.84240800	-1.03638300
H	0.71803600	-3.46598300	-2.69738700
C	3.09803600	-0.53970900	0.16938400
C	3.69755400	-0.70242900	-1.24291800
C	4.19496100	-0.19334200	1.19098800
H	2.65513600	-1.50449000	0.46964600
C	4.78063900	-1.78955700	-1.24542900
H	4.13553900	0.26745500	-1.54484000
H	2.88467400	-0.92122600	-1.95211500
C	5.26467700	-1.29781000	1.19879800
H	4.67783600	0.76476000	0.92691100
H	3.74523600	-0.07002500	2.19024400
C	5.86933800	-1.50576900	-0.19884400
H	5.22386700	-1.87453100	-2.25119000
H	4.31217400	-2.76818100	-1.02858100
H	6.05384700	-1.05053100	1.92758000
H	4.80492200	-2.24251800	1.54341100
H	6.60646200	-2.32534100	-0.17720700
H	6.42195200	-0.59336400	-0.49157200
C	-3.13681400	-0.70117800	-0.27439900
C	-3.65263900	-0.54413200	1.17057100
C	-4.28986600	-0.65332100	-1.29083600
H	-2.66656300	-1.69591300	-0.34814500
C	-4.68215200	-1.63600500	1.48952900
H	-4.11925300	0.45421800	1.26713100
H	-2.78616000	-0.56038100	1.84995000
C	-5.31202600	-1.75653500	-0.96914900
H	-4.79810900	0.32677700	-1.24661400
H	-3.89200300	-0.76723800	-2.31294300
C	-5.83406000	-1.63978600	0.47207500
H	-5.07085900	-1.49679500	2.51171000
H	-4.18048700	-2.62153900	1.47882300
H	-6.14736800	-1.71560400	-1.68726800
H	-4.83144500	-2.74341400	-1.10427600
H	-6.53806100	-2.46027300	0.68853400
H	-6.40740100	-0.69907700	0.57223000
O	-0.48109500	0.15421200	1.78926800
C	0.33357600	-0.49929000	2.72361500
H	1.41082300	-0.26092700	2.55999700
H	0.25373900	-1.60741200	2.63173800
C	-0.07272400	-0.06340200	4.13176100
H	0.55194100	-0.55671600	4.89497600
H	0.03532400	1.02698800	4.23808300
H	-1.12605100	-0.32052000	4.32405400

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Ru	-0.09339000	0.02276300	-0.08014500
N	1.95616600	0.42247200	-0.13610900
N	-0.05877800	1.96202000	0.02332200
N	-2.12486000	0.46484300	0.03959300
C	2.25550000	1.71778500	-0.02335900
H	3.28817100	2.07727200	-0.05281700
C	1.15990600	2.62916400	0.10825000
C	-2.38886200	1.75979100	0.14324800
H	-3.40926500	2.14175500	0.23600000
C	-1.26007000	2.65202200	0.16272000
C	1.18167100	4.01835400	0.29672600
H	2.14127200	4.53558500	0.36093600
C	-1.24900300	4.03878600	0.34718200
H	-2.19530000	4.57266400	0.45584200
C	-0.02420200	4.72318100	0.40424500
H	-0.01174900	5.80470100	0.54873800
C	-3.18517400	-0.55128600	0.00201000
C	-4.54281900	-0.13543200	0.58323400
C	-3.34325600	-1.07274700	-1.44126700
H	-2.77110400	-1.38810200	0.59738600
C	-5.51764200	-1.32458800	0.55478800
H	-4.97651800	0.68811700	-0.01476800
H	-4.41506600	0.24002700	1.61279800
C	-4.33113300	-2.24676200	-1.48736200
H	-3.70205500	-0.24280700	-2.07863500
H	-2.35398300	-1.37261400	-1.81863000
C	-5.68725200	-1.87265600	-0.87039100
H	-6.49269100	-1.02193700	0.97097300
H	-5.12952000	-2.12541100	1.21063900
H	-4.46132000	-2.58633600	-2.52814900
H	-3.89805700	-3.09784500	-0.93058600
H	-6.36243500	-2.74438200	-0.86681400
H	-6.17182500	-1.10132000	-1.49816300
C	3.06048400	-0.53099400	-0.36949600
C	4.00146100	-0.14131400	-1.52392000
C	3.85304600	-0.79714900	0.92458300
H	2.56319400	-1.47305700	-0.65702900
C	5.04828000	-1.24320100	-1.75233500
H	4.52232700	0.80374400	-1.28745300
H	3.40507700	0.03694500	-2.43355600
C	4.91395900	-1.88470700	0.69956000
H	4.33872500	0.14347200	1.24405100
H	3.15448900	-1.08666500	1.72590200
C	5.84499200	-1.53210400	-0.47057000
H	5.72677000	-0.95445200	-2.57176400
H	4.53658100	-2.16698500	-2.08024100
H	5.49520300	-2.04025000	1.62326400
H	4.40499800	-2.84298000	0.48543300
H	6.56719900	-2.34680200	-0.64392500

H	6.43831800	-0.63718400	-0.20445400
C	0.48087800	-2.79478500	1.05448100
H	0.09924200	-3.80328800	0.79165400
H	1.47711600	-2.69505700	0.57228300
C	0.64035000	-2.69280900	2.57261600
H	-0.33742000	-2.80289100	3.06635000
H	1.32068000	-3.46940500	2.96020100
H	1.04626300	-1.70388700	2.84190900
O	-0.43481800	-1.83828700	0.57224200
H	-0.12396800	0.10747000	-1.66622400

