
Methyl formate as a hydrogen energy carrier

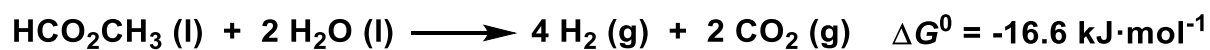
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Supplementary Methods

Thermodynamic of methyl formate dehydrogenation



$$\Delta_r G^\circ = 4\Delta_f G^\circ[\text{H}_2(\text{g})] + 2\Delta_f G^\circ[\text{CO}_2(\text{g})] - 2\Delta_f G^\circ[\text{H}_2\text{O}(\text{l})] - \Delta_f G^\circ[\text{HCOOCH}_3(\text{l})]$$

$$= 2 \times (-394.4 \text{ kJ}\cdot\text{mol}^{-1}) - 2 \times (-237.1 \text{ kJ}\cdot\text{mol}^{-1}) - (-298.0 \text{ kJ}\cdot\text{mol}^{-1})$$

$$= -16.6 \text{ kJ}\cdot\text{mol}^{-1}$$

Supplementary Table 1. $\Delta_f G^\circ$ of different material.

Entry	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{H}_2(\text{g})^3$	$\text{CO}_2(\text{g})^3$	$\text{H}_2\text{O}(\text{l})^3$	$\text{HCOOCH}_3(\text{l})^4$
1	$\Delta_f G^\circ$	0.0	-394.4	-237.1	-298.0

Gas Chromatogram of the collected reaction gas mixture.

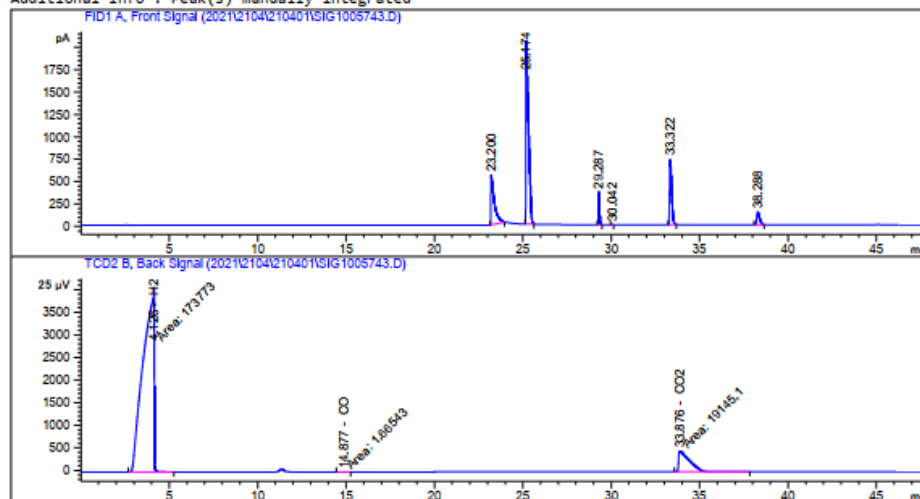
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Additional Info : Peak(s) manually integrated



External Standard Report

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Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

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Signal 2: TCD2 B, Back Signal

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11.339		-	-	-	N2	
14.877	MM	1.66543	5.26440e-4	8.76750e-4	CO	

GC Lab 1.132 5/2/2021 4:47:39 PM AK

Page 1 of 2

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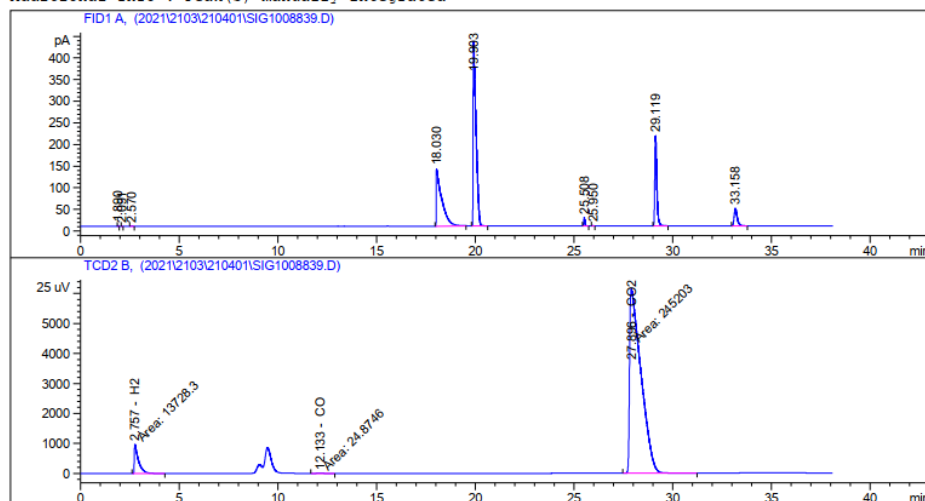
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Supplementary Fig. 1 Typical GC spectra using Ar carrier gas with CO quantification limit of 78 ppm.

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Signal 2: TCD2 B,

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21.000	2		-	-	-		CH4
27.896	2	MM	2.45203e5	1.53561e-4	37.65369		CO2

GC Lab 1.126 06/05/2021 09:20:22 AL

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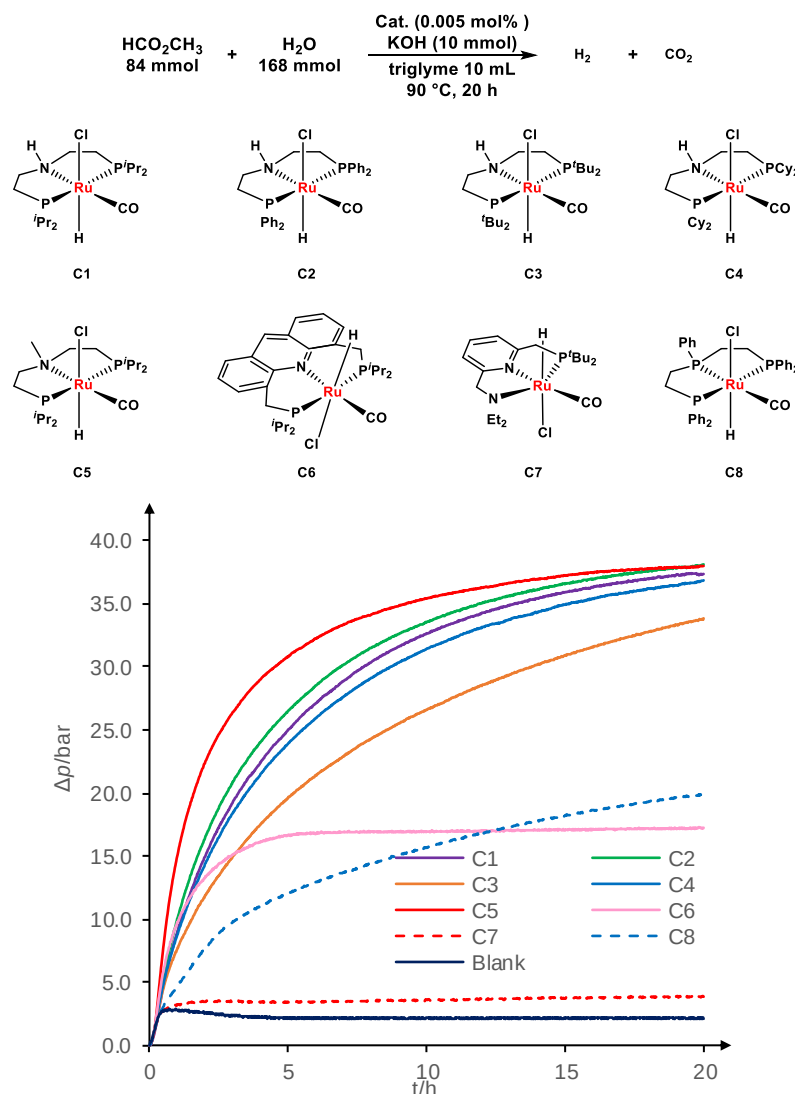
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Totals : 97.69558

Supplementary Fig. 2 Typical GC spectra using He carrier gas with CO quantification limit of 10 ppm.

Measurement of methyl formate (MF) dehydrogenation.

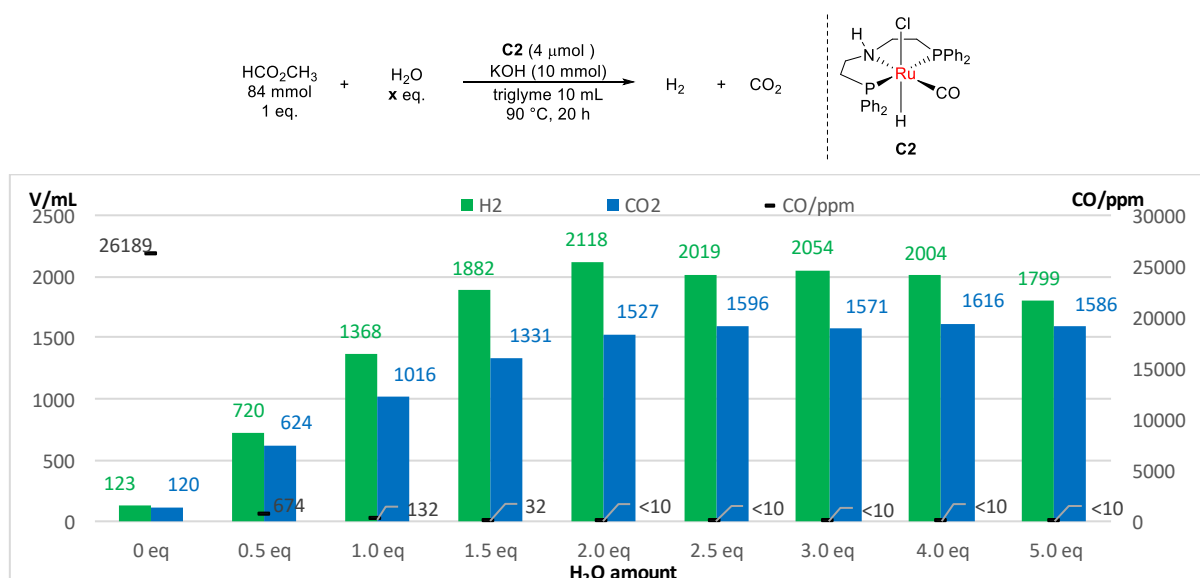
Supplementary Table 2. Catalyst variation in the dehydrogenation of methyl formate.



Entry	Cat.	Δp (bar)	V (mL)	H ₂ :CO ₂ (%)	CO (ppm)	TON[H ₂]	TOF[H ₂] _{max} (h ⁻¹)
1	C1	37.4	3,540	58:42	<10	20,968	5,286
2	C2	38.1	3,645	58:42	<10	21,590	5,677
3	C3	33.9	3,163	58:42	<10	19,058	3,643
4	C4	36.9	3,488	57:43	<10	20,304	4,312
5	C5	38.0	3,564	57:43	undetectable	20,746	8,376
6	C6	17.3	1,542	57:43	227	8,976	4,171
7	C7	3.9	230	56:43	2,672	1,315	408
8	C8	20.0	1,768	57:43	270	10,292	1,999
9	-	2.1	36	65:33	18,684	-	-

Reaction conditions: under argon atmosphere 4 μmol catalyst and 10 mmol KOH (0.561 g) were added to a 100 mL autoclave. Then 10.0 mL solvent triglyme, 168 mmol H₂O (3.0 mL) and 84 mmol MF (5.2 mL) were injected by a syringe under ice-bath. After that, the autoclave was flushed with N₂ (5 bar) and the pressure was released three times. The reaction was performed at 90 $^\circ\text{C}$ for 20 h. After that the autoclave was cooled down using ice-bath and the pressure was carefully released through a room temperature (25 $^\circ\text{C}$) condenser (the water temperature was controlled by a thermostat) to a manual burette to get the gas volume. The gas was analyzed by GC. Additional CO₂ was collected via burette by adding HCl aqueous solution to the reaction liquid phase. All experiments were performed at least twice, and the average gas pressures and values are shown with standard deviations <5 %.

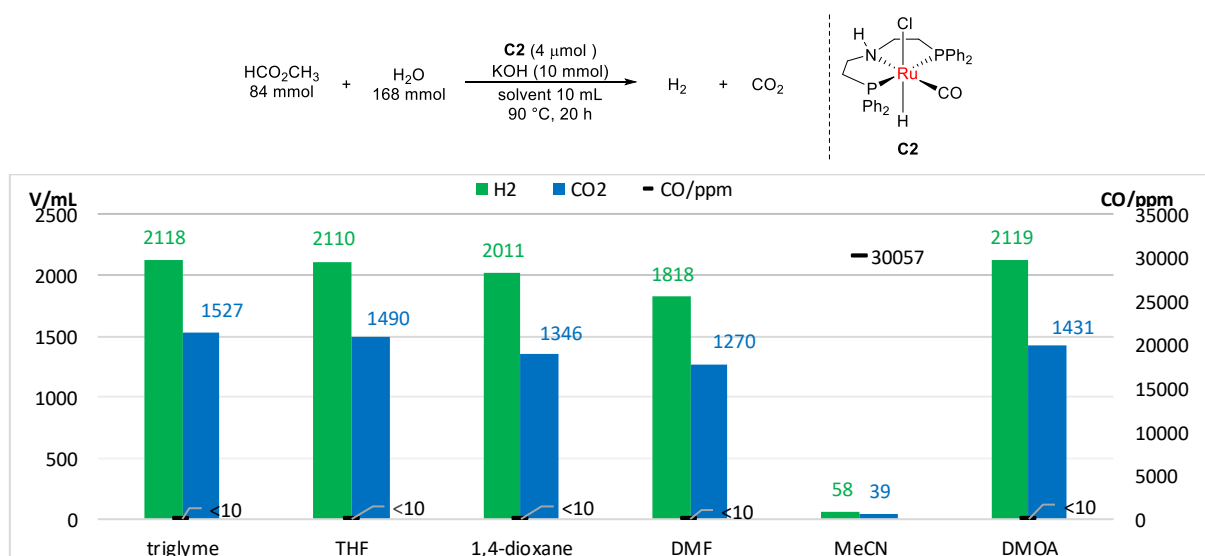
Supplementary Table 3. Water amount variation in the dehydrogenation of methyl formate.



Entry	H ₂ O (eq.)	Δp (bar)	V (mL)	H ₂ :CO ₂ (%)	CO (ppm)	TON
1	0	3.3	250	49:48	26,189	1,251
2	0.5	12.5	1,345	54:46	674	7,417
3	1.0	24.2	2,385	57:43	132	13,883
4	1.5	33.8	3,213	58:42	32	19,031
5	2.0	38.1	3,645	58:42	<10	21,590
6	2.5	38.3	3,615	56:44	<10	20,674
7	3.0	39.0	3,625	57:43	<10	21,101
8	4.0	39.9	3,620	55:45	<10	20,333
9	5.0	38.7	3,385	54:47	<10	18,667

Reaction conditions: under argon atmosphere 4 μmol **C2** catalyst (2.4 mg) and 10 mmol KOH (0.561 g) were added to a 100 mL autoclave. Then 10.0 mL solvent triglyme, H_2O (x eq. to MF) and 84 mmol MF (5.2 mL) were injected by a syringe under ice-bath. After that, the autoclave was flushed with N_2 (5 bar) and the pressure was released three times. The reaction was performed at 90 $^\circ\text{C}$ for 20 h. After that the autoclave was cooled down using ice-bath and the pressure was carefully released through a room temperature (25 $^\circ\text{C}$) condenser (the water temperature was controlled by a thermostat) to a manual burette to get the gas volume. The gas was analyzed by GC. Additional CO_2 was collected via burette by adding HCl aqueous solution to the reaction liquid phase. Experiments were at least performed twice, and the average values were shown. Standard deviations are <5 % of the average.

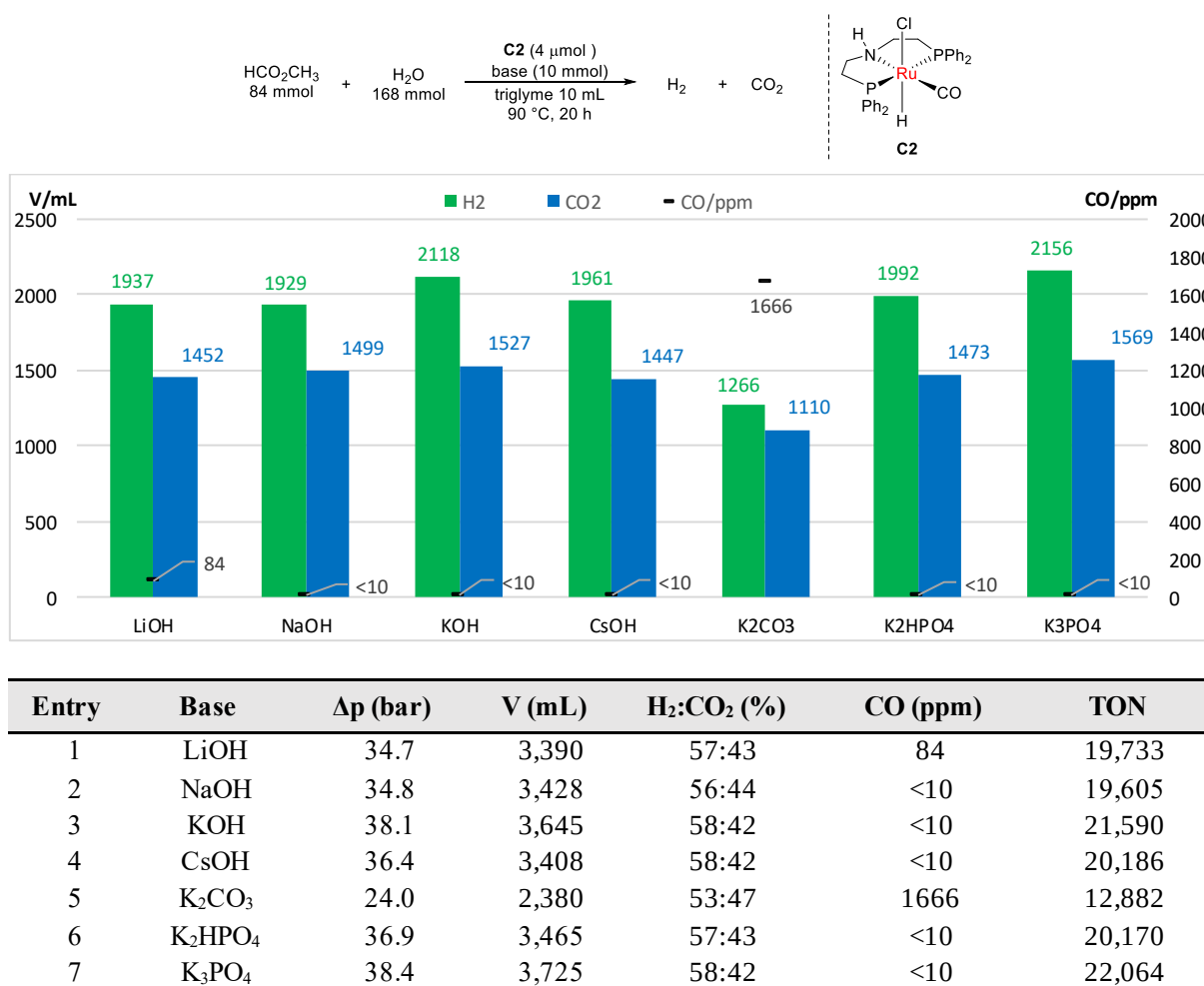
Supplementary Table 4. Solvent variation in the dehydrogenation of methyl formate.



Entry	Solvent	Δp (bar)	V (mL)	H ₂ :CO ₂ (%)	CO (ppm)	TON
1	triglyme	38.1	3,645	58:42	<10	21,590
2	THF	37.9	3,600	58:42	<10	21,324
3	dioxane	34.9	3,357	59:41	<10	20,227
4	DMF	32.4	3,088	59:41	<10	18,606
5	MeCN	3.1	100	58:39	30057	593
6	DMOA	37.4	3,550	59:41	<10	21,390

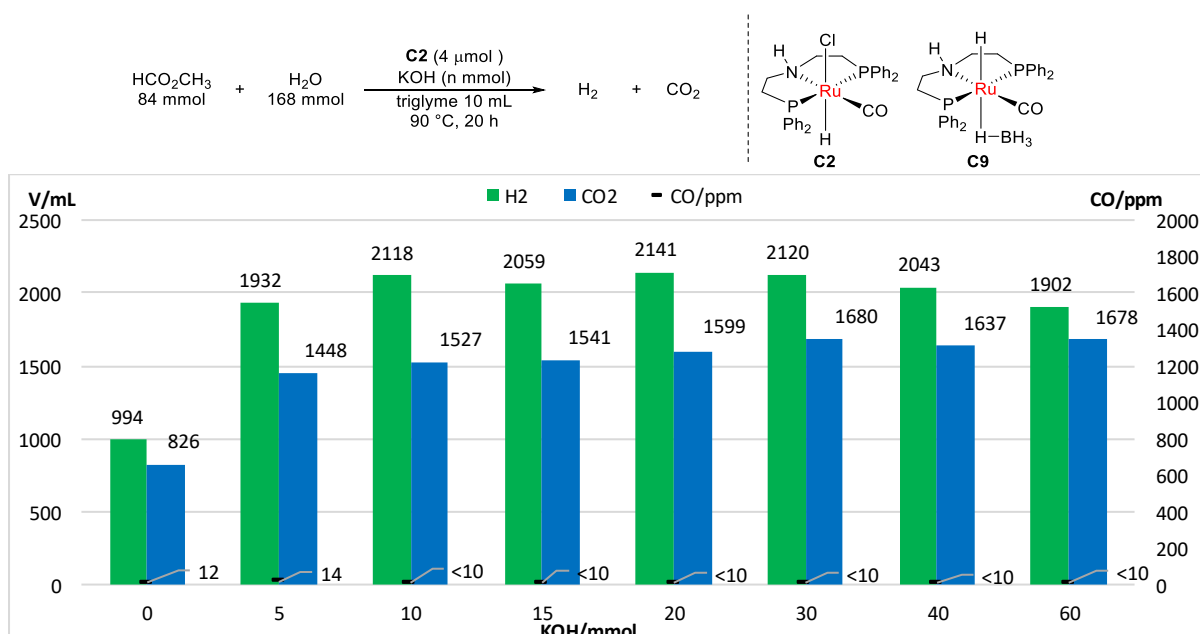
Reaction conditions: under argon atmosphere 4 μmol **C2** catalyst (2.4 mg) and 10 mmol KOH (0.561 g) were added to a 100 mL autoclave. Then 10.0 mL solvent, 168 mmol H₂O (3.0 mL) and 84 mmol MF (5.2 mL) were injected by a syringe under ice-bath. After that, the autoclave was flushed with N₂ (5 bar) and the pressure was released three times. The reaction was performed at 90 $^\circ\text{C}$ for 20 h. After that the autoclave was cooled down using ice-bath and the pressure was carefully released through a room temperature (25 $^\circ\text{C}$) condenser (the water temperature was controlled by a thermostat) to a manual burette to get the gas volume. The gas was analyzed by GC. Additional CO₂ was collected via burette by adding HCl aqueous solution to the reaction liquid phase. Experiments were at least performed twice, and the average values were shown. Standard deviations are <5 % of the average.

Supplementary Table 5. Base variation in the dehydrogenation of methyl formate.



Reaction conditions: under argon atmosphere 4 μmol **C2** catalyst (2.4 mg) and 10 mmol base were added to a 100 mL autoclave. Then 10.0 mL triglyme, 168 mmol H₂O (3.0 mL) and 84 mmol MF (5.2 mL) were injected by a syringe under ice-bath. After that, the autoclave was flushed with N₂ (5 bar) and the pressure was released three times. The reaction was performed at 90 °C for 20 h. After that the autoclave was cooled down using ice-bath and the pressure was carefully released through a room temperature (25 °C) condenser (the water temperature was controlled by a thermostat) to a manual burette to get the gas volume. The gas was analyzed by GC. Additional CO₂ was collected via burette by adding HCl aqueous solution to the reaction liquid phase. Experiments were at least performed twice, and the average values were shown. Standard deviations are <5 % of the average.

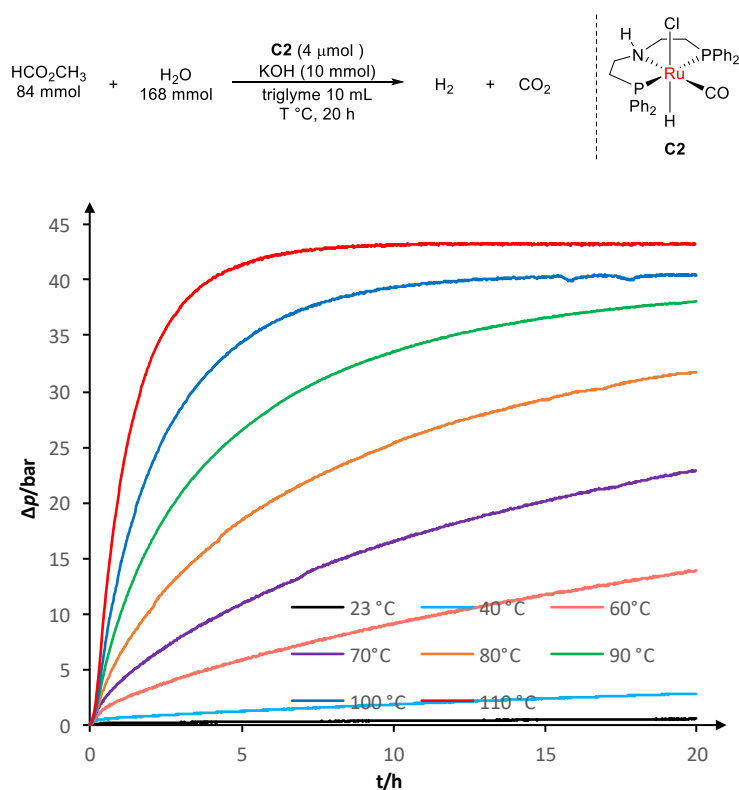
Supplementary Table 6. Base amount variation in the dehydrogenation of methyl formate.



Entry ^a	KOH (mmol)	Δp (bar)	V (mL)	H ₂ :CO ₂ (%)	CO (ppm)	TON
1	0	20.4	1,820	55:45	12	10,223
2	5	35.7	3,380	57:43	14	19,675
3	10	38.1	3,645	58:42	<10	21,590
4	15	37.3	3,600	57:43	<10	20,956
5	20	37.4	3,740	57:43	<10	21,771
6	30	35.6	3,800	56:44	<10	21,732
7	40	33.4	3,680	56:44	<10	21,046
8	60	29.4	3,580	53:47	<10	19,377
9 ^b	0	21.8	1,980	55:45	<10	11,121

^aReaction conditions: under argon atmosphere 4 μmol catalyst and n mmol KOH were added to a 100 mL autoclave. Then 10.0 mL triglyme, 168 mmol H_2O (3.0 mL) and 84 mmol MF (5.2 mL) were injected by a syringe under ice-bath. After that, the autoclave was flushed with N_2 (5 bar) and the pressure was released three times. The reaction was performed at 90°C for 20 h. After that the autoclave was cooled down using ice-bath and the pressure was carefully released through a room temperature (25°C) condenser (the water temperature was controlled by a thermostat) to a manual burette to get the gas volume. The gas was analyzed by GC. Additional CO_2 was collected via burette by adding HCl aqueous solution to the reaction liquid phase. Experiments were at least performed twice, and the average values were shown. Standard deviations are $<5\%$ of the average. ^bCat. **C9** was used instead of **C2**.

Supplementary Table 7. Temperature variation in the dehydrogenation of methyl formate.

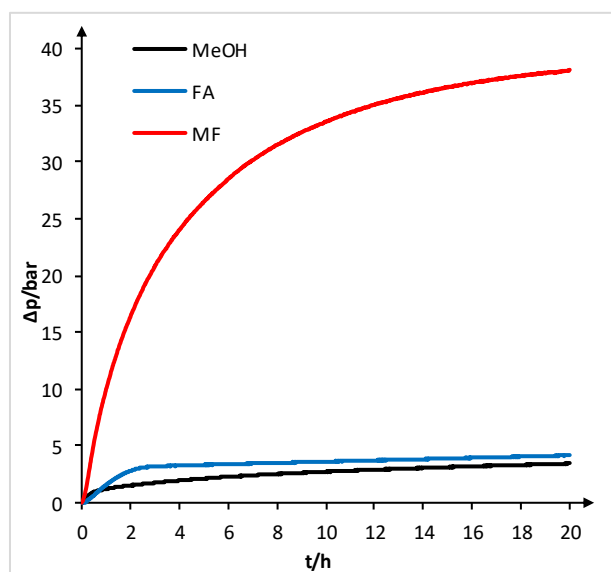


Entry	T (°C)	Δp (bar)	V (mL)	H ₂ :CO ₂ (%)	CO (ppm)	TON
1	23	0.6	86	51:49	<10	448
2	40	2.8	278	52:48	<10	1,476
3	60	13.9	1,485	56:44	<10	8,493
4	70	22.9	2,355	57:43	<10	13,709
5	80	31.7	3,165	57:43	<10	18,424
6	90	38.1	3,645	58:42	<10	21,590
7	100	40.4	3,650	58:42	<10	21,620
8	110	43.2	3,745	57:43	39	21,800

Reaction conditions: under argon atmosphere 4 μmol **C2** catalyst (2.4 mg) and 10 mmol KOH (0.561 g) were added to a 100 mL autoclave. Then 10.0 mL triglyme, 168 mmol H_2O (3.0 mL) and 84 mmol MF (5.2 mL) were injected by a syringe under ice-bath. After that, the autoclave was flushed with N_2 (5 bar) and the pressure was released three times. The reaction was performed at T $^\circ\text{C}$ for 20 h. After that the autoclave was cooled down using ice-bath and the pressure was carefully released through a room temperature (25 $^\circ\text{C}$) condenser (the water temperature was controlled by a thermostat) to a manual burette to get the gas volume. The gas was analyzed by GC. Additional CO_2 was collected via burette by adding HCl aqueous solution to the reaction liquid phase. Experiments were at least performed twice, and the average values were shown. Standard deviations are <5 % of the average.

Dehydrogenation comparison of MF, FA, and methanol.

Supplementary Table 8. Comparison test for dehydrogenation of MeOH, FA, and MF using C2 catalyst.

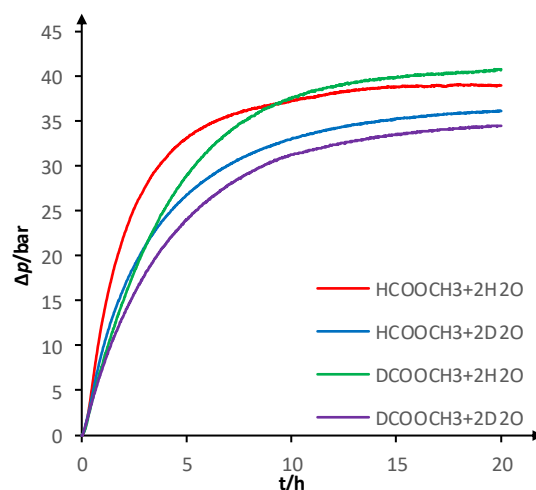


Entry	Substrate	Δp (bar)	V (mL)	H ₂ :CO ₂ (%)	CO (ppm)	Gas evolution curve slope ($\Delta p/\Delta t_{0.6-1.5h}$)	Ratio of gas evolution rate
1	MeOH	3.5	311	79:21	<10	0.4	1.0
2	FA	4.2	359	52:47	3652	1.6	4.0
3	MF	38.1	3,645	58:42	<10	8.0	20.0

General conditions: under argon atmosphere 4 μmol C2 catalyst (2.4 mg) and 10 mmol KOH (0.561 g) were added to a 100 mL autoclave. Then 10.0 mL triglyme, 168 mmol H₂O (3.0 mL) and 84 mmol substrate were injected by a syringe under ice-bath. After that, the autoclave was flushed with N₂ (5 bar) and the pressure was released three times. The reaction was performed at 90 °C for 20 h. After that the autoclave was cooled down using ice-bath and the pressure was carefully released through a room temperature (25 °C) condenser (the water temperature was controlled by a thermostat) to a manual burette to get the gas volume. The gas was analyzed by GC. Additional CO₂ was collected via burette by adding HCl aqueous solution to the reaction liquid phase. Experiments were at least performed twice, and the average values were shown. Standard deviations are <5 % of the average.

KIE measurements for the dehydrogenation of MF.

Supplementary Table 9. KIE measurements.



Entry	Substrates	Slope	KIE
1	$\text{HCOOCH}_3 + 2\text{H}_2\text{O}$	12.31	1.00
2	$\text{HCOOCH}_3 + 2\text{D}_2\text{O}$	8.79	1.40
3	$\text{DCOOCH}_3 + 2\text{H}_2\text{O}$	7.75	1.59
4	$\text{DCOOCH}_3 + 2\text{D}_2\text{O}$	6.83	1.80

General conditions: under argon atmosphere 4 μmol **C2** catalyst (2.4 mg) and 10 mmol K_3PO_4 (2.12 g) were added to a 100 mL autoclave. Then 10.0 mL triglyme, 168 mmol water and 64 mmol MF were injected by a syringe under ice-bath. After that, the autoclave was flushed with N_2 (5 bar) and the pressure was released three times. The reaction was performed at 90 °C for 20 h. The pressure data was automatically generated by the pressure monitor. Experiments were at least performed twice, and the average values were shown. Standard deviations are <5 % of the average.

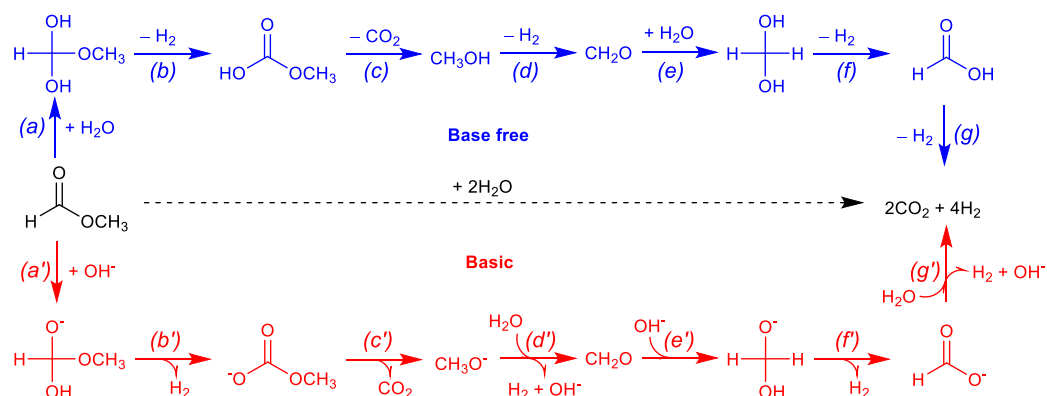
DFT calculations.