TS-7

C	0.00717000	4.91453000	-0.05374100
C	1.21888600	4.22475000	-0.22482000
C	1.20539600	2.82674400	-0.28217000
C	-1.18980600	2.80675500	0.00101500
C	-1.19608600	4.20878700	0.06716900
C	2.31863900	1.92175200	-0.41943200
C	-2.29132000	1.89304500	0.07121800
H	-3.32065800	2.24888300	0.16311300
H	3.33787300	2.31026500	-0.50779300
H	0.00505000	6.00448800	-0.00149000
H	2.16720200	4.76050800	-0.29658100
H	-2.14063200	4.73423200	0.22104400
N	-2.00103000	0.59924400	-0.03515300
N	2.05670600	0.63197300	-0.44533400
N	0.01222600	2.14726600	-0.19307400
Ru	-0.00717400	0.21566300	-0.22963800
C	0.59799800	-2.88165800	-0.63003100
H	1.19767400	-2.86958800	0.30395300
H	-0.13473800	-0.06691500	-2.02759300
O	-0.42244300	-1.90628100	-0.57472200
H	-0.29950000	-0.90542400	-1.63505100
C	-0.02590100	-4.26245900	-0.82522400
H	0.74671500	-5.04820000	-0.86355300
H	-0.71167600	-4.48721100	0.00609500
H	-0.60455700	-4.29152600	-1.76152800
H	1.30771400	-2.67972400	-1.46491600
C	3.14715400	-0.34970900	-0.51277200
C	4.45964500	0.11205100	-1.16484000
C	3.41250500	-0.90280800	0.90401700
H	2.74469500	-1.17858700	-1.12203100
C	5.44031600	-1.07100900	-1.24537100
H	4.92571700	0.91313900	-0.56228900
H	4.26198100	0.52692400	-2.16799600
C	4.40180900	-2.07370200	0.84505100
H	3.82834000	-0.08140300	1.51671600
H	2.45422900	-1.17781000	1.36907000
C	5.70876300	-1.67412800	0.14275800

H	6.38394700	-0.74544300	-1.71309400
H	5.01452700	-1.84848400	-1.90637500
H	4.60871200	-2.43959400	1.86415300
H	3.93381800	-2.91474400	0.29998700
H	6.38245600	-2.54259400	0.05577000
H	6.23764400	-0.92650400	0.76304600
C	-3.06357700	-0.41714100	-0.11327300
C	-4.24454300	-0.19432300	0.84474100
C	-3.55702300	-0.56900200	-1.56639600
H	-2.56177500	-1.36219300	0.15614700
C	-5.22747100	-1.37196000	0.74570900
H	-4.78097100	0.73738300	0.58741300
H	-3.86626000	-0.08086500	1.87433300
C	-4.55416900	-1.73098700	-1.67429900
H	-4.03402600	0.37748400	-1.88332600
H	-2.68992500	-0.73625600	-2.22316800
C	-5.72615700	-1.56453600	-0.69492200
H	-6.07675700	-1.21175500	1.43011900
H	-4.71958400	-2.29382000	1.08365100
H	-4.92516900	-1.81322500	-2.70929500
H	-4.02212500	-2.67446800	-1.45405700
H	-6.40105300	-2.43443700	-0.75263300
H	-6.32416600	-0.68199600	-0.99073900
O	0.35070500	-0.01152000	1.72901600
C	-0.63239900	-0.72055500	2.44731300
H	-0.92560100	-1.65003600	1.91342100
H	-1.55665200	-0.10803400	2.55391700
C	-0.07980700	-1.07141500	3.82818200
H	-0.83554200	-1.60164500	4.43074100
H	0.80667400	-1.71749200	3.73297100
H	0.22052400	-0.15762500	4.36318800

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C	-1.36475900	2.68971200	-0.41299000
C	-1.48226000	4.06437100	-0.65518700
C	-0.32030400	4.83004100	-0.83709300
C	0.94095100	4.22067400	-0.78607200
C	1.03738400	2.84365400	-0.54075300
H	-2.47218400	4.52217200	-0.70138300
H	-0.39904600	5.90206800	-1.02492600
H	1.85158700	4.80360100	-0.93738900
C	2.20987500	2.01452100	-0.49086700
H	3.20628200	2.43931100	-0.64145200
C	-2.39988800	1.71243400	-0.22411300
H	-3.45462100	2.00077700	-0.27652300
N	2.02004200	0.72029500	-0.29554900
N	-0.11665800	2.10324200	-0.34784200
N	-2.02603100	0.45889300	-0.01650300