Model and Method

DFT computations were carried out with Gaussian 16 program.⁵ Since geometry optimization including solvation effect has serious convergence problems, especially in searching transition states, structures were first optimized in gas phase at the B3PW91 level⁶⁻⁷ of theory with the TZVP basis set⁸ for non-metal elements and the effective core potential (ECP) of Hay and Wadt with double- ζ valence basis set⁹ (LanL2DZ) for Ru and K; and all optimized structures were characterized either as energy minima having only real vibrational frequencies or authentic transition states having one imaginary frequency. In order to verify the validity of transition states (TS) having low imaginary frequency values, the tight thresholds (0.000015 for maximum force, 0.00001 for RMS force, 0.00006 for maximum displacement and 0.00004 for RMS displacement) as well as superfine grid (175,974 grid) were applied for the optimization of TS geometries (low imaginary frequency values below 150 cm^{-1}). Connection between a reactant/product and a transition state was validated with intrinsic reaction coordinate (IRC) or quasi-IRC calculations. In the quasi-IRC calculations, the geometry of a transition state was at first shifted by perturbing the geometries very slightly along the reaction coordinate and released for equilibrium optimization. Then, we refined the energies at the M06L-SCRF level¹⁰ under the consideration of solvation effect of triglyme as solvent based on the solute electron density (SMD) model¹¹ with the def2-TZVP basis set¹²⁻¹³ on the B3PW91 optimized gas phase geometries. The Gibbs free energies were further corrected to standard state in solution with a standard concentration of 1 mol/L ($p = 24.5$ atm) from standard state in gas phase ($p = 1$ atm). The optimized 3D structure were displayed by CYLview program.¹⁴ For discussion and comparison, we used the M06L computed Gibbs free energies at 298 K if not noted otherwise. In our computation we used the conjugated parent amine (**HRu-H**) and amido (**Ru amido**) Ru PNP complexes with Ph substitution at the phosphorous centers.

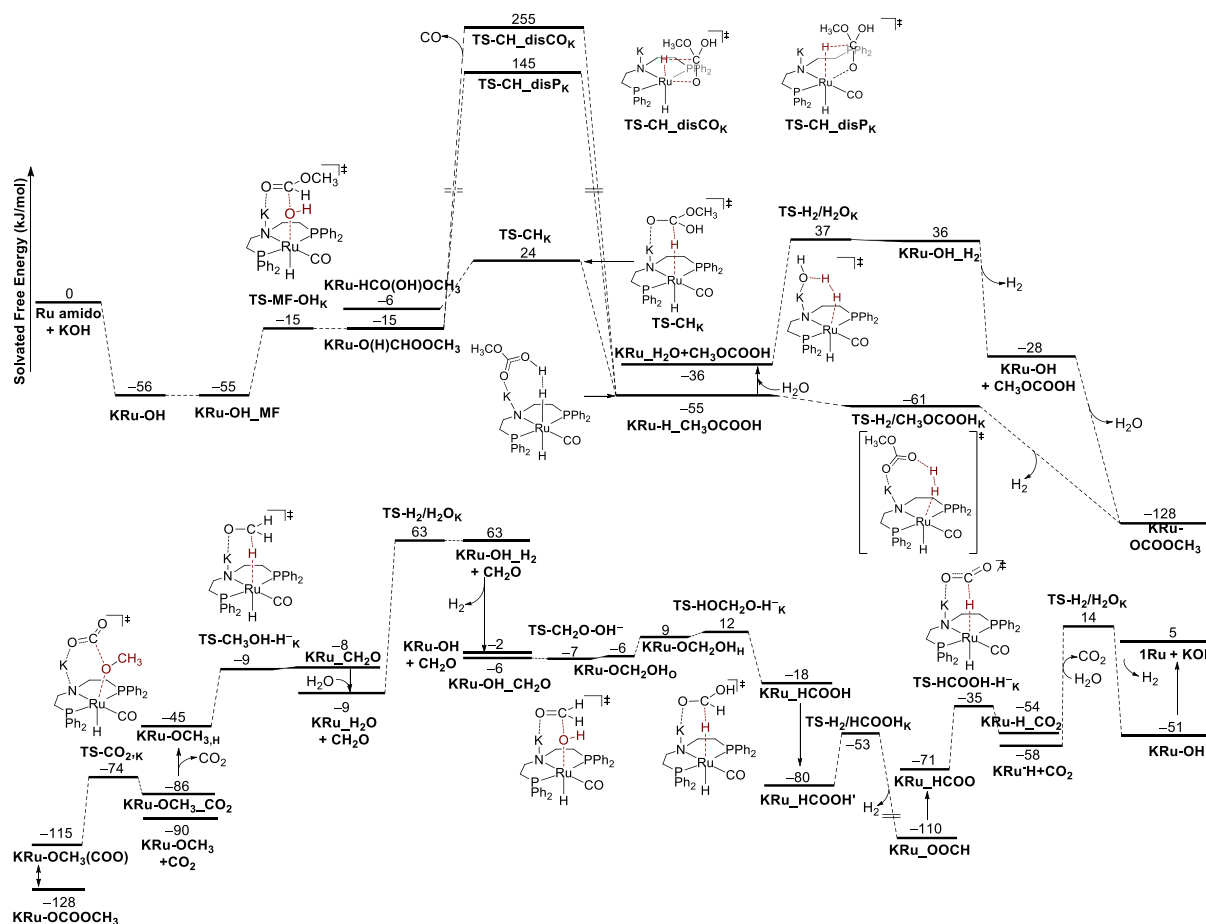
Supplementary Fig. 3 shows the reaction sequences of methyl formate (MF) and H_2O under base free (blue) and basic conditions (red). in the absence of base, the first step is MF hydration to methoxymethanediol (a) [$\text{HCOOCH}_3 + \text{H}_2\text{O} = \text{CH}_3\text{OCH}(\text{OH})_2$]; which is dehydrogenated to methyl hydrogen carbonate (b) [$\text{CH}_3\text{OCH}(\text{OH})_2 = \text{H}_2 + \text{CH}_3\text{OCOOH}$]; followed by the decomposition to CH_3OH and CO_2 (c) [$\text{CH}_3\text{OCOOH} = \text{CH}_3\text{OH} + \text{CO}_2$]. The next step is CH_3OH dehydrogenation to CH_2O (d) [$\text{CH}_3\text{OH} = \text{CH}_2\text{O} + \text{H}_2$], followed by subsequent CH_2O hydration to HOCH_2OH (e) [$\text{CH}_2\text{O} + \text{H}_2\text{O} = \text{HOCH}_2\text{OH}$]; which is dehydrogenated to HCOOH (f) [$\text{HOCH}_2\text{OH} = \text{HCOOH} + \text{H}_2$]; the last step is HCOOH dehydrogenation (g) [$\text{HCOOH} =$

$\text{CO}_2 + \text{H}_2$]. Under strong basic conditions, the deprotonated intermediates are generated which then follow similar reaction sequences (a')-(g').

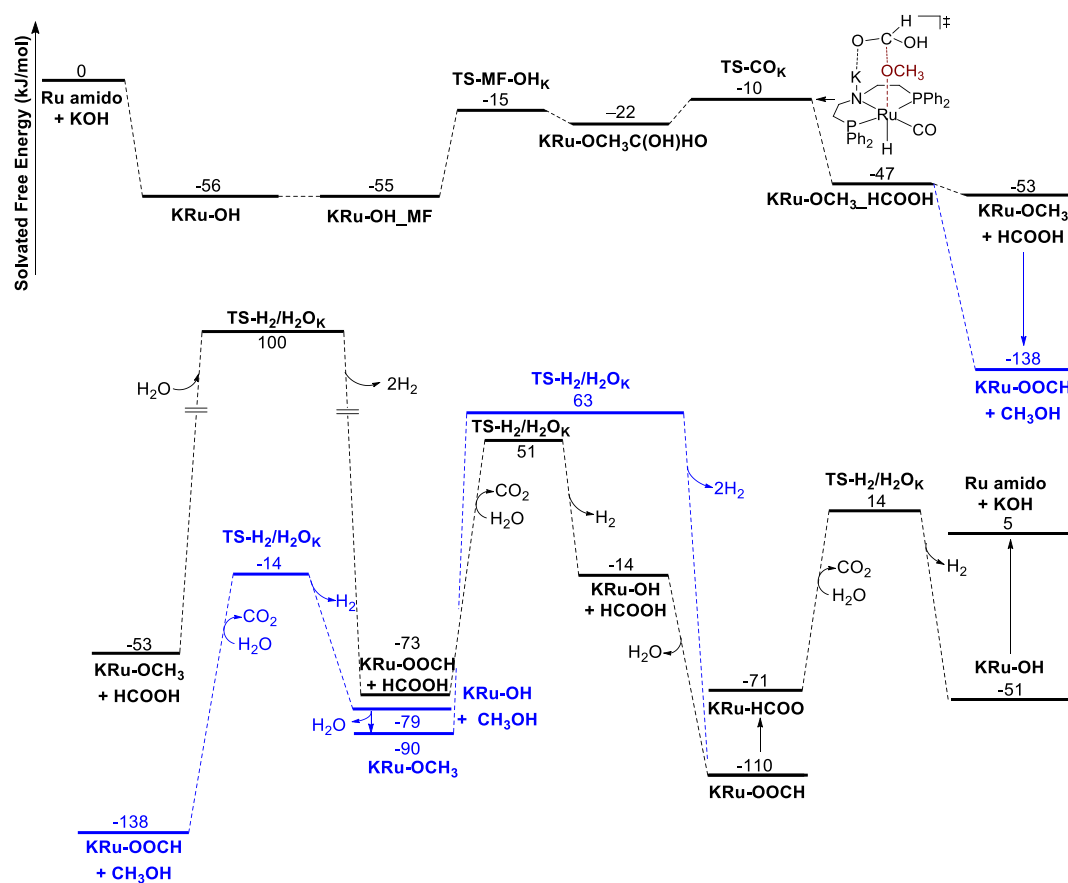


Supplementary Fig. 3 Proposed reaction sequence of MF and H_2O under base free (blue) and basic conditions (red)

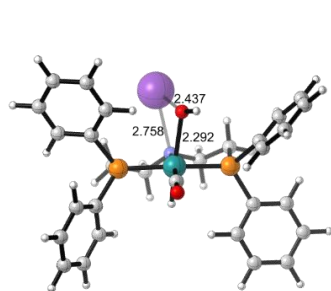
Detailed Gibbs free energy profiles for MF dehydrogenation under basic conditions



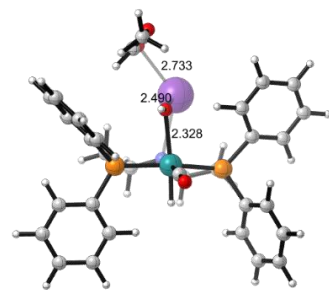
Supplementary Fig. 4 Gibbs free energy profile of aqueous MF dehydrogenation to H₂ and CO₂ via direct dehydrogenation route under basic condition with KOH.



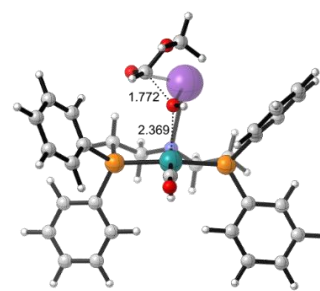
Supplementary Fig. 5 Gibbs free energy profile of aqueous dehydrogenation of MF to H₂ and CO₂ *via* decoupling of C-O route under basic condition with KOH.



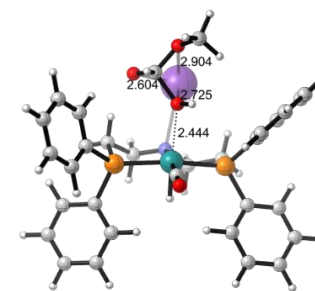
KRu-OH



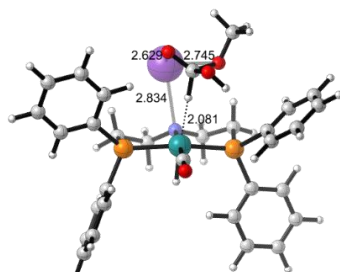
KRu-OH_MF



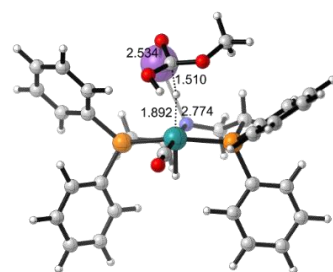
TS-MF-OH_K



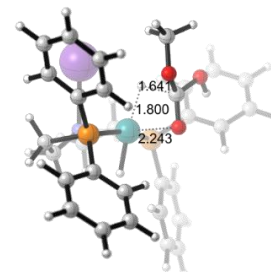
KRu-O(H)CHOOCH₃



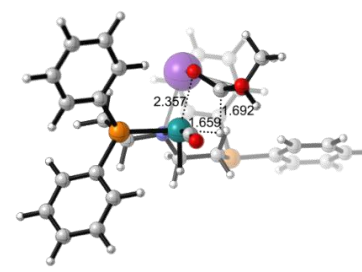
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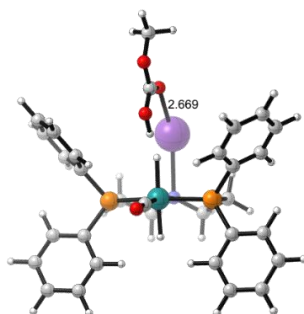
TS-CH_K



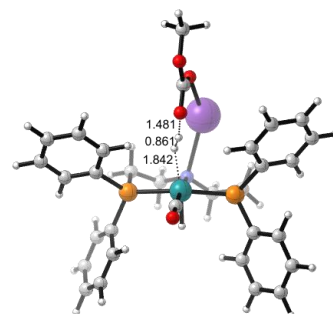
TS-CH_{disCO}_K



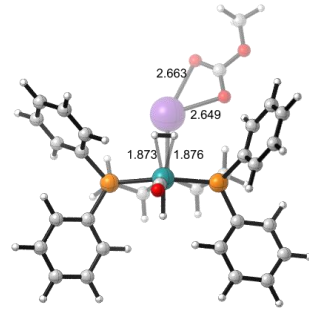
TS-CH_{disP}_K



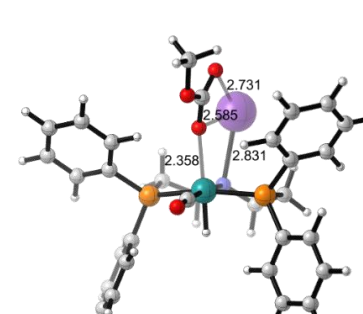
KRu_CH₃OCOOH



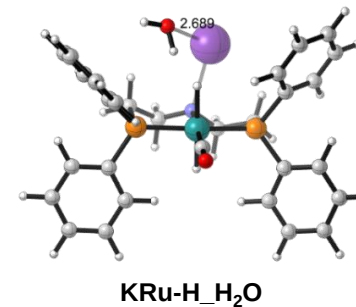
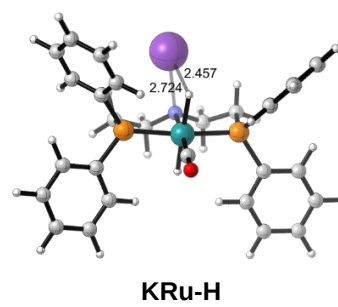
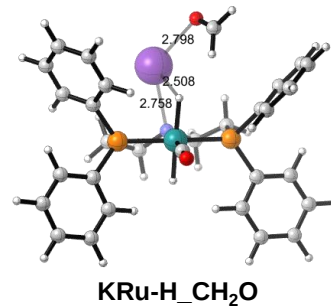
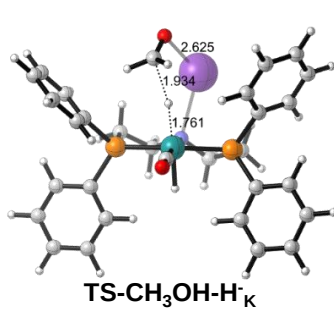
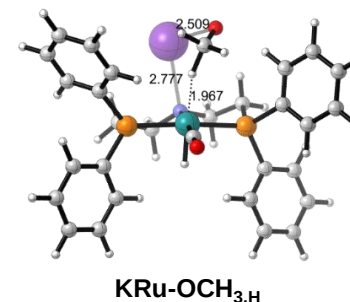
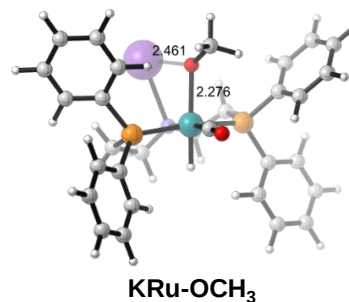
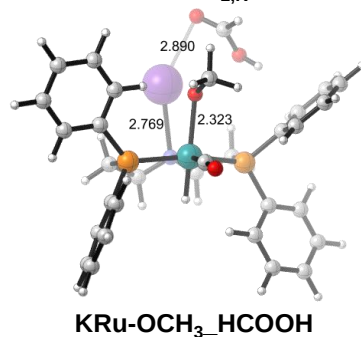
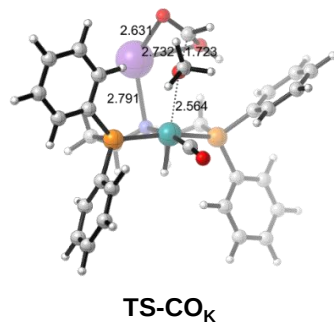
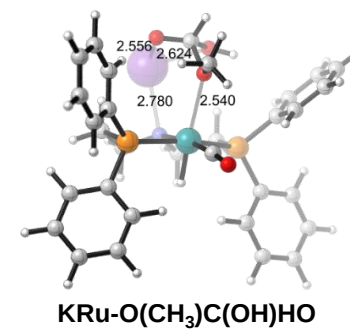
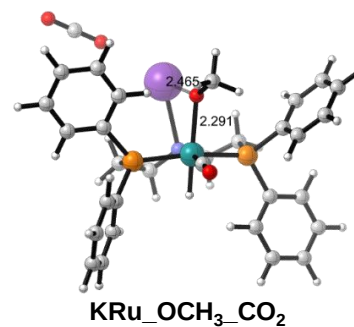
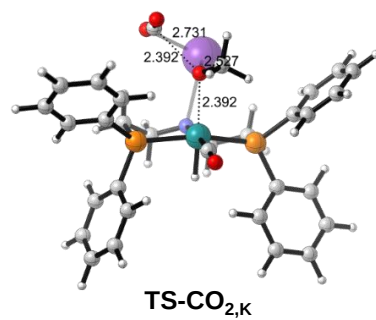
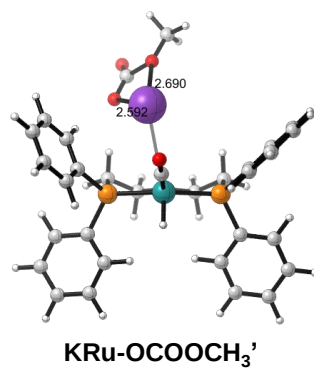
TS-H₂/CH₃OCOOH_K

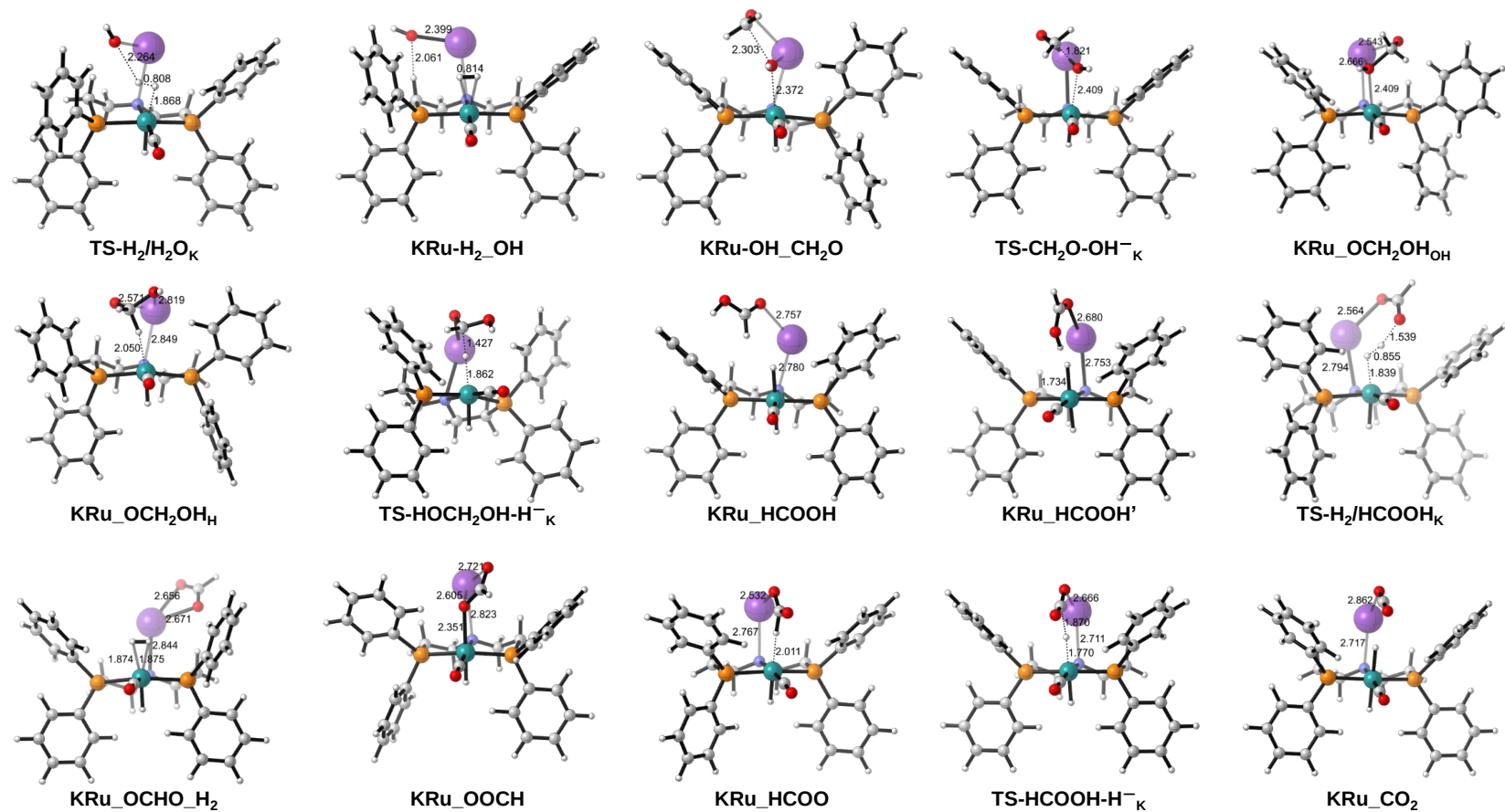


KRu-OCOCH₃_H₂



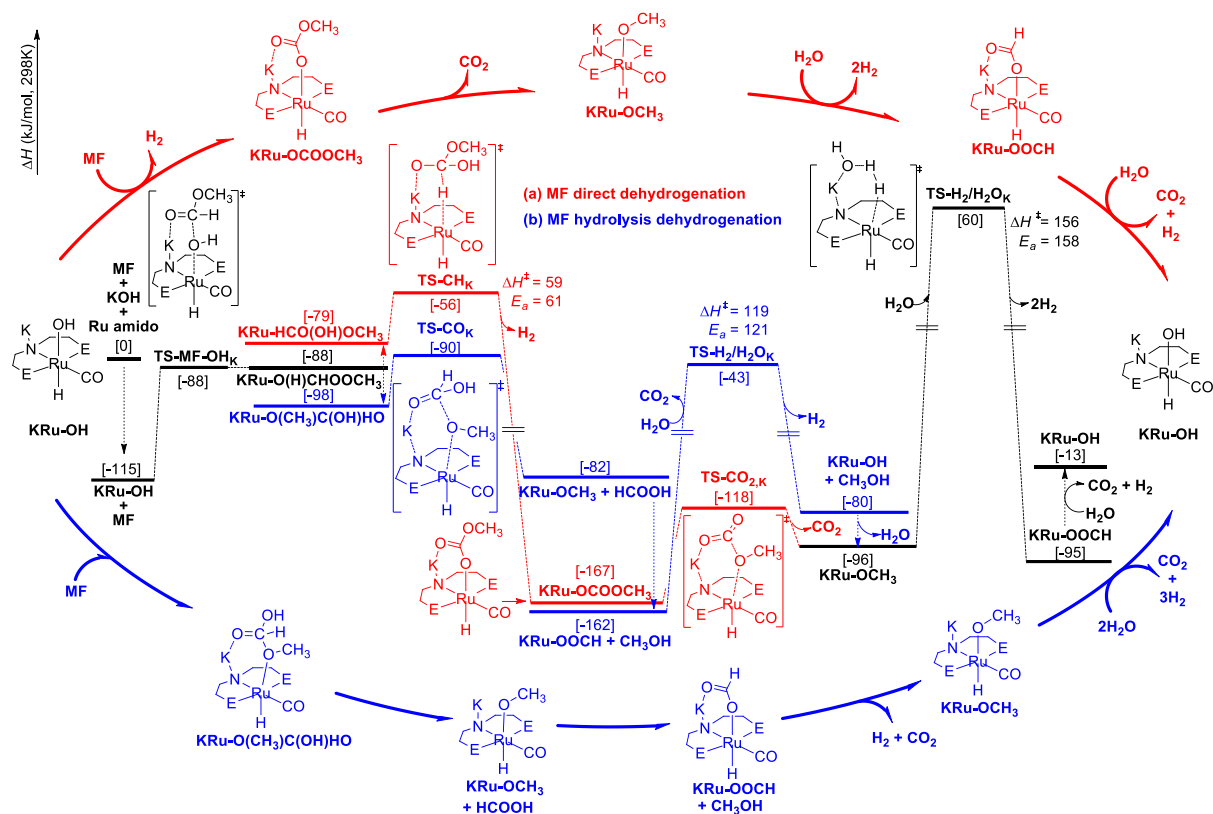
KRu-OCOCH₃





Supplementary Fig. 6 Optimized structures with critical bond distances (Å; purple ball for K, green ball for Ru, yellow ball for P, blue ball for N, grey ball for C and white ball for H).

Enthalpy profile for MF dehydrogenation under basic conditions



Supplementary Fig. 7. Enthalpy profile for MF dehydrogenation under basic conditions with KOH.

Activation energy under basic condition

Eyring equation can be written as

$$k = \frac{k_B T}{h} e^{-\frac{\Delta G^\ddagger}{RT}} = \frac{k_B T}{h} e^{\frac{\Delta S^\ddagger}{R}} e^{-\frac{\Delta H^\ddagger}{RT}}$$

Arrhenius equation:

$$k = Ae^{-\frac{E_a}{RT}}$$

For ideal gas:

$$E_a = \Delta U^\ddagger + RT = \Delta H^\ddagger - p\Delta V + RT$$

In constant pressure:

$$E_a = \Delta H^\ddagger - \Delta n^\ddagger RT + RT$$

In solution:

$$E_a = \Delta H^\ddagger - 0 + RT = \Delta H^\ddagger + RT$$

The theoretical predicted activation energy are shown in Supplementary Table 10.

Supplementary Table 10. Calculated energy barriers *via* different mechanisms

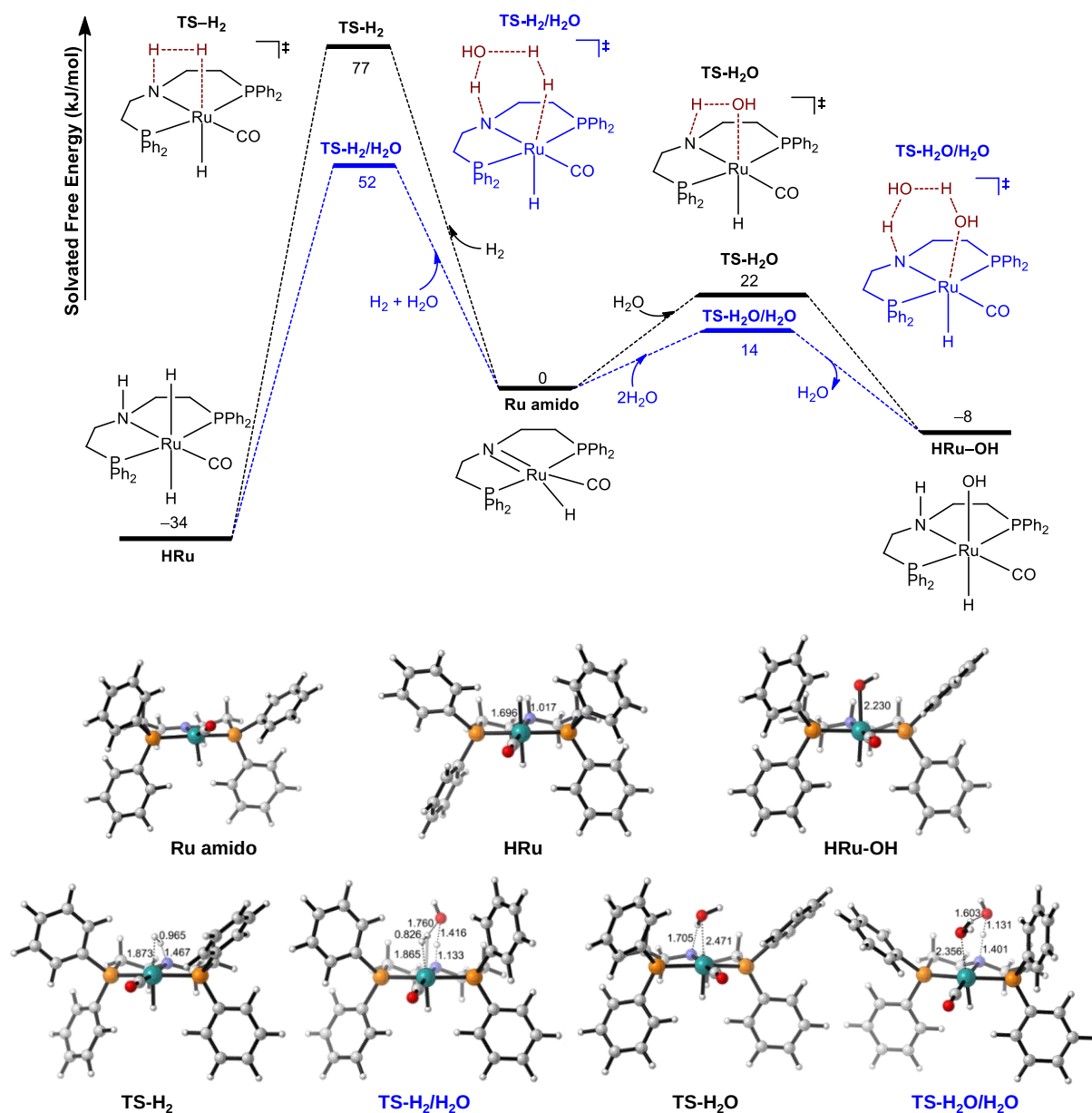
(Unit: kJ·mol⁻¹).

Mechanism	E_a	$\Delta H^\ddagger$	$\Delta G^\ddagger$
Exp.	65	---	---
MF dehydrogenation	61	59	80
MF hydrolysis dehydrogenation	121	119	124
HCOOH dehydrogenation	121	119	124
CH ₃ OH dehydrogenation	158	156	153

It was found that the Arrhenius activation energy (E_a) *via* MF dehydrogenation and MF hydrolysis dehydrogenation mechanisms as well as HCOOH and CH₃OH are 61, 121, 121 and 158 kJ·mol⁻¹, respectively, and they have the same order as the computed activation enthalpy ($\Delta H^\ddagger$) and activation Gibbs free energy ($\Delta G^\ddagger$)

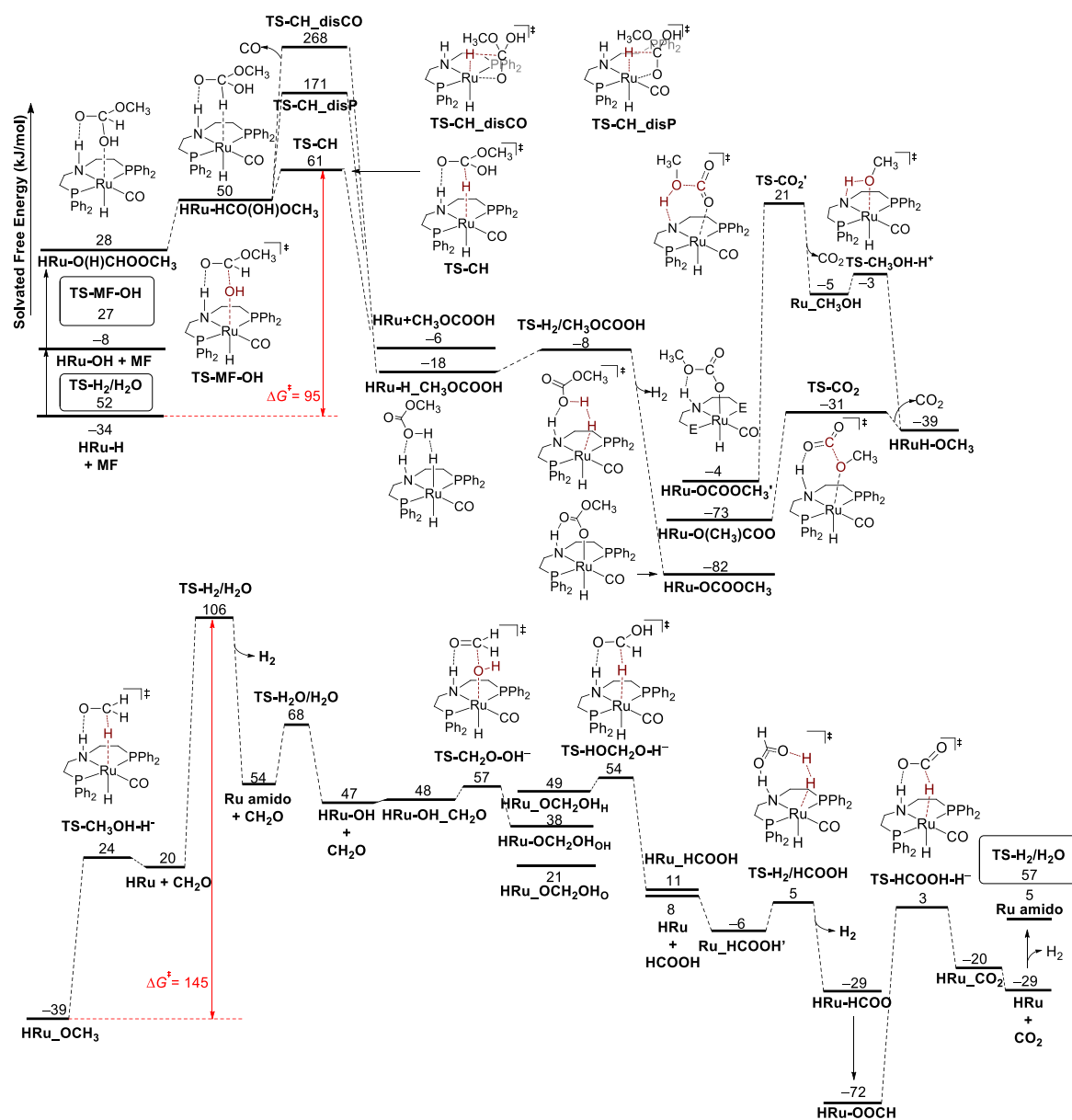
MF dehydrogenation under base free conditions