Ru	0.05156700	0.20614000	-0.05887300
H	-1.11090500	-2.26216200	-1.57369300
C	-0.09503400	-1.86903600	-1.78765200
C	0.81678500	-2.80452500	-2.52461000
O	-0.00937600	-0.52197200	-2.13702300
H	1.85016500	-2.43645700	-2.47285200
H	0.76018800	-3.82942900	-2.12839500
H	0.50871700	-2.82157000	-3.58321500
O	0.45056800	-1.77350700	-0.10578100
C	-0.10883700	-2.74451300	0.78892100
H	-0.37110700	-2.20814500	1.71521100
H	-1.04071100	-3.16565100	0.35650300
C	0.89811800	-3.85002700	1.08161100
H	0.47223400	-4.58344700	1.78543600
H	1.18967500	-4.38234400	0.16372000
H	1.80516900	-3.42203000	1.53339700
C	3.13824700	-0.22117000	-0.20051700
C	4.38774100	0.12519500	-1.02275500
C	3.49570700	-0.44294100	1.28452500
H	2.72757700	-1.17539300	-0.57586900
C	5.42054700	-1.00770200	-0.89842600
H	4.84551300	1.06013800	-0.65024500
H	4.10950800	0.29248300	-2.07672300
C	4.53985200	-1.55955700	1.41874700
H	3.89851800	0.50466900	1.68899900
H	2.57360800	-0.65793500	1.84556600
C	5.78865200	-1.27357800	0.57015400
H	6.32229500	-0.76288300	-1.48367500
H	4.99951600	-1.92950000	-1.34167600
H	4.81582500	-1.69168900	2.47809800
H	4.08938300	-2.51538100	1.09097600
H	6.50291000	-2.11102800	0.63845800
H	6.30601200	-0.38466900	0.97743800
C	-3.07506400	-0.57592200	0.05977000
C	-4.21636500	-0.27875100	1.04972700
C	-3.63986500	-0.87143500	-1.34448100
H	-2.56025000	-1.48250200	0.41889700
C	-5.18314600	-1.47272900	1.10841300
H	-4.77290600	0.61983400	0.72851600
H	-3.79663900	-0.06010300	2.04522900
C	-4.61003800	-2.05964800	-1.29720300
H	-4.16939800	0.03079700	-1.70273400
H	-2.80758400	-1.04050500	-2.04526600
C	-5.73876400	-1.81896600	-0.28231200
H	-6.00639500	-1.25671500	1.80886700
H	-4.64749600	-2.34991400	1.51684300
H	-5.02655700	-2.24759800	-2.30040700
H	-4.05165200	-2.97218600	-1.01487000
H	-6.39617700	-2.70185800	-0.22163500
H	-6.36874300	-0.98200100	-0.63722900

O	0.35956300	0.15140200	1.92488800
C	-0.64361300	0.40269300	2.87636800
H	-1.60863800	-0.08357800	2.61028400
H	-0.31056500	-0.07118400	3.82389200
C	-0.87692800	1.89602200	3.12543000
H	0.07478800	2.38807500	3.37857400
H	-1.28324900	2.38590700	2.22878200
H	-1.58507000	2.05056900	3.95766100

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C	-1.23778900	2.82924600	-0.48443900
C	-1.22742000	4.20411500	-0.74280700
C	-0.01565200	4.91007200	-0.75617300
C	1.19172200	4.23781500	-0.51534000
C	-2.34494000	1.93243300	-0.40458600
C	1.18859800	2.86048000	-0.27026700
H	-2.17544200	4.71329200	-0.92741100
H	-0.01234800	5.98310300	-0.95202300
H	2.14358100	4.77247800	-0.51902300
N	-0.02675700	2.17398100	-0.25624500
Ru	-0.04159700	0.33218100	0.14230400
H	-1.59419000	-0.70413000	-2.38227300
C	-0.68396400	-1.32262200	-2.23257000
O	0.31726800	-0.61413100	-1.61950400
N	-2.06742000	0.66429700	-0.12850600
N	1.99421600	0.70693900	0.18500400
C	2.28931400	1.97966100	-0.04712900
C	-0.19311700	-1.87817700	-3.56756300
H	-0.97115300	-2.50428100	-4.02774000
H	0.70903900	-2.48718700	-3.41093200
O	-1.19926300	-2.46135300	-1.42465200
C	-0.44763300	-2.83092800	-0.28528000
H	-0.26173800	-1.95286700	0.39205900
H	-1.11571900	-3.49246900	0.29139700
C	0.87950400	-3.52440600	-0.58094600
H	1.56223200	-2.83822500	-1.10041400
H	0.71424700	-4.40643400	-1.21819300
H	1.35681500	-3.85547700	0.35645900
H	0.05324900	-1.04731500	-4.24556900
H	3.32154100	2.33830400	-0.10172900
H	-3.36687900	2.28118300	-0.57219500
C	3.06948000	-0.29763300	0.22603200
C	3.61590400	-0.56211700	-1.19166700
C	4.20629600	0.02269000	1.21264900
H	2.58337300	-1.22675000	0.56870700
C	4.64550600	-1.70050500	-1.16914200
H	4.08878000	0.36529600	-1.56500400

H	2.76553700	-0.78352800	-1.85489100
C	5.22673700	-1.12655600	1.23436800
H	4.71680700	0.95428600	0.90829800
H	3.78814000	0.19579700	2.21775300
C	5.77813600	-1.41827600	-0.17011400
H	5.05305600	-1.85766700	-2.18133300
H	4.13754600	-2.64205600	-0.88859700
H	6.04758400	-0.88749000	1.93021100
H	4.73585100	-2.03524700	1.63006500
H	6.48073300	-2.26713500	-0.13468900
H	6.35886600	-0.54365600	-0.51863300
C	-3.14611400	-0.32014400	0.05322300
C	-3.48267600	-0.45149900	1.55300400
C	-4.42061300	-0.08448600	-0.77255800
H	-2.71394500	-1.27774300	-0.28552500
C	-4.46576000	-1.60983200	1.77427500
H	-3.93273400	0.50023900	1.89337000
H	-2.54981600	-0.58297600	2.12181600
C	-5.38760600	-1.26293700	-0.56736900
H	-4.92503200	0.84637800	-0.45350400
H	-4.16301900	0.02870300	-1.83950100
C	-5.73230100	-1.45113300	0.91875700
H	-4.72937000	-1.68013100	2.84263900
H	-3.96521800	-2.56053800	1.51164200
H	-6.30497200	-1.10560900	-1.15830800
H	-4.91533600	-2.18407800	-0.95508800
H	-6.39699800	-2.32144000	1.04814600
H	-6.29770100	-0.56816900	1.27177000
O	-0.35628700	0.18235200	2.09739700
C	0.67080900	0.15311000	3.07104300
H	0.26002600	0.60283500	3.99793600
H	1.53308700	0.77557400	2.76214200
C	1.13508000	-1.27382400	3.36956700
H	0.28107600	-1.89464200	3.68177400
H	1.57870800	-1.73581200	2.47308700
H	1.88896200	-1.28913600	4.17444000