Gibbs free energy profile for activation of H₂O, H₂ and CH₃OH

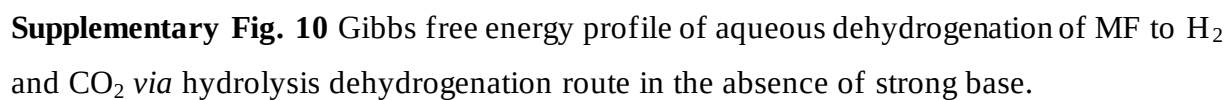


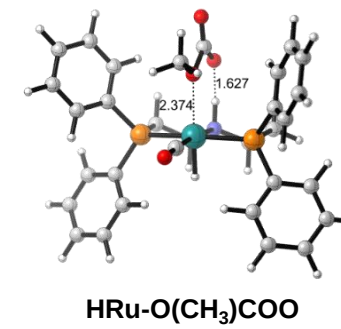
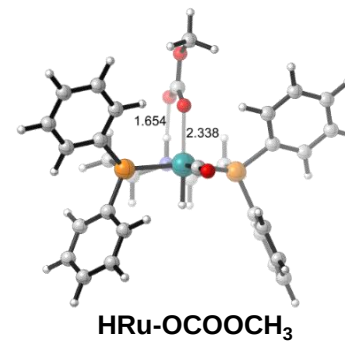
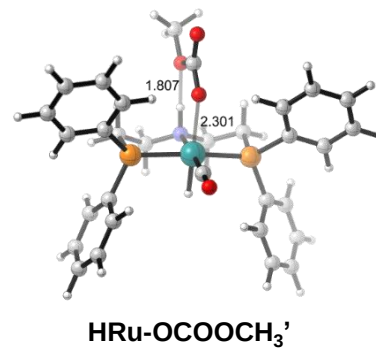
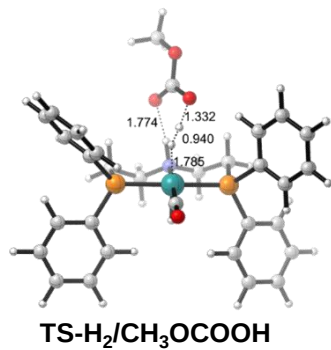
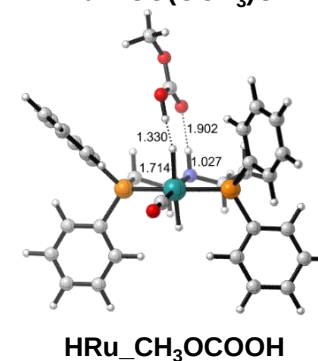
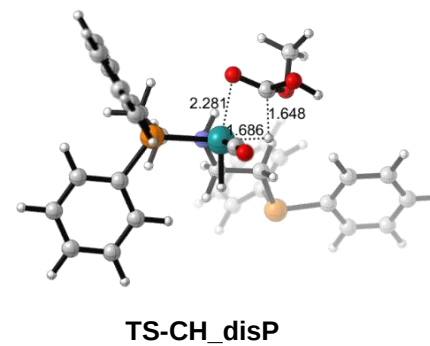
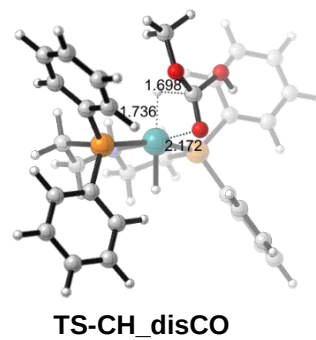
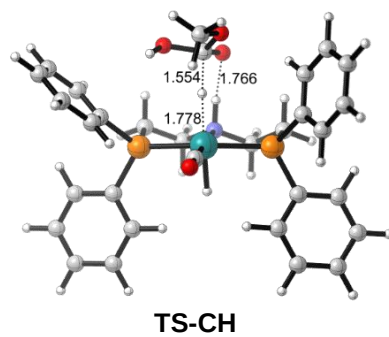
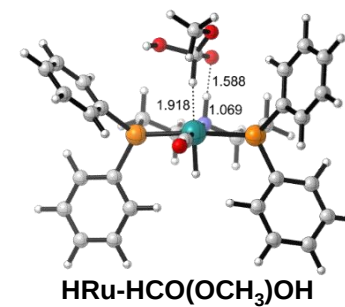
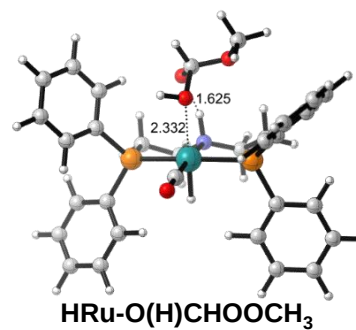
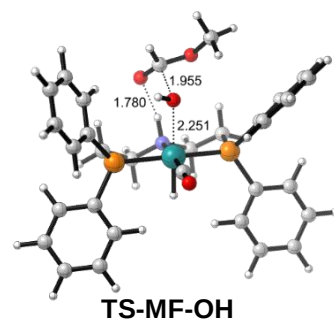
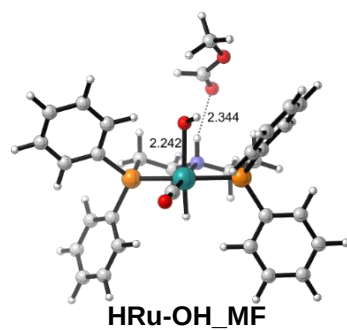
Supplementary Fig. 8. Gibbs free energy profile for activation of H₂O and H₂ with and without H₂O assistance; optimized structures with critical bond distances (Å; green ball for Ru, yellow ball for P, blue ball for N, grey ball for C, red ball for O and white ball for H).

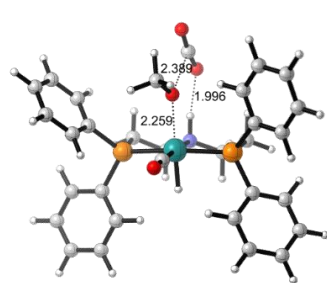
Detailed Gibbs free energy profiles for MF dehydrogenation under base free conditions



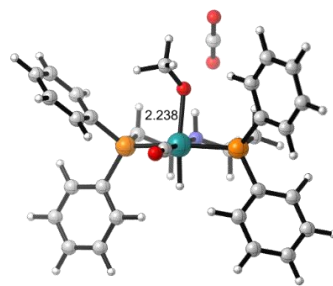
Supplementary Fig. 9 Gibbs free energy profile of aqueous dehydrogenation of MF to H₂ and CO₂ via direct dehydrogenation route in the absence of strong base.



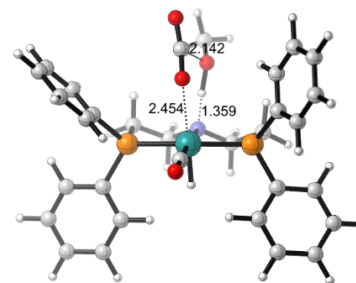




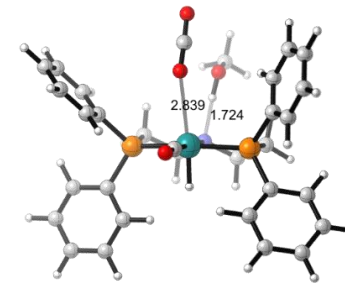
TS-CO₂



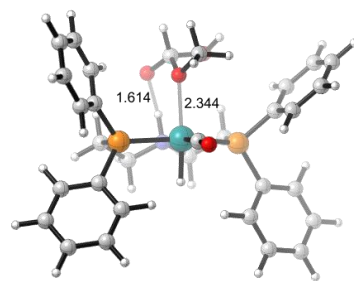
HRu-OCH₃-CO₂



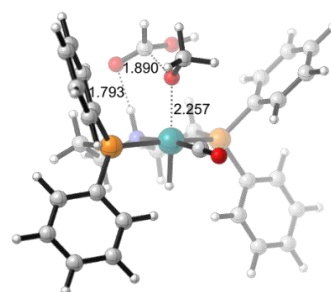
TS-CO₂'



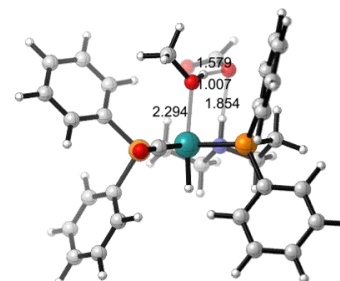
Ru-CO₂-CH₃OH



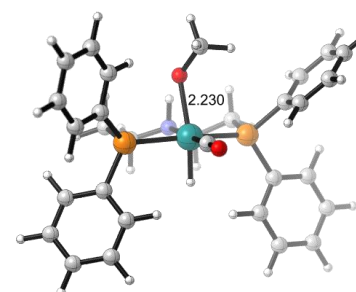
HRu-O(CH₃)C(OH)HO



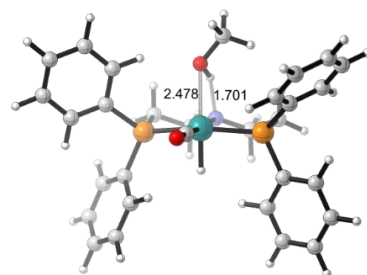
TS-CO



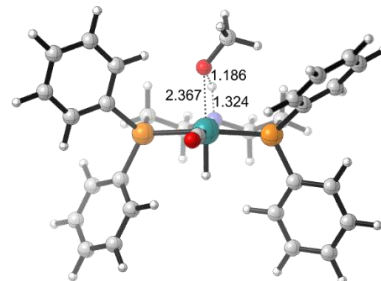
HRu-O(H)CH₃-HCOO



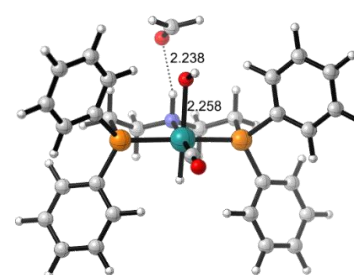
HRu-OCH₃



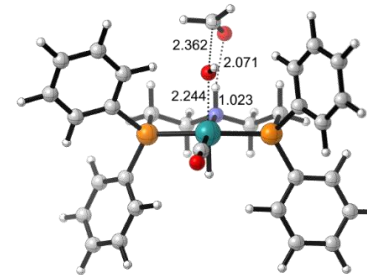
Ru-CH₃OH



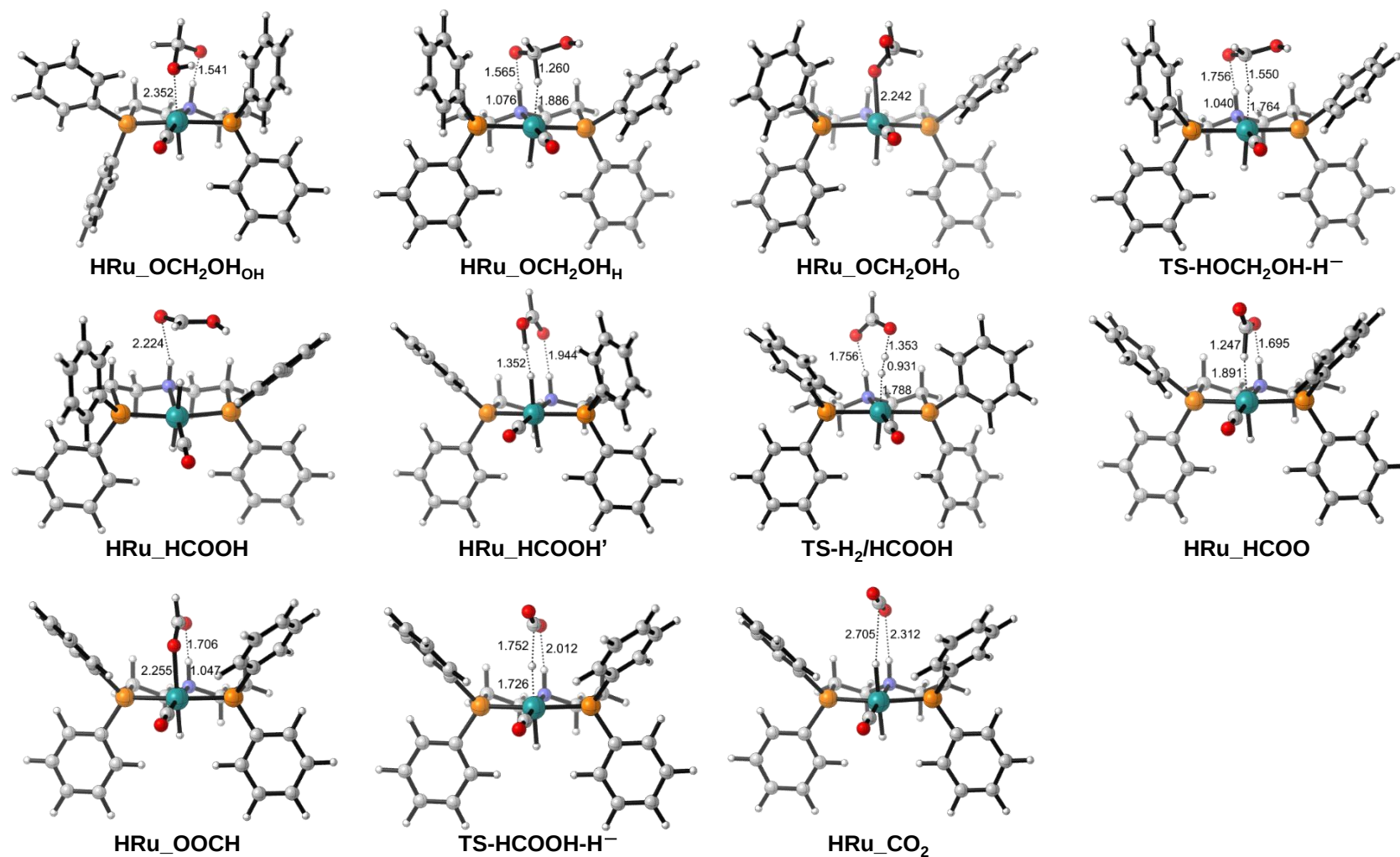
TS-CH₃OH-H⁺



HRu-OH-CH₂O



TS-CH₂O-OH⁻



Supplementary Fig. 11 Optimized structures with critical bond distances (Å; green ball for Ru, yellow ball for P, blue ball for N, grey ball for C and white ball for H).