TS-10

C	-0.96319300	2.55781500	-1.12015100
C	-0.91853700	3.82051600	-1.72926600
C	0.32896600	4.41837100	-1.96978000
C	1.51282600	3.76621200	-1.59882900
C	1.43586100	2.50291200	-0.99035300
H	-1.84655100	4.33097600	-1.99372000
H	0.37656100	5.40190100	-2.44073800
H	2.48664000	4.22850100	-1.77220700
C	2.49738700	1.64500900	-0.54533000
H	3.54327800	1.93991000	-0.67493000
C	-2.11614000	1.78557700	-0.73463300

H	-3.12405500	2.18550800	-0.87617100
N	2.16372400	0.47278200	-0.01588000
N	0.20747300	1.92193000	-0.78336200
N	-1.90712400	0.59637800	-0.18762400
Ru	0.10132100	0.13002700	0.03951600
C	-0.02842800	-2.18941200	-1.06195300
C	0.82880000	-3.32529600	-0.54182200
O	0.43278900	-1.21011600	-1.72909800
H	-0.05424600	-1.47315500	0.63029300
H	1.73581300	-2.93733600	-0.06896200
H	0.26494000	-3.93579000	0.17347100
H	1.10553000	-3.95657000	-1.40432700
O	-1.29620800	-2.64695000	-1.30626800
C	-2.01914100	-1.95994700	-2.36588300
H	-2.17668200	-0.90980900	-2.08075200
H	-1.39298400	-1.96294700	-3.27210400
C	-3.31942400	-2.71077300	-2.57358600
H	-3.89857200	-2.23973000	-3.38256500
H	-3.12673100	-3.75778100	-2.85007100
H	-3.93376500	-2.70295500	-1.66155500
C	-3.03976800	-0.17272600	0.36755400
C	-3.14126900	0.08049900	1.88664500
C	-4.40721300	0.05381000	-0.30035100
H	-2.75614900	-1.23130100	0.22976900
C	-4.19645200	-0.83826400	2.51581500
H	-3.41876400	1.14030500	2.03904900
H	-2.14585100	-0.04723900	2.33479200
C	-5.45837900	-0.88344600	0.31850100
H	-4.73804300	1.09634700	-0.14247500
H	-4.33760300	-0.10257800	-1.39049700
C	-5.56557100	-0.68127200	1.83768900
H	-4.27538200	-0.62893100	3.59542700
H	-3.86146100	-1.88847100	2.42525500
H	-6.43605600	-0.72153200	-0.16476600
H	-5.17723600	-1.93299800	0.11243800
H	-6.29558400	-1.38865000	2.26512100
H	-5.95501500	0.33422500	2.03902600
C	3.24146000	-0.47778200	0.31832000
C	3.77459000	-1.15509900	-0.96162200
C	4.40616000	0.10980100	1.13746900
H	2.75447600	-1.24580900	0.94419200
C	4.78798800	-2.25504500	-0.61628400
H	4.25978100	-0.38000900	-1.58366800
H	2.92622900	-1.54031500	-1.54664100
C	5.40679800	-0.99889500	1.50111300
H	4.93106200	0.88532400	0.55133200
H	4.01163200	0.59772200	2.04353600
C	5.93695800	-1.71198900	0.24745900
H	5.18080000	-2.70866300	-1.54123000
H	4.27215100	-3.06557900	-0.06740800

H	6.24049600	-0.57622500	2.08549600
H	4.90655500	-1.73518800	2.15731500
H	6.62311300	-2.52673800	0.53199000
H	6.53029200	-0.99545200	-0.35089600
O	-0.11964500	0.79288100	1.91817600
C	0.90959500	0.51243200	2.83141400
H	1.06733700	-0.58408000	2.94430600
H	1.87843800	0.93022200	2.47831600
C	0.54831900	1.12573900	4.18435700
H	-0.38968900	0.69311300	4.56508800
H	1.34407600	0.94160100	4.92499400
H	0.40595800	2.21235500	4.08239100

3''

Ru	0.07298800	-0.01797000	-0.08929000
N	-1.97020500	0.29679000	0.02256100
N	0.03187200	1.84968300	0.14278700
N	2.08925100	0.39234300	-0.15985700
C	-2.28453400	1.57362300	0.17683500
H	-3.32122000	1.91904800	0.22322300
C	-1.19379300	2.49543600	0.27220200
C	2.35832100	1.67735500	-0.00706700
H	3.37434500	2.07435800	-0.07024800
C	1.23688200	2.54556100	0.19652300
C	-1.21707900	3.87989300	0.47466800
H	-2.17930500	4.38460800	0.57935700
C	1.21138900	3.93003300	0.39683600
H	2.15583100	4.47599300	0.43676400
C	-0.01382200	4.59712700	0.53734800
H	-0.03087700	5.67637300	0.69428900
Cl	0.03892600	-0.28544200	-2.46482700
O	0.26426900	-0.92920200	1.64035000
C	-0.80642500	-1.16689000	2.53877200
H	-1.34071400	-0.22043100	2.75519000
H	-1.55099600	-1.86672000	2.10320800
C	-0.24027200	-1.75738500	3.82741600
H	0.47622000	-1.05831400	4.28374700
H	-1.04539800	-1.96303100	4.55166200
H	0.28729700	-2.69973600	3.61573900
C	3.13612400	-0.59840700	-0.43271700
C	4.43133100	-0.05895600	-1.05755700
C	3.43809800	-1.40068600	0.85112600
H	2.67054200	-1.28675000	-1.16356400
C	5.38176900	-1.22419600	-1.37837900
H	4.93808700	0.62377100	-0.35028400
H	4.19711500	0.51785600	-1.96758500
C	4.40395000	-2.55463100	0.54754500