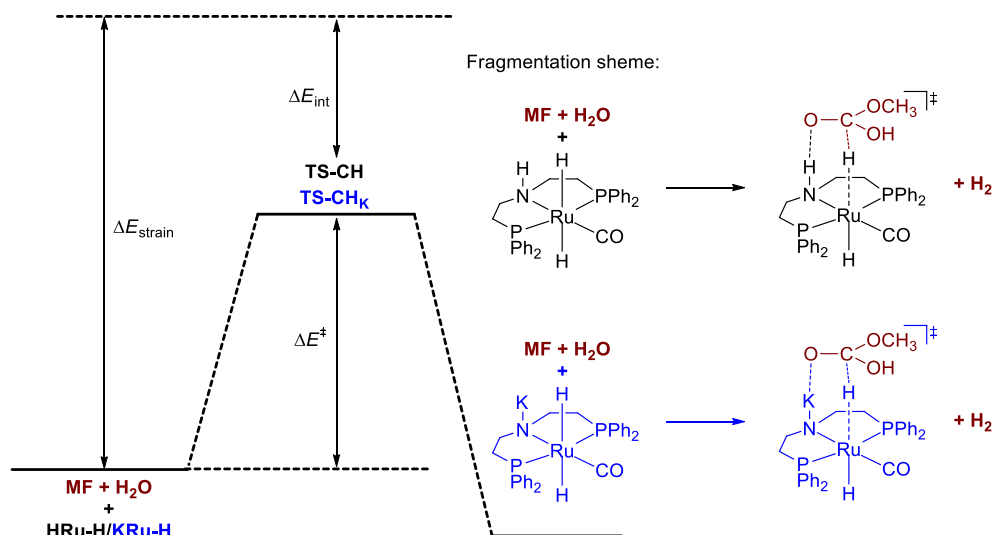
Activation strain model on the basis of key transition states

To understand the lower energy barriers under basic condition, we dissected the electronic activation energy of the key transition states into the deformation and interaction effect of substrate and catalyst by using the proposed activation strain model (ASM). The electronic activation energy $\Delta E^\ddagger$ is defined as the electronic energy difference between the optimized TS and the sum of substrate and catalyst in their optimized structures; and the geometrical strain energy ΔE_{strain} ($\Delta E_{\text{strain}} = \Delta E_{\text{strain/sub}} + \Delta E_{\text{strain/cat}}$) is defined as the electronic energy difference between the sum of the structurally deformed substrate ($\Delta E_{\text{strain/sub}}$) and catalyst ($\Delta E_{\text{strain/cat}}$) individually taken from the optimized TS and the sum of reactant and catalyst in their optimized structures. Accordingly, the difference between ΔE_{strain} and $\Delta E^\ddagger$ is the interaction energy ΔE_{int} ($\Delta E_{\text{int}} = \Delta E_{\text{strain}} - \Delta E^\ddagger$) between substrate and catalyst in the TS.

Activation strain model on the basis of the TS-CH/TS-CH_K

Since the formation of HRu-OCH₃OOCH₃/KRu-OCH₃OOCH₃ *via* transition states TS-CH/TS-CH_K are the rate-determining steps for MF dehydrogenation in the presence and absence of strong base, the AMS analysis was first performed based on the rate-determining states. As the reaction energy ΔE_r of [KRu-H + H₂O = KRu-OH + H₂] is thermodynamically neutral ($\Delta E_r = -1 \text{ kJ}\cdot\text{mol}^{-1}$), the KRu-H is used as reference state instead of KRu-OH for understanding the origin of lower energy barrier with similar reactant and TS structures. The ASM analysis (Supplementary Table 11) shows slightly lower strain energy ΔE_{strain} in the presence of K⁺ than H⁺ by 5 kJ·mol⁻¹ (133 vs. 138 kJ·mol⁻¹). Meanwhile, the stabilization effect (ΔE_{int}) of K⁺ cation is higher than H⁺ by 14 kJ·mol⁻¹ (-100 vs. -86 kJ·mol⁻¹). Totally, the energy barrier in the presence of base is lower than that under base free condition by 19 kJ·mol⁻¹ (33 vs. 52 kJ·mol⁻¹).

1 **Supplementary Table 11.** ASM analysis of the transition states TS-CH/TS-CH_K (kJ·mol⁻¹).

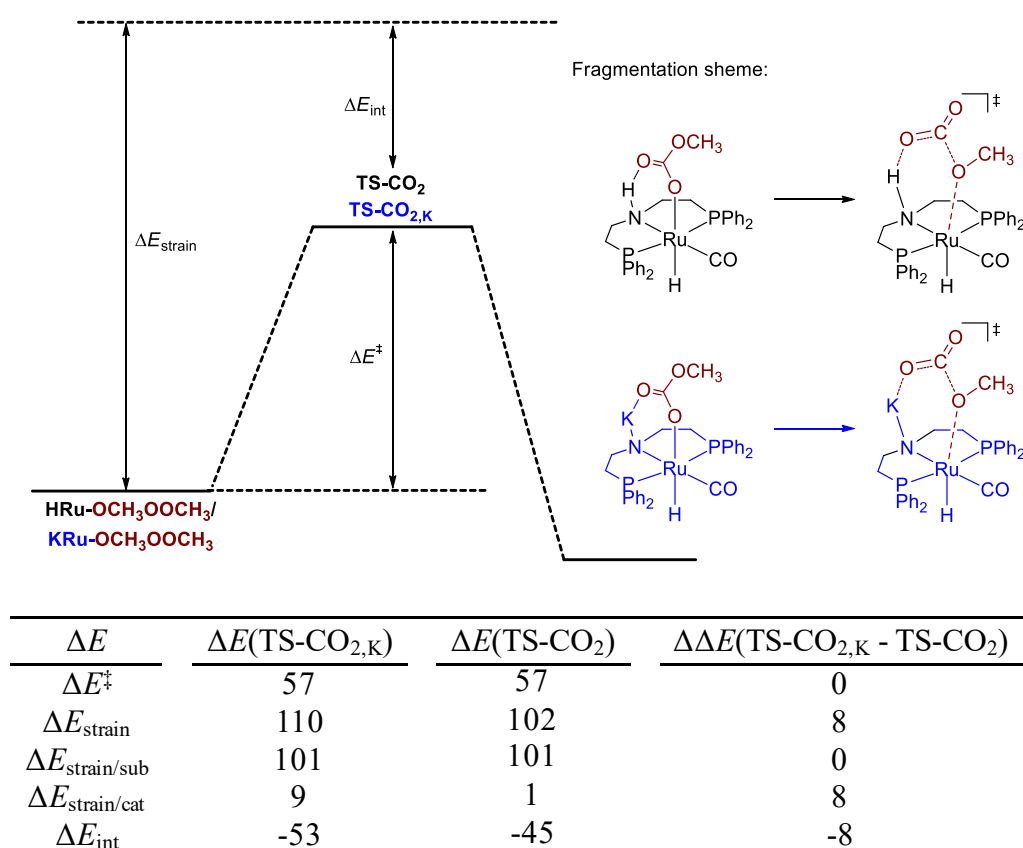


ΔE	$\Delta E(\text{TS-CH}_K)$	$\Delta E(\text{TS-CH})$	$\Delta \Delta E(\text{TS-CH}_K - \text{TS-CH})$
$\Delta E^\ddagger$	33	52	-19
ΔE_{strain}	133	138	-5
$\Delta E_{\text{strain/sub}}$	120	130	-10
$\Delta E_{\text{strain/cat}}$	14	8	5
ΔE_{int}	-100	-86	-14

Activation strain model on the basis of the HRu-OCH₃OOCH₃ and KRu-OCH₃OOCH₃ for CO₂ formation

The energy barriers of the decoupling of C-O route in the presence and absence of strong base are similar. Using the same strategy, transition states of TS-CO₂ and TS-CO_{2,K} were also analyzed by ASM model (Supplementary Table 12). The ASM analysis reveals that the slightly higher total strain energy ΔE_{strain} (110 vs. 102 kJ·mol⁻¹) under basic condition is origin from the deformation of the catalyst $\Delta E_{\text{strain/cat}}$ (9 vs. 1 kJ·mol⁻¹), the stabilization effect (ΔE_{int}) of K⁺ cations (-53 vs. -45 kJ·mol⁻¹) offset the deformation energy and makes the energy barrier comparable (57 vs. 57 kJ·mol⁻¹).

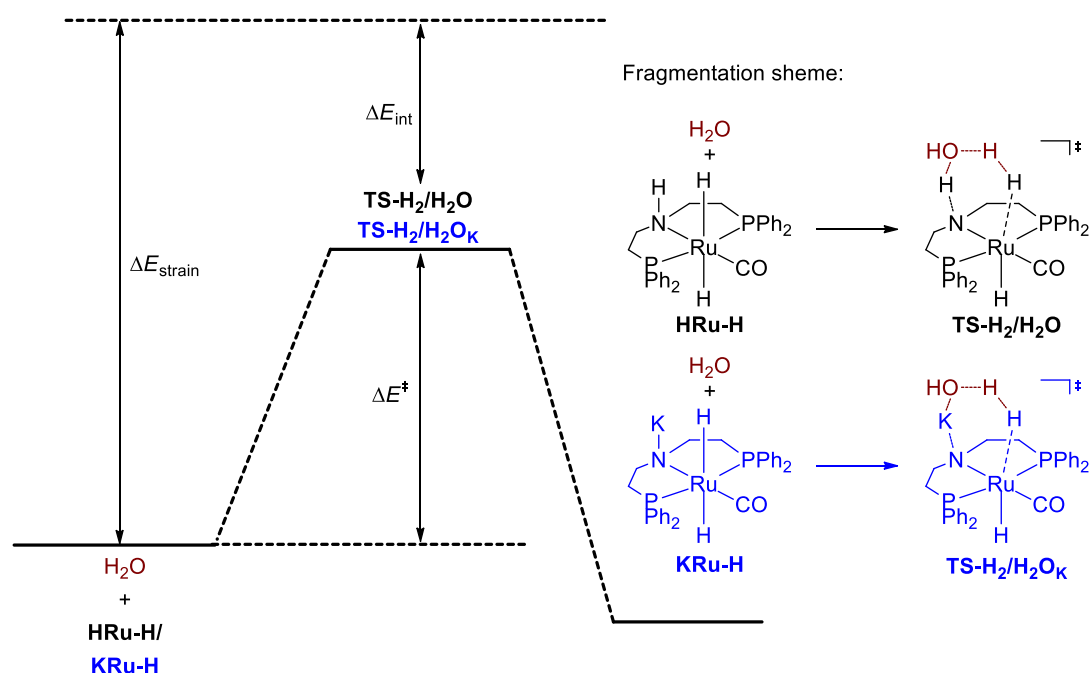
Supplementary Table 12. ASM analysis of the transition states TS-CO_{2,K} and TS-CO₂ (kJ·mol⁻¹).



Activation strain model on the basis of the HRu-OCH₃OOCH₃ and KRu-OCH₃OOCH₃ for CO₂ formation

The ASM analysis (Supplementary Table 13) shows that although the higher total strain energy ΔE_{strain} is found under basic condition than that in the absence of base (624 vs. 485 kJ·mol⁻¹), the stabilization effect (ΔE_{int}) of K⁺ cation (-592 vs. -429 kJ·mol⁻¹) significantly lowers the energy barrier of TS-H₂/H₂O_K than that under base-free condition of TS-H₂/H₂O by 24 kJ·mol⁻¹ (32 vs. 56 kJ·mol⁻¹).

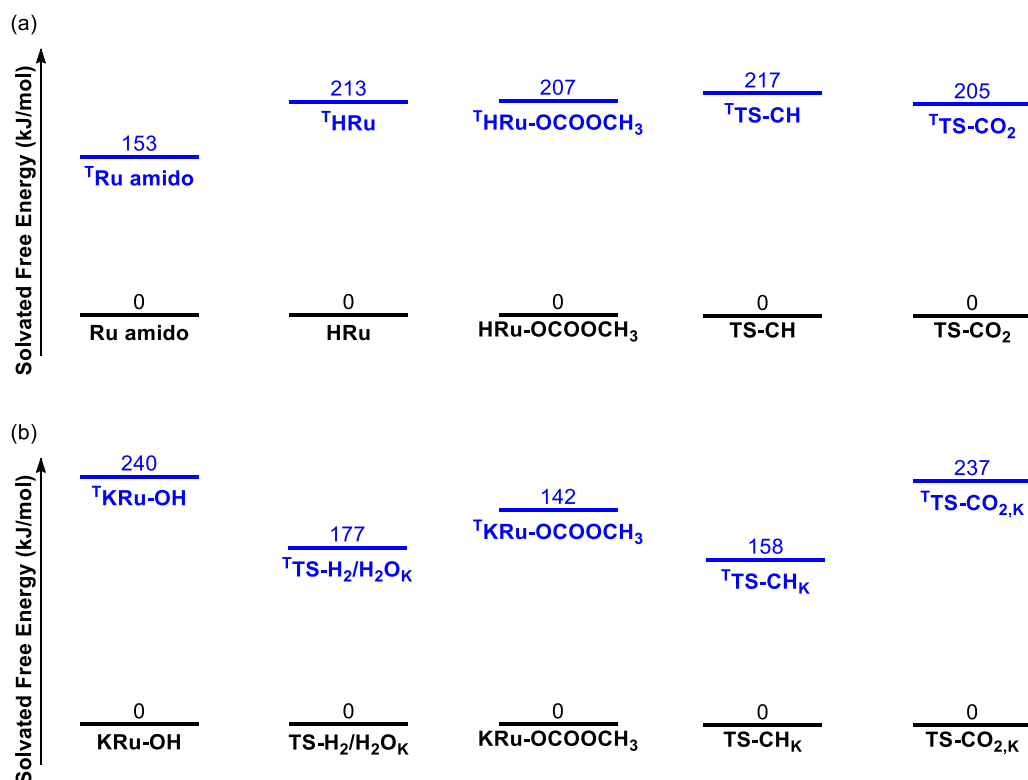
Supplementary Table 13. ASM analysis of the transition states TS-H₂/H₂O_K and TS-H₂/H₂O (kJ·mol⁻¹).



ΔE	$\Delta E(\text{TS-H}_2/\text{H}_2\text{O}_K)$	$\Delta E(\text{TS-H}_2/\text{H}_2\text{O})$	$\Delta\Delta E(\text{TS-H}_2/\text{H}_2\text{O}_K - \text{TS-H}_2/\text{H}_2\text{O})$
$\Delta E^\ddagger$	31	55	24
ΔE_{strain}	624	485	-139
$\Delta E_{\text{strain/sub}}$	583	436	-147
$\Delta E_{\text{strain/cat}}$	40	48	8
ΔE_{int}	-592	-429	163

Gibbs free energy of key intermediates and transition states in singlet and triplet state

The triplet state of the key intermediates and transition states were calculated. As shown in **Supplementary Fig. 12**, the triplet state of the intermediates and the transition states can be ruled out since the free energy of all tested structures in triplet state are more than 140 kJ·mol⁻¹ higher than that in singlet state. This is because that all these complexes are closed-shell 18-valence-electron states.



Supplementary Fig. 12 Gibbs free energy difference of key intermediates and transition states between their singlet (black) and triplet state (blue).

Computed energetic data and Cartesian coordinates (DFT)

Supplementary Table 14. Computed Energetic Data for All Optimized Structures

Species	Imag	ZPE ^a	H_{corr}^a	G_{corr}^a	$E_{e,scr}^b$	E_{scr}^c	H_{scr}^c	$G_{scr,1atm}^c$	$G_{scr,1M}^d$
H ₂	0	0.01007	0.01337	-0.00143	-1.16898	-1.15891	-1.15561	-1.17041	-1.16740
HCOOCH ₃ (MF)	0	0.06207	0.06754	0.03527	-229.12668	-229.06461	-229.05914	-229.09141	-229.08840
HCOOH	0	0.03392	0.03802	0.00984	-189.82093	-189.78701	-189.78291	-189.81109	-189.80808
CH ₃ OH	0	0.05124	0.05550	0.02850	-115.75287	-115.70163	-115.69737	-115.72437	-115.72136
H ₂ O	0	0.02137	0.02515	0.00373	-76.45292	-76.43155	-76.42777	-76.44919	-76.44618
HOCH ₂ OH	0	0.0575	0.06220	0.03330	-191.00539	-190.94789	-190.94319	-190.97209	-190.96908
CH ₃ OCH ₂ OH	0	0.08544	0.09148	0.05798	-230.31021	-230.22477	-230.21873	-230.25223	-230.24922
CO ₂	0	0.01183	0.01539	-0.00951	-188.64806	-188.63623	-188.63267	-188.65757	-188.65456
CH ₂ O	0	0.02666	0.03047	0.00566	-114.53317	-114.50651	-114.50270	-114.52751	-114.52450
CH ₃ OCOOH	0	0.06768	0.07392	0.03925	-304.39881	-304.33113	-304.32489	-304.35956	-304.35655
CH ₃ OCHOHOH	0	0.08976	0.09679	0.06071	-305.56779	-305.47803	-305.47100	-305.50708	-305.50407
KOH	0	0.01079	0.01519	-0.00591	-675.80938	-675.79859	-675.79419	-675.81529	-675.81228
RuH	0	0.52349	0.55662	0.45721	-2031.80546	-2031.28197	-2031.24884	-2031.34825	-2031.34524
TS-H ₂	1 (-1105.8)	0.51722	0.55034	0.44990	-2031.75612	-2031.23890	-2031.20578	-2031.30622	-2031.30321
Ru amido	0	0.50295	0.53603	0.43456	-2030.60255	-2030.09960	-2030.06652	-2030.16799	-2030.16498
HRu_H ₂ O	0	0.54804	0.58420	0.47827	-2108.27144	-2107.72340	-2107.68724	-2107.79317	-2107.79016
TS-H ₂ /H ₂ O	1 (-224.2)	0.54304	0.57834	0.47546	-2108.23737	-2107.69433	-2107.65903	-2107.76191	-2107.75890
Ru_H ₂ O_H ₂	0	0.54292	0.57910	0.47285	-2108.24535	-2107.70243	-2107.66625	-2107.77250	-2107.76952
Ru_H ₂ O	0	0.52847	0.56361	0.45918	-2107.06601	-2106.53754	-2106.50240	-2106.60683	-2106.60382
TS-H ₂ O	1 (-928.4)	0.52523	0.55977	0.45627	-2107.06170	-2106.53647	-2106.50193	-2106.60543	-2106.60242
HRu-OH	0	0.53035	0.56517	0.46214	-2107.07911	-2106.54876	-2106.51394	-2106.61697	-2106.61396
Ru_2H ₂ O	0	0.55327	0.59078	0.48144	-2183.53633	-2182.98306	-2182.94555	-2183.05489	-2183.05189
TS-H ₂ O/H ₂ O	1	0.55119	0.58795	0.48043	-2183.53535	-2182.98416	-2182.94740	-2183.05492	-2183.05191

	(-226.0)								
HRu-OH_H ₂ O	0	0.55544	0.59247	0.48567	-2183.55017	-2182.99473	-2182.95770	-2183.06450	-2183.06147
HRu-OH_MF	0	0.59315	0.63494	0.51242	-2336.21593	-2335.62278	-2335.58099	-2335.70351	-2335.70050
TS-MF-OH ^f	1 (-130.9/-131.7 ^g)	0.59460	0.63432	0.52053	-2336.21290	-2335.61830	-2335.57858	-2335.69237	-2335.68936
HRu- O(H)CHOOCH ₃	0	0.59571	0.63542	0.52171	-2336.21343	-2335.61772	-2335.57801	-2335.69172	-2335.68871
HRu- HCO(OH)OCH ₃	0	0.59309	0.63340	0.51625	-2336.20230	-2335.60921	-2335.5689	-2335.68605	-2335.68304
TS-CH	1 (-450.7)	0.59114	0.63054	0.51725	-2336.19635	-2335.60521	-2335.56581	-2335.67910	-2335.67609
TS-CH_disCO	1 (-597.4)	0.58142	0.61868	0.51049	-2222.76519	-2222.18377	-2222.14651	-2222.25470	-2222.25169
TS-CH_disP	1 (-529.5)	0.59006	0.63072	0.50944	-2336.14663	-2335.55657	-2335.51591	-2335.63719	-2335.63419
HRu_CH ₃ OCOOH	0	0.59165	0.63183	0.51411	-2336.22341	-2335.63176	-2335.59158	-2335.70930	-2335.70629
HRu- O(CH ₃)C(OH)HO	0	0.59538	0.63521	0.52196	-2336.21541	-2335.62003	-2335.58020	-2335.69345	-2335.69044
TS-CO ^f	1 (-97.4/-97.9 ^g)	0.59467	0.63441	0.52097	-2336.21343	-2335.61876	-2335.57902	-2335.69245	-2335.68944
HRu- O(H)CH ₃ _HCOO	0	0.59470	0.63582	0.51810	-2336.24796	-2335.65326	-2335.61214	-2335.72986	-2335.72685
HRu-OCH ₃	0	0.55799	0.59455	0.48747	-2146.38296	-2145.82497	-2145.78841	-2145.89549	-2145.89248
TS-H ₂ /CH ₃ OCOOH	1 (-698.1)	0.58821	0.62804	0.51166	-2336.21725	-2335.62904	-2335.58921	-2335.70559	-2335.70258
HRu-OCOOCH ₃	0	0.57424	0.61356	0.49820	-2335.06454	-2334.49030	-2334.45098	-2334.56634	-2334.56333
HRu-OCOOCH ₃ '	0	0.57428	0.61377	0.49809	-2335.05766	-2334.48338	-2334.44389	-2334.55957	-2334.55656
HRu-O(CH ₃)COO	0	0.57386	0.61320	0.49912	-2335.06199	-2334.48813	-2334.44879	-2334.56287	-2334.55986
TS-CO ₂ ^f	1 (-63.7/-63.7 ^g)	0.57161	0.61125	0.49576	-2335.04276	-2334.47115	-2334.43150	-2334.54700	-2334.54399
HRu_OCH ₃ _CO ₂	0	0.57082	0.61185	0.49084	-2335.04050	-2334.46968	-2334.42865	-2334.54966	-2334.54665

TS-CO ₂ [†]	1 (-503.9)	0.56597	0.60618	0.48904	-2335.01608	-2334.45011	-2334.40990	-2334.52704	-2334.52403
Ru-CH ₃ OH	0	0.55678	0.59360	0.48568	-2146.36788	-2145.81110	-2145.77428	-2145.88220	-2145.87923
TS-CH ₃ OH-H ⁺	1 (-930.4)	0.55309	0.58943	0.48281	-2146.36447	-2145.81138	-2145.77504	-2145.88166	-2145.87865
TS-CH ₃ OH-H ⁻	1 (-55.3/-41.1 ⁹)	0.55248	0.58847	0.48254	-2146.35323	-2145.80075	-2145.76476	-2145.87069	-2145.86768
HRu-OH-CH ₂ O	0	0.55951	0.59846	0.48453	-2221.62551	-2221.06600	-2221.02705	-2221.14098	-2221.13798
TS-CH ₂ O-OH ⁻	1 (-42.5/-41.6 ⁹)	0.56034	0.59807	0.48715	-2221.62486	-2221.06452	-2221.02679	-2221.13771	-2221.13470
HRu-OCH ₂ OH _{OH}	0	0.56290	0.59990	0.49261	-2221.63756	-2221.07466	-2221.03766	-2221.14495	-2221.14195
HRu-OCH ₂ OH _O	0	0.56372	0.60128	0.49096	-2221.64238	-2221.07866	-2221.04110	-2221.15142	-2221.14841
HRu-OCH ₂ OH _H	0	0.56009	0.59716	0.48935	-2221.62998	-2221.06989	-2221.03282	-2221.14063	-2221.13762
TS-HOCH ₂ OH-H ⁻	1 (-379.7)	0.5586	0.59536	0.48827	-2221.62690	-2221.06830	-2221.03154	-2221.13863	-2221.13562
HRu-HCOOH	0	0.55863	0.59673	0.48434	-2221.63929	-2221.08066	-2221.04256	-2221.15495	-2221.15194
HRu-HCOOH [†]	0	0.55828	0.59599	0.48423	-2221.64570	-2221.08742	-2221.04971	-2221.16147	-2221.15846
TS-H ₂ /HCOOH	1 (-655.0)	0.55501	0.59234	0.48285	-2221.64014	-2221.08513	-2221.04780	-2221.15729	-2221.15428
HRu-OCHO-H ₂	0	0.55677	0.59478	0.48502	-2221.65533	-2221.09856	-2221.06055	-2221.17031	-2221.16731
HRu-HCOO	0	0.54104	0.57786	0.46717	-2220.48661	-2219.94557	-2219.90875	-2220.01944	-2220.01643
HRu-OOCH	0	0.53792	0.57497	0.46305	-2220.46628	-2219.92836	-2219.89131	-2220.00323	-2220.00022
TS-HCOOH-H ⁻	1 (-296.1)	0.53553	0.57229	0.46258	-2220.45319	-2219.91766	-2219.88090	-2219.99061	-2219.98760
HRu-CO ₂	0	0.53612	0.57375	0.46020	-2220.45964	-2219.92352	-2219.88589	-2219.99944	-2219.99643
KRu-H	0	0.50909	0.54427	0.43885	-2631.16129	-2630.65220	-2630.61702	-2630.72244	-2630.71943
KRu-OH	0	0.51572	0.55269	0.44373	-2706.44528	-2705.92956	-2705.89259	-2706.00155	-2705.99854
KRu-OH-MF	0	0.57859	0.62222	0.49629	-2935.58601	-2935.00742	-2934.96379	-2935.08972	-2935.08671
TS-MF-OH _K [†]	1 (-123.3/-128.1 ⁹)	0.57966	0.62163	0.50046	-2935.57523	-2934.99557	-2934.95359	-2935.07477	-2935.07176
KRu-	0	0.58053	0.62287	0.50157	-2935.57602	-2934.99549	-2934.95315	-2935.07445	-2935.07144

O(H)CHOOCH ₃									
KRu- HCO(OH)OCH ₃	0	0.57932	0.62164	0.50064	-2935.57146	-2934.99214	-2934.94982	-2935.07082	-2935.06781
TS-CH _K	1 (-563.2)	0.57655	0.61798	0.49989	-2935.55929	-2934.98274	-2934.94131	-2935.0594	-2935.05639
TS-CH_disCO _K	1 (-564.4)	0.56674	0.60602	0.49271	-2822.11843	-2821.55169	-2821.51241	-2821.62572	-2821.62271
TS-CH_disP _K	1 (-556.8)	0.57579	0.61784	0.49762	-2935.51121	-2934.93542	-2934.89337	-2935.01359	-2935.01058
KRu_CH ₃ OCOOH	0	0.57720	0.61982	0.49467	-2935.57655	-2934.99935	-2934.95673	-2935.08188	-2935.07887
KRu- O(CH ₃)C(OH)HO	0	0.58145	0.62347	0.50333	-2935.58051	-2934.99906	-2934.95704	-2935.07718	-2935.07417
TS-CO _K ^f	1 (-100.8/-104.9 ^g)	0.58076	0.62234	0.50394	-2935.57643	-2934.99567	-2934.95409	-2935.07249	-2935.06948
KRu-OCH ₃ _HCOOH	0	0.57885	0.62209	0.49886	-2935.58545	-2935.00660	-2934.96336	-2935.08659	-2935.08359
KRu-CH ₃ OCOOH'	0	0.57718	0.61927	0.49629	-2935.58605	-2935.00887	-2934.96678	-2935.08976	-2935.08675
TS-H ₂ /CH ₃ OCOOH _K	1 (-324.7)	0.57383	0.61611	0.49223	-2935.58407	-2935.01024	-2934.96796	-2935.09184	-2935.08883
KRu-OCOOCH ₃ _H ₂	0	0.57567	0.61847	0.49250	-2935.60168	-2935.02601	-2934.98321	-2935.10918	-2935.10617
KRu-OCOOCH ₃	0	0.55936	0.60107	0.47907	-2934.4291	-2933.86974	-2933.82803	-2933.95003	-2933.94702
KRu-H_H ₂ O	0	0.53313	0.57148	0.45892	-2707.63089	-2707.09776	-2707.05941	-2707.17197	-2707.16896
TS-H ₂ /H ₂ O _K ^f	1 (-65.9/-66.7 ^g)	0.53088	0.56850	0.45801	-2707.60232	-2707.07145	-2707.03383	-2707.14431	-2707.14130
KRu-OH_H ₂	0	0.53144	0.56970	0.45798	-2707.60248	-2707.07104	-2707.03278	-2707.14450	-2707.14149
KRu-OCOOCH ₃ '	0	0.55904	0.60146	0.47479	-2934.41981	-2933.86077	-2933.81835	-2933.94502	-2933.94201
TS-CO _{2K} ^f	1 (-85.4/-87.6 ^g)	0.55635	0.59814	0.47787	-2934.40730	-2933.85095	-2933.80916	-2933.92944	-2933.92643
KRu-OCH ₃ _CO ₂	0	0.55548	0.59868	0.47050	-2934.40455	-2933.84907	-2933.80587	-2933.93405	-2933.93104
KRu-OCH ₃	0	0.54344	0.58205	0.46935	-2745.75034	-2745.2069	-2745.16829	-2745.28099	-2745.27798
KRu-OCH ₃ H	0	0.54130	0.57978	0.46696	-2745.73067	-2745.18937	-2745.15089	-2745.26371	-2745.26070
TS-CH ₃ OH-H ⁻ _K	1	0.53798	0.57603	0.46457	-2745.71476	-2745.17679	-2745.13873	-2745.25020	-2745.24719

Convergence $\Delta E=3.1\text{e-}05$	(-7.3)								
KRu-H_CH ₂ O	0	0.53734	0.57692	0.46100	-2745.71065	-2745.17331	-2745.13373	-2745.24965	-2745.24664
KRu-OH_CH ₂ O	0	0.54554	0.58619	0.46845	-2820.99637	-2820.45083	-2820.41018	-2820.52792	-2820.52491
TS-CH ₂ O-OH ⁻ _K Convergence $\Delta E=4.6\text{e-}05$	1 (-15.3/-14.2 ⁹)	0.54629	0.58576	0.47095	-2820.99927	-2820.45298	-2820.41351	-2820.52832	-2820.52531
KRu-OCH ₂ OH _{OH}	0	0.54877	0.58815	0.47445	-2821.00239	-2820.45362	-2820.41424	-2820.52794	-2820.52493
KRu-OCH ₂ OH _H	0	0.54645	0.58618	0.47093	-2820.99285	-2820.4464	-2820.40667	-2820.52192	-2820.51891
TS-HOCH ₂ OH-H ⁻ _K	1 (-175.6)	0.54371	0.58281	0.46911	-2820.98992	-2820.44621	-2820.40711	-2820.52081	-2820.51780
KRu_HCOOH	0	0.54403	0.58404	0.46692	-2820.99933	-2820.45530	-2820.41529	-2820.53241	-2820.52940
KRu_HCOOH'	0	0.54366	0.58336	0.46576	-2821.02189	-2820.47823	-2820.43853	-2820.55613	-2820.55312
TS-H ₂ /HCOOH _K	1 (-334.0)	0.54031	0.58032	0.4612	-2821.00701	-2820.4667	-2820.42669	-2820.54581	-2820.54280
KRu-OOCH	0	0.52610	0.5653	0.44982	-2819.84965	-2819.32355	-2819.28435	-2819.39983	-2819.39682
KRu-HCOO	0	0.52398	0.56316	0.44796	-2819.83293	-2819.30895	-2819.26977	-2819.38497	-2819.38196
TS-HCOOH-H ⁻ _K	1 (-284.9)	0.52063	0.55936	0.44448	-2819.81587	-2819.29524	-2819.25651	-2819.37139	-2819.36838
KRu-H_CO ₂	0	0.52135	0.56092	0.44274	-2819.82143	-2819.30008	-2819.26051	-2819.37869	-2819.37569
^T Ru amido	0	0.50042	0.53386	0.43084	-2030.54055	-2030.04013	-2030.00670	-2030.10971	-2030.10670
^T HRu-H	0	0.51976	0.55457	0.44719	-2031.71398	-2031.19423	-2031.15942	-2031.26679	-2031.26378
^T HRu-OCOOCH ₃	0	0.57092	0.61143	0.49189	-2334.97940	-2334.40849	-2334.36798	-2334.48752	-2334.48451
^T TS-CH	1 (-474.3)	0.58790	0.62850	0.51008	-2336.10646	-2335.51855	-2335.47796	-2335.59638	-2335.59337
^T TS-CO ₂	1 (-148.5)	0.56826	0.60922	0.48707	-2334.95614	-2334.38787	-2334.34691	-2334.46907	-2334.46606
^T KRu-OH	0	0.51568	0.55336	0.43938	-2706.34969	-2705.83401	-2705.79633	-2705.91031	-2705.90730
^T TS-H ₂ /H ₂ O _K	1 (-156.6)	0.52573	0.56468	0.45164	-2707.52839	-2707.00266	-2706.96371	-2707.07674	-2707.07373
^T KRu-OCOOCH ₃	0	0.55699	0.59967	0.47136	-2934.36708	-2933.81009	-2933.76740	-2933.89572	-2933.89271

[†] TS-CH _k	1 (-514.6)	0.57223	0.61471	0.49307	-2935.49216	-2934.91993	-2934.87745	-2934.99909	-2934.99608
[†] TS-CO _{2,k}	1 (-147.2)	0.55572	0.59799	0.47489	-2934.31408	-2933.75836	-2933.71608	-2933.83919	-2933.83618

^aThe ZPE, H_{corr} and G_{corr} designate the zero-point energy, enthalpy and Gibbs free energy correction to energy, enthalpy and Gibbs free energy calculated at B3PW91/TZVP(LanL2DZ for Ru and K) level.

^bThe $E_{\text{e,scrf}}$ designate the single point energy at the M06L-SCRF(SMD)/def2-TZVP level under the consideration of triglyme as solvent.

^cThe E_{scrf} , H_{scrf} and $G_{\text{scrf,1atm}}$ designates the solvated total energy, enthalpy and Gibbs free energy calculated by $E_{\text{e,scrf}}$ with ZPE, H_{corr} and G_{corr} .

^dThe $G_{\text{scrf,1M}}$ are given with the correction for standard concentration of 1 mol/L ($p = 24.5$ atm) from standard state in gas phase ($p = 1$ atm).

^fThe tight thresholds were applied.

^gThe superfine grid (175,974 grid) were applied.