H	3.89098700	-0.71116400	1.58794500
H	2.49380400	-1.75665900	1.29003500
C	5.69254200	-2.05621600	-0.12461800
H	6.31203600	-0.83690700	-1.82524600
H	4.91277600	-1.87175200	-2.14168000
H	4.63926800	-3.09822300	1.47732500
H	3.90182600	-3.27909500	-0.12011300
H	6.34638000	-2.90566900	-0.38246000
H	6.25646200	-1.43059000	0.59257300
C	-3.02915600	-0.70769900	-0.17523700
C	-4.18303000	-0.62918000	0.84226600
C	-3.56338200	-0.65653300	-1.62118400
H	-2.52688800	-1.68242700	-0.03922900
C	-5.17800800	-1.77523300	0.60123000
H	-4.71442600	0.33342100	0.73418200
H	-3.77877800	-0.66420800	1.86705000
C	-4.57125500	-1.78858100	-1.86274200
H	-4.05188900	0.32341300	-1.77711500
H	-2.71455100	-0.71101700	-2.31919500
C	-5.71573900	-1.75848300	-0.83806500
H	-6.00667900	-1.71044600	1.32522500
H	-4.67073100	-2.73925200	0.79099400
H	-4.96863100	-1.72027700	-2.88847300
H	-4.04604200	-2.75926500	-1.79667800
H	-6.39997600	-2.60768500	-0.99920600
H	-6.31313000	-0.83985400	-0.98905700

TS-4'

C	-1.29261300	2.52781600	-0.30497300
C	-1.37872700	3.93371200	-0.23156100
C	-0.20320400	4.67608600	-0.10646200
C	1.04964300	4.03648400	-0.03357000
C	1.08684300	2.64111200	-0.11402800
H	-2.35341800	4.42451300	-0.24698800
H	-0.25648600	5.76457900	-0.04276700
H	1.96931300	4.61034200	0.09039900
C	2.25487700	1.76348900	-0.06585000
H	3.25808900	2.20209200	-0.03315000
C	-2.34960100	1.55052400	-0.31507300
H	-3.39921400	1.85580600	-0.28737600
N	2.06625900	0.47358500	-0.10345800
N	-0.06291200	1.93935400	-0.28081800
N	-2.00012300	0.26804500	-0.26584000
Ru	-0.00168200	-0.06911700	-0.19298700
H	-1.23839600	-1.78040500	-1.82994300
C	-0.14252400	-1.67928200	-1.67772400
C	0.60366100	-2.99890700	-1.72865300
O	0.42690300	-0.60904600	-2.18301200
Cl	-0.05851900	0.16767800	2.22514500
H	0.04226800	-1.66758300	0.18079700

H	1.63223400	-2.89289100	-1.35714200
H	0.08869000	-3.77092700	-1.13831000
H	0.64833500	-3.33566700	-2.77923700
C	3.18525500	-0.47365400	-0.15031900
C	4.58445400	0.11556600	-0.37304500
C	3.15398200	-1.35287000	1.11551500
H	2.93901000	-1.11477100	-1.01836600
C	5.62123900	-1.01694200	-0.48232500
H	4.85599900	0.76693200	0.47879500
H	4.60022900	0.73759100	-1.28461100
C	4.19671300	-2.47497900	1.02187300
H	3.35717800	-0.70935500	1.98980800
H	2.13726800	-1.74917200	1.25426300
C	5.60412000	-1.91946500	0.75981900
H	6.62523800	-0.58920100	-0.63709200
H	5.39704200	-1.62327500	-1.37929900
H	4.18242300	-3.07220800	1.94787800
H	3.91765600	-3.16259300	0.20126500
H	6.32945400	-2.74143100	0.64247200
H	5.93176500	-1.33298300	1.63821400
C	-3.05745100	-0.74524900	-0.06196500
C	-3.61663700	-0.66402500	1.37181900
C	-4.18386000	-0.69923300	-1.11041000
H	-2.54509600	-1.71584700	-0.15945500
C	-4.61955700	-1.79999800	1.61546000
H	-4.11803500	0.31234000	1.50500000
H	-2.77668400	-0.69596500	2.08272100
C	-5.17974200	-1.84296400	-0.86030300
H	-4.71835700	0.26581600	-1.04875800
H	-3.75131800	-0.76367100	-2.12267900
C	-5.74414000	-1.79605900	0.56829100
H	-5.03760900	-1.71647400	2.63184000
H	-4.08668100	-2.76811100	1.57711900
H	-5.99484700	-1.79937400	-1.60108700
H	-4.66534000	-2.80929400	-1.01709600
H	-6.42931900	-2.64355900	0.73474600
H	-6.34675800	-0.87614800	0.68781800

5''

Ru	0.00002900	-0.11848200	0.05710400
N	-2.02940700	0.28448100	0.03194000
N	-0.00003500	1.82055600	0.00324600
N	2.02943300	0.28464200	0.03361300
C	-2.31740200	1.57851900	-0.01654200
H	-3.34991100	1.94130000	-0.04271300
C	-1.20697400	2.49725300	-0.04087900
C	2.31736700	1.57868900	-0.01492800
H	3.34986400	1.94153900	-0.04046500
C	1.20688500	2.49733700	-0.04014100
C	-1.21667500	3.89705500	-0.11454000

H	-2.16933100	4.42884000	-0.14834600
C	1.21653800	3.89713700	-0.11381700
H	2.16917800	4.42898600	-0.14705300
C	-0.00008300	4.59328200	-0.14591700
H	-0.00010200	5.68307800	-0.20149000
Cl	0.00021500	-2.47833600	-0.29202700
H	-0.00064700	-0.04567100	1.62741700
C	3.13404900	-0.69940400	0.06230000
C	3.95218100	-0.67863700	-1.24213700
C	4.03887000	-0.53078800	1.29633300
H	2.63533500	-1.67981400	0.13161900
C	5.03686700	-1.76621000	-1.21220900
H	4.42569600	0.31312900	-1.36585600
H	3.27185100	-0.82405300	-2.09664500
C	5.12016700	-1.62224000	1.31857000
H	4.52346700	0.46301400	1.27182600
H	3.41937700	-0.56735000	2.20700000
C	5.94193600	-1.62309900	0.02072300
H	5.63412100	-1.72565300	-2.13787800
H	4.54955900	-2.75793500	-1.19531700
H	5.77684700	-1.48191500	2.19280800
H	4.63497400	-2.60722100	1.44426000
H	6.68893000	-2.43339200	0.04222700
H	6.50759400	-0.67495500	-0.05129100
C	-3.13401000	-0.69958300	0.06019000
C	-4.03522500	-0.53435200	1.29735300
C	-3.95587600	-0.67508200	-1.24177400
H	-2.63523200	-1.68024300	0.12548300
C	-5.11668500	-1.62563600	1.31962000
H	-4.51946100	0.45973700	1.27707200
H	-3.41302500	-0.57369400	2.20605100
C	-5.04044300	-1.76277600	-1.21175600
H	-4.42995700	0.31689000	-1.36148100
H	-3.27801100	-0.81803600	-2.09866700
C	-5.94206500	-1.62292000	0.02407900
H	-5.77089700	-1.48753900	2.19606100
H	-4.63131900	-2.61103200	1.44133600
H	-5.64028600	-1.71977600	-2.13563900
H	-4.55308200	-2.75454100	-1.19884700
H	-6.68905400	-2.43321900	0.04548300
H	-6.50786700	-0.67455400	-0.04383000

TS-7'

C	0.04192700	4.86620700	0.13397100
C	1.25032100	4.15974500	0.07480500
C	1.21729600	2.76692500	-0.08538100
C	-1.18247900	2.79375700	-0.10317500
C	-1.18224300	4.18655800	0.05233200
C	2.31893400	1.83596800	-0.16850800
C	-2.31187200	1.89194300	-0.18228000

H	-3.33568000	2.27467000	-0.16110000
H	3.35039700	2.19857700	-0.14367300
H	0.05257700	5.94985000	0.26202500
H	2.20860800	4.67392600	0.16688200
H	-2.12934000	4.72372100	0.12624600
N	-2.04869700	0.60821100	-0.30373900
N	2.03150500	0.55856800	-0.30181800
N	0.01305800	2.12552800	-0.19500400
Ru	-0.03909100	0.18299500	-0.28829400
Cl	-0.00263800	0.10029300	2.12216900
C	0.48542900	-2.92721600	-0.41667000
H	0.88323400	-2.88819500	0.61838200
H	-0.00547600	-0.00689300	-2.05036800
O	-0.46801100	-1.90839600	-0.61593700
H	-0.17897400	-0.84803200	-1.71712500
C	-0.16917100	-4.28556900	-0.66587400
H	0.54593300	-5.10856400	-0.50127400
H	-1.02156200	-4.42114000	0.01737400
H	-0.54572700	-4.34754100	-1.69875500
C	-3.10762500	-0.40986600	-0.37607700
C	-3.19458400	-1.14645200	0.97764300
C	-4.48640400	0.08843900	-0.82771200
H	-2.72708000	-1.15068200	-1.10238700
C	-4.18257500	-2.31645100	0.87801300
H	-3.51746700	-0.42808900	1.75289900
H	-2.18967000	-1.49557000	1.25007700
C	-5.46074100	-1.09714900	-0.94000100
H	-4.89134100	0.80469700	-0.08864800
H	-4.40526400	0.62008100	-1.79164800
C	-5.56488900	-1.86150100	0.38847400
H	-4.26451700	-2.81358500	1.85835100
H	-3.77200100	-3.06747700	0.17801700
H	-6.45254100	-0.73704700	-1.25951400
H	-5.10478300	-1.78333000	-1.73039400
H	-6.24030500	-2.72587500	0.27683100
H	-6.02122500	-1.20117700	1.14963500
C	3.11177200	-0.43829000	-0.37236700
C	4.46645900	0.04605900	-0.91248000
C	3.28419200	-1.08756400	1.01658100
H	2.73319700	-1.21617700	-1.05994700
C	5.43938000	-1.14263900	-1.01098400
H	4.90344900	0.79799700	-0.23038900
H	4.33495100	0.52918800	-1.89576200
C	4.26436900	-2.26515700	0.93966300
H	3.66461500	-0.31490200	1.70937200
H	2.30210100	-1.39193200	1.40491100
C	5.61577100	-1.83695600	0.34880200
H	6.41234800	-0.79864200	-1.39830000
H	5.04837800	-1.86996300	-1.74630200
H	4.40165300	-2.69947200	1.94319600

H	3.82303800	-3.06140200	0.31182000
H	6.28610300	-2.70621700	0.24685200
H	6.11098600	-1.13791100	1.04837500
H	1.35968400	-2.81338000	-1.09880300

TS-8'

C	1.29118700	2.62034900	-0.03098900
C	1.37206900	4.01927400	0.00524400
C	0.19103800	4.77516000	0.00325800
C	-1.05676700	4.13933600	-0.04178900
C	-1.11477800	2.73888700	-0.07531000
H	2.35036200	4.50230900	0.02703700
H	0.24438300	5.86473600	0.02836900
H	-1.98260400	4.71689800	-0.05685000
N	0.05449000	2.01302600	-0.05379700
Ru	-0.04313400	0.10390700	-0.13377600
H	1.07353300	-2.09955200	1.49670900
C	0.05699600	-2.39915300	1.16876200
O	-0.38239100	-2.06601100	0.04629900
Cl	0.05281500	0.03176000	-2.54763200
C	-2.27259800	1.87692100	-0.11406700
C	2.35240000	1.64561000	-0.06301800
N	1.99545900	0.37399300	-0.08469600
N	-2.05197500	0.58111600	-0.15426200
C	-0.64693800	-3.40579100	2.02325200
H	-0.76021200	-2.99350700	3.03784700
H	-1.63341500	-3.64326300	1.60429500
H	-0.04323500	-4.32607200	2.10627000
O	-0.32347800	-0.26827700	1.90086500
H	3.40102200	1.95681600	-0.09025000
H	-3.28113000	2.29860400	-0.08973100
C	0.61889500	0.23748000	2.81416400
H	1.59910700	-0.29218300	2.72593100
H	0.83579800	1.30709000	2.61038600
C	0.08647000	0.08556700	4.23886100
H	-0.09407500	-0.97484000	4.47570900
H	0.80285900	0.48653000	4.97459300
H	-0.86762500	0.62332400	4.34527600
C	-3.13778900	-0.40223000	-0.11695100
C	-4.52529300	0.13399200	0.26092200
C	-3.18764500	-1.17483800	-1.45083900
H	-2.81568700	-1.11616900	0.66608800
C	-5.53230200	-1.02483500	0.35618700
H	-4.87489100	0.84591800	-0.51011900
H	-4.47592900	0.68083000	1.21814000
C	-4.20447000	-2.32087300	-1.36900700
H	-3.46637900	-0.46770400	-2.25266200
H	-2.18335700	-1.54734100	-1.69244600
C	-5.59663900	-1.82283100	-0.95459500

H	-6.52829300	-0.63403100	0.62205300
H	-5.22936600	-1.69787400	1.17978400
H	-4.25320800	-2.84199800	-2.33890200
H	-3.84692300	-3.06480400	-0.63228500
H	-6.29710900	-2.66829600	-0.85195200
H	-6.00145600	-1.17316400	-1.75292200
C	3.02452300	-0.67055900	-0.23799400
C	3.58804700	-0.67632100	-1.67305000
C	4.15317100	-0.59926900	0.80627200
H	2.48855400	-1.62468600	-0.09570600
C	4.56608300	-1.84470600	-1.85724500
H	4.10928500	0.28257900	-1.85138800
H	2.74896200	-0.72595700	-2.38359100
C	5.12229800	-1.77706100	0.61844400
H	4.70964800	0.34843400	0.69221300
H	3.72102400	-0.59922400	1.82109600
C	5.68931800	-1.81669400	-0.80936300
H	4.98681100	-1.82047400	-2.87561600
H	4.00998700	-2.79681100	-1.77372600
H	5.93736700	-1.71428400	1.35800000
H	4.58529500	-2.72199700	0.82387800
H	6.35256900	-2.68885600	-0.93137100
H	6.31587400	-0.91991400	-0.97320100

9'			
C	1.14484000	2.46690400	-0.55157300
C	1.18031800	3.86423500	-0.62775800
C	-0.01845700	4.59013800	-0.65671900
C	-1.24902300	3.92075800	-0.61313100
C	-1.28061400	2.52312200	-0.53775500
H	2.14648600	4.37034300	-0.66623700
H	0.00647600	5.67910800	-0.71498700
H	-2.19056700	4.47230100	-0.63891100
N	-0.08288700	1.82308200	-0.50006500
Ru	-0.12622300	-0.06304500	-0.42107400
H	1.50309400	-0.52302100	2.11286600
C	0.54229300	-0.99945500	2.40201500
O	-0.35784900	-0.95318600	1.32892700
Cl	-0.04893200	-0.37556000	-2.78373100
C	-2.40958400	1.64277800	-0.43345600
C	2.23247900	1.53585700	-0.47319400
N	1.91270900	0.25775200	-0.34759600
N	-2.14067600	0.35309000	-0.34287500
C	-0.32239500	1.05070800	3.31819600
H	-0.90260800	1.34363500	4.20672900
H	-0.98588600	1.13733800	2.43865000
C	0.89752200	1.95896300	3.16204000
H	1.46700200	1.72428600	2.25005600
H	0.57895800	3.01102700	3.08631200
H	1.57074500	1.85851100	4.02726500

C	0.76693700	-2.44316000	2.83072800
H	1.41272200	-2.48060600	3.71991700
H	-0.20436100	-2.89743300	3.07325900
H	1.23393400	-3.01145600	2.01347000
O	0.00698300	-0.32644000	3.54259900
H	3.26974400	1.88105100	-0.48730700
H	-3.42734600	2.03599400	-0.37644800
C	2.96797700	-0.76906200	-0.27798000
C	3.45577300	-1.14213300	-1.69214500
C	4.15047100	-0.40910000	0.63854300
H	2.47132000	-1.65750400	0.15005400
C	4.45880600	-2.30361500	-1.62260700
H	3.93429400	-0.25215000	-2.14081400
H	2.58716600	-1.38768800	-2.32183700
C	5.13382800	-1.58749100	0.71694400
H	4.68347600	0.47210600	0.23888300
H	3.77777000	-0.13801600	1.64074300
C	5.63071800	-1.99162200	-0.67965700
H	4.82831500	-2.53535400	-2.63472700
H	3.93552100	-3.21070200	-1.26741400
H	5.98231300	-1.32604600	1.37001100
H	4.62726000	-2.44881000	1.19062800
H	6.30661400	-2.85946200	-0.60768300
H	6.22771200	-1.16285900	-1.10414200
C	-3.16421300	-0.65284000	-0.05315300
C	-4.56082200	-0.11573200	0.28389300
C	-3.22896500	-1.67880500	-1.20235900
H	-2.75849000	-1.17308200	0.83938100
C	-5.50071800	-1.27556100	0.65230500
H	-4.97607000	0.42078000	-0.59002300
H	-4.50252700	0.60488300	1.11753400
C	-4.17673700	-2.83187000	-0.84594800
H	-3.57539100	-1.16163800	-2.11522900
H	-2.21479900	-2.04688800	-1.42337400
C	-5.57530300	-2.31836800	-0.47289900
H	-6.50452200	-0.88384300	0.88472000
H	-5.12974000	-1.75854100	1.57482100
H	-4.23676500	-3.53801600	-1.68986100
H	-3.75501200	-3.39480500	0.00712100
H	-6.22696200	-3.15584800	-0.17395200
H	-6.04209000	-1.85744800	-1.36322700

TS-10'

C	-0.93415600	2.76685700	-0.42536300
C	-0.90596200	4.16328100	-0.60472700
C	0.32784700	4.80981000	-0.72155700
C	1.52709800	4.08000800	-0.63778800
C	1.45493400	2.69340100	-0.46449600
H	-1.83978000	4.72800900	-0.62893800
H	0.36150800	5.89239700	-0.85685100

H	2.49604100	4.57895900	-0.69574100
C	2.54869600	1.74320900	-0.34090500
H	3.58194600	2.09146200	-0.44016200
C	-2.06284200	1.90917300	-0.18356500
H	-3.07480200	2.31629400	-0.13311700
N	2.25747700	0.48442700	-0.14009100
N	0.24471800	2.07119300	-0.40566700
N	-1.82128300	0.61696200	0.02582900
Ru	0.15649800	0.12207200	0.00887500
C	-0.04771800	-1.93333100	-1.25671700
C	0.71534700	-3.19325000	-0.89497400
O	0.51445400	-0.93913800	-1.84562100
Cl	0.34770100	0.68775700	2.33923300
H	-0.03463900	-1.46487000	0.50919600
H	1.65161000	-2.94577400	-0.38422600
H	0.10586900	-3.84108700	-0.25324300
H	0.93674600	-3.73258000	-1.83174400
C	3.30322400	-0.54167000	-0.07487300
C	4.72798900	-0.09671000	-0.43200500
C	3.26816800	-1.21507600	1.31206100
H	2.98076500	-1.28775100	-0.82719400
C	5.68877700	-1.29701100	-0.39050000
H	5.07436400	0.66278000	0.29367500
H	4.74571700	0.36991500	-1.43203700
C	4.24050200	-2.40062200	1.36854000
H	3.53626700	-0.45905100	2.07106000
H	2.23387600	-1.51681100	1.53926100
C	5.66737400	-1.98527000	0.98207900
H	6.70967800	-0.96677900	-0.64302500
H	5.39258100	-2.02401100	-1.16936300
H	4.22622200	-2.84227800	2.37810300
H	3.89469400	-3.19291600	0.67734900
H	6.33912200	-2.85955400	0.98228900
H	6.05904600	-1.28509900	1.74313000
C	-2.93102400	-0.27217100	0.43915100
C	-2.96623500	-0.38854800	1.97690400
C	-4.32262000	0.09844300	-0.10221000
H	-2.65944800	-1.26492200	0.04184900
C	-4.00687100	-1.42886700	2.41333100
H	-3.21580000	0.60283400	2.39752600
H	-1.96278900	-0.64089900	2.34713100
C	-5.35117200	-0.96537300	0.31754200
H	-4.64734700	1.07110000	0.30958600
H	-4.29260800	0.20457900	-1.20016200
C	-5.39916700	-1.12082800	1.84496900
H	-4.04129700	-1.47591500	3.51404300
H	-3.68385700	-2.42888700	2.06850100
H	-6.34559300	-0.70153200	-0.07865800
H	-5.07946100	-1.93650700	-0.13661500
H	-6.11679000	-1.90950300	2.12561100

H	-5.77374300	-0.18029600	2.29058400
O	-1.34237600	-2.26939800	-1.59166300
C	-1.97176600	-1.42958100	-2.59738900
H	-2.11967500	-0.41739800	-2.19039700
H	-1.29014600	-1.34123600	-3.45775100
C	-3.27857900	-2.09749900	-2.97863800
H	-3.78680600	-1.50821900	-3.75723600
H	-3.09926500	-3.10914200	-3.37131100
H	-3.95309100	-2.17838900	-2.11403300

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