Supplementary Table 15. Computed Optimized Structures

H₂ H 0.00000000 0.00000000 0.37255500 H 0.00000000 0.00000000 -0.37255500	CH₃OCH₂OH C -0.01679199 0.03515855 0.51765542 H -0.89044750 -0.11448505 1.15975692 H 0.88814518 0.12715209 1.13023164 O -0.09928197 1.23992207 -0.19927176 H -0.93009689 1.23870328 -0.68648924 O 0.03693350 -1.09876221 -0.29540677 C 1.23858093 -1.21207051 -1.03725950 H 1.16815126 -2.13121853 -1.61757965 H 1.37699537 -0.36493828 -1.71542235 H 2.10822904 -1.27702681 -0.37009873
HCOOCH₃ (MF) C -0.82828900 0.43159500 0.00000000 O -1.30032000 -0.67052900 -0.00000100 O 0.47438000 0.72513700 0.00000000 C 1.36636000 -0.39848400 0.00000100 H 2.36855300 0.02246400 0.00000100 H 1.20923900 -1.01158700 0.88827200 H 1.20923900 -1.01158900 -0.88826900 H -1.40793800 1.36518600 -0.00000300	CO₂ C 0.00000028 -0.00000009 0.00004925 O 0.00000028 -0.00000009 -1.15889474 O 0.00000028 -0.00000009 1.15889474
HCOOH C -0.81124213 0.44271237 -0.00000302 O -1.24923741 -0.67146657 -0.00000010 O 0.49061001 0.76137837 -0.00000019 H -1.41667086 1.35899386 -0.00000148 H 0.99563415 -0.06697857 0.00000145	CH₂O C 0.00000000 0.00000000 -0.52590900 H 0.00000000 0.93988700 -1.11405200 H 0.00000000 -0.93988700 -1.11405200 O 0.00000000 0.00000000 0.67294400
CH₃OH C 0.04654400 0.66052600 0.00000000 H 1.08924600 0.97928300 0.00000000 H -0.43789100 1.07871700 0.89168600 H -0.43789100 1.07871700 -0.89168600 O 0.04654400 -0.75521600 0.00000000 H -0.86508600 -1.05814400 0.00000000	CH₃OCOOH C 0.14798966 0.39254436 0.00000444 O 1.11779226 -0.32076804 -0.00000477 O -1.12267144 -0.03447077 0.00000051 H -1.08415520 -0.99902099 -0.00000344 O 0.14548587 1.72074344 0.00000153 C 1.44112157 2.32872452 -0.00000452 H 2.00176390 2.03844919 -0.88922847 H 1.25727167 3.40019930 -0.00000628 H 2.00177015 2.03845312 0.88921677
H₂O O 0.00000000 0.00000000 0.11710900 H 0.00000000 0.76127400 -0.46843500 H 0.00000000 -0.76127400 -0.46843500	CH₃OCHOHOH C -0.47254346 0.06574104 -0.07775286 O -0.50819611 0.77375509 1.13899077 O -1.58596171 -0.72965297 -0.25478867 H -1.53970629 -1.42907360 0.41010932 O 0.65166064 -0.73735982 -0.05878290 C 1.88079048 -0.03187154 -0.00842292 H 1.99295243 0.51095374 0.93274403 H 2.66943946 -0.77720098 -0.09827562 H 1.96286875 0.67462616 -0.84417562 H -0.45567908 0.76284311 -0.92916392 H -1.28275102 1.34534204 1.12172192
HOCH₂OH C 0.00000000 0.00000000 0.52787200 H -0.89131100 -0.07550500 1.15828700 H 0.89131100 0.07550500 1.15828700 O 0.00000000 1.16956500 -0.24619000 H -0.80690500 1.17764500 -0.77238700 O 0.00000000 -1.16956500 -0.24619000 H 0.80690500 -1.17764500 -0.77238700	KOH K 0.00000000 -0.00515295 -0.77569743 H 0.00000000 0.02744309 2.48583680 O 0.00000000 0.01759123 1.53086746
HRu H -0.00609990 1.49770200 0.07407080 Ru -0.00703640 -0.18427520 0.11359910 C -0.09013810 -0.36830830 -1.72406110 O -0.14769350 -0.48637180 -2.87300320 N 0.08018200 -0.01040570 2.33618500 P -2.27986320 0.01703310 0.47591880 P 2.30093690 -0.14981390 0.29753370 H -0.01047670 -1.86109710 0.36798260 C 2.51281270 -0.27325340 2.15182270 C -2.36505740 0.16587690 2.33885950 H 3.48147290 0.10163960 2.48639890	KRu-H P 2.29537480 -0.04555479 0.24080236 P -2.27396659 0.04381057 0.15497883 C 2.47172976 1.05955437 1.74727967 C -2.40412600 1.45601066 1.36590737 H 2.76217252 2.05782575 1.40255653 H -2.38135953 2.38630674 0.78811581 H 3.26704121 0.70052683 2.40360846 H -3.34189356 1.42680500 1.92580318 C 1.12640134 1.10970360 2.45375313 C -1.19249988 1.37028614 2.27784921 H 1.17350300 1.89328157 3.23408476

H -3.22807250 0.74395510 2.67478680	H -1.22258160 2.21845562 2.98794539
H 2.46298590 -1.33555990 2.40651730	H 0.97449175 0.15345383 2.98758789
H -2.50444450 -0.85527400 2.70525520	H -1.28886724 0.45709223 2.89674710
C -1.06474960 0.74247120 2.87417830	N 0.04550736 1.36787256 1.52090940
C 1.37973690 0.49172390 2.81375140	O 0.01882801 -2.55319712 -1.97587197
H -0.93895370 1.77785000 2.55045480	H -0.07230602 0.86950022 -1.35259865
H 1.43273480 1.55029480 2.54747250	C 0.01585614 -1.65311423 -1.24615723
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C -3.48651880 -1.34582240 0.15217600	C 4.43454477 1.62686233 -0.71391597
C 4.82517200 -3.71642940 -1.28298290	C 2.90350536 0.79116602 -2.36554508
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C -5.73540860 -2.2278230 0.08300900	H 3.28379289 1.39023661 -4.39032533
C 5.32171990 -2.42823690 -1.42421910	H 5.26882892 2.75616427 -3.80253693
C -3.86999370 -3.66471350 -0.39335910	C 3.35474886 -1.51891329 0.62026259
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H 1.85313620 -2.96781920 0.17853050	C 5.43571005 -2.74896343 0.59739743
H -5.26142020 -0.18076440 0.52605030	H 5.17060969 -0.83617626 -0.32023762
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C 4.63464040 3.69652760 -0.85183390	C -2.75276444 -2.31721967 1.58513659
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C -3.49037350 2.60213270 0.57550830	C -3.52525885 -3.30097686 2.19135264
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H -4.38302010 2.56920590 -3.17707200	H -2.25597478 -0.71955646 -2.63061586
H 2.94875620 4.11075690 -2.11773140	C -4.75966816 1.37719012 -3.54075506
H -4.34802200 4.56831980 0.61381190	H -5.76998326 2.73362220 -2.21499290
H 5.16761660 4.59976260 -1.12824290	H -3.57608314 -0.06583117 -4.60798459
H -4.93364500 4.55338420 -1.79388950	H -5.33035019 1.67643763 -4.41317000
TS-H₂	KRu-OH
H 1.32998070 -0.32797860 -0.08626910	P -2.31038204 0.36062073 0.39307816
Ru -0.22212910 0.07821080 -0.02813260	P 2.26531948 0.19622017 0.19708265
C -0.62222870 -1.73582180 -0.22525740	C -2.38890277 0.56051223 2.25498971
O -0.84792320 -2.86059350 -0.35511030	C 2.43806708 -0.30485366 1.97460627
N 0.04187370 2.25190530 0.18442650	H -2.75403391 -0.38950250 2.65849223
P -0.05115090 0.60438350 -2.29742490	H 2.31288396 -1.39131029 2.00039302
P -0.10398000 0.17146200 2.31282280	H -3.11721061 1.32328404 2.53904393
H -1.90709500 0.88968560 0.07976360	H 3.41643091 -0.04841370 2.38850431
C -0.05767820 2.01063570 2.60773880	C -0.99298618 0.87350473 2.77723495
C -0.09748940 2.46452940 -2.24175030	C 1.30191834 0.37388880 2.72508712
H 0.42733700 2.25376810 3.55491920	H -0.99838929 0.74790272 3.87708945
H 0.34657230 2.91455330 -3.13083210	H 1.36158198 0.09052895 3.79321720
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H -1.15351280 2.74518020 -2.21435850	H 1.47691627 1.46767129 2.70374262
C 0.60102170 2.91664010 -0.96769880	N 0.00911716 0.02455453 2.16112657
C 0.64525810 2.66650110 1.42773030	Ru -0.04987600 0.18654282 -0.03999199
H 1.68452590 2.71623310 -1.05834870	C -0.15106796 0.48079658 -1.87677386
H 1.72148090 2.41642790 1.45546760	O -0.21776678 0.72529166 -3.00718622
H 0.49358260 4.01040630 -0.87477760	H -0.11237961 1.77375601 0.19307922
H 0.57691810 3.76098570 1.54536090	K -0.67795340 -2.64293073 2.02023846
H -1.28379340 1.62446970 0.14031780	C -3.45321560 -1.06835200 0.10397317

C -1.50507240 -0.42976640 3.35003540	C -4.78845105 -1.07268034 0.51871172
C -1.41076190 0.15567560 -3.46439590	C -2.92347984 -2.20167925 -0.51601039
C -3.62509290 -1.44022370 4.86839340	C -5.58202153 -2.19356183 0.31813409
C -3.56166370 -0.51248630 -5.12172090	H -5.21440955 -0.19199318 0.98829086
C -1.99951800 -1.71365510 3.11363500	C -3.72503480 -3.32482969 -0.71309041
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H -2.91183540 0.85530160 -2.09066440	C 4.95185603 -2.76036356 -0.92495446
H -1.72541840 1.34161770 4.56103190	H 4.25187212 -1.95506296 0.92853419
H -0.18280520 -0.69618350 -5.01372960	C 4.02613878 -1.79564419 -2.91997060
H -3.58979660 0.45287510 5.88385210	H 2.58267101 -0.23892938 -2.63332866
H -2.07501830 -1.28507520 -6.46560740	C 4.87797925 -2.70964425 -2.31020192
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H -4.80280300 0.31047750 -3.57054430	H 3.95852361 -1.75147395 -4.00144043
H -4.44970310 -1.83064250 5.45441300	H 5.47967339 -3.38070164 -2.91325442
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C 1.37359440 -0.46804350 3.22405560	C 4.64158070 1.74992990 0.20322711
C 1.48475510 0.19374010 -3.23070600	C 2.59604475 2.97034587 -0.12439415
C 3.65743720 -1.33612860 4.57963480	C 5.36136601 2.93445453 0.13950732
C 3.80488170 -0.48588690 -4.63305950	H 5.17001688 0.81201603 0.33721999
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	H 0.69452488 -2.23441739 -0.98925796
Ru amido	KRu-OH_MF
H 0.01608250 0.73664670 -1.02469600	P -2.14119849 0.37173649 0.25692285
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C -0.17044770 -1.47916820 -1.34457560	C -2.28546937 -0.17814984 2.02175291
O -0.25165950 -2.22503120 -2.22475170	C 2.50849191 0.85664103 2.28753237
N 0.03886120 0.22257770 2.08111330	H -2.12893352 -1.26053138 2.03100900
P -2.32643740 0.02977410 0.45521870	H 2.89268571 -0.12175423 2.59256822
P 2.27489920 -0.27547340 0.36189210	H -3.26762601 0.04042961 2.44797100
C 2.42864530 -0.29279760 2.20894750	C 3.22717983 1.59916462 2.64178494
C -2.39381740 0.10811680 2.30753570	C -1.16573213 0.52106190 2.77811487
H 3.40258610 0.06590280 2.55049440	C 1.11038931 1.08744757 2.84218582
H -3.28646330 0.60945290 2.68678860	H -1.19681166 0.19715052 3.83528659
H 2.29315950 -1.33171440 2.52155080	H 1.13214537 0.89284747 3.93140486
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H 5.75985910 -3.83664480 0.71842790	C 3.24703589 -1.65297871 -0.55070942
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C 3.16302360 1.27369300 -0.11952840	H 7.01409018 -1.15290405 0.17796998
C -3.06193660 1.60991720 -0.15138910	H 3.80230161 -3.60559085 -1.25328242
C 4.45821930 3.67459340 -0.71937850	H 6.21366826 -3.28995692 -0.78447111
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C 3.07347840 3.63470070 -0.62278630	C 4.27590449 4.79227291 -1.09909463
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H 1.34557050 2.39830940 -0.27313060	H 3.52115837 5.65743629 0.71761492
H -4.46415160 1.88327110 1.46540050	H 4.68926193 5.72450130 -1.46779917
H 5.14006220 0.41965360 -0.07624180	C -3.20054849 1.88647214 0.16971848
H -1.79661950 1.63444260 -1.88063670	C -4.58395179 1.81476725 0.34957215
H 6.27860350 2.53722850 -0.60157160	C -2.61304773 3.12566899 -0.07163590
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	H -1.82492628 -4.21965492 -2.05536003
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Ru_H₂O	TS-MF-OH_k
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P 2.28592800 0.01573700 0.32978900	P 2.28348300 0.65551700 0.29646000
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C 2.43159800 -0.11893900 2.18761400	C 2.43151200 0.75018900 2.15414600
H -2.49152400 -1.20317500 2.43382400	H -2.20044700 -1.34798100 2.05391600
H 2.46239600 -1.17861800 2.44980100	H 2.77248000 -0.22446000 2.51562500
H -3.38688700 0.31351500 2.54436500	H -3.34042700 -0.05725300 2.52881500
H 3.35027200 0.34782000 2.54694200	H 3.17665600 1.48931600 2.45519700
C -1.24672800 0.51703100 2.80998700	C -1.23114900 0.45130900 2.77204600
C 1.20756900 0.53142900 2.81001100	C 1.04826200 1.05833900 2.71443400
H -1.27701300 0.40693000 3.90288800	H -1.21296000 0.13345600 3.83129900
H 1.23638800 0.42485400 3.90311100	H 1.08647500 0.93645800 3.81351200
H -1.22460800 1.58402300 2.57623000	H -1.45742000 1.53500900 2.79732100
H 1.17424900 1.59725100 2.57207400	H 0.82228700 2.12738900 2.54412700
N -0.01679100 -0.08155700 2.26538900	N 0.04896200 0.18343200 2.13058000
O -0.00204900 -0.10127200 -2.97718300	C -0.80466900 -3.47165400 0.07618800
H -0.01320600 -1.78930500 0.01266000	Ru 0.01000900 0.30826000 -0.04300000
H 0.25608700 -2.63175700 1.24805500	C -0.04653300 0.53843900 -1.89673200
C -0.00794700 -0.09095000 -1.82259700	O -0.09480000 0.75396000 -3.03430300
Ru -0.01587600 -0.08002800 0.02978700	O -1.38305300 -3.32034000 1.16196200
H -0.03268500 1.58540800 0.15916600	H -0.07058900 1.87315000 0.14710000
O 0.39228300 -3.02619600 2.14978100	K 0.82328600 -2.51324600 2.32418100
H -0.00852100 -1.07105600 2.52042300	C -3.48342100 -0.74986400 -0.66124500
C -3.42467200 -1.34750600 -0.30098300	C -3.90281000 -2.00939900 -0.23510200
C -3.17542200 -2.65994400 0.10565300	C -3.93165000 -0.26623800 -1.89383400
C -4.43845400 -1.11489100 -1.22886400	C -4.77296700 -2.75824900 -1.02081100
C -3.94714700 -3.70805300 -0.37235500	H -3.51890000 -2.43280400 0.68464300
H -2.35212600 -2.86450300 0.78104600	C -4.79596100 -1.01805000 -2.67548100
C -5.20103600 -2.16859400 -1.72090000	H -3.61030500 0.70923500 -2.24275700
H -4.63586500 -0.10867000 -1.57735700	C -5.22424800 -2.26653800 -2.23784300
C -4.96502900 -3.46534600 -1.28815400	H -5.09206300 -3.73591700 -0.67599500

H -3.74461000	-4.72070600	-0.04083200	H -5.13549400	-0.62759200	-3.62865300
H -5.98197700	-1.97020200	-2.44681200	H -5.90258100	-2.85420100	-2.84685900
H -5.56217400	-4.28590400	-1.67007400	C 3.53056100	-0.61488200	-0.21828000
C 3.41849500	-1.29080800	-0.32154700	C 4.50904000	-1.14672600	0.62213800
C 3.38352700	-2.58044100	0.21260900	C 3.46814800	-1.06815200	-1.53869700
C 4.23718100	-1.04179100	-1.42348000	C 5.39995000	-2.10935600	0.15657200
C 4.17728700	-3.58554800	-0.32243100	H 4.59970400	-0.80341800	1.64673700
H 2.72084000	-2.81503000	1.03813500	C 4.36293700	-2.01920600	-2.00699000
C 5.02035200	-2.05328900	-1.96570400	H 2.71343400	-0.66435600	-2.20574300
H 4.26714900	-0.05276000	-1.86502600	C 5.32911900	-2.54817200	-1.15803500
C 4.99957100	-3.32604500	-1.41226800	H 6.15688300	-2.50870900	0.82324200
H 4.14523300	-4.57966300	0.11020000	H 4.30329800	-2.35232600	-3.03736700
H 5.64831600	-1.84209600	-2.82432000	H 6.02519900	-3.29566100	-1.52182100
H 5.61395300	-4.11449900	-1.83271100	C 3.09581700	2.20637100	-0.30277500
C 3.22906500	1.56523300	-0.03631400	C 4.46562700	2.41687100	-0.12893300
C 2.60514200	2.61617900	-0.70144100	C 2.33471700	3.19187500	-0.92565200
C 4.56306600	1.70663800	0.35681800	C 5.05795100	3.59517300	-0.55960600
C 3.30020900	3.79069800	-0.97059000	H 5.08011600	1.65218000	0.33375300
H 1.56372500	2.50609500	-0.98251300	C 2.92942700	4.37100800	-1.36087100
C 5.25344600	2.88137800	0.09633500	H 1.27382900	3.02453400	-1.06611000
H 5.07269200	0.89083900	0.85898300	C 4.28957400	4.57612000	-1.17736500
C 4.62219600	3.92639400	-0.57103600	H 6.12283100	3.74594600	-0.41934300
H 2.80331000	4.60161600	-1.49187200	H 2.32537100	5.12827100	-1.84842100
H 6.28700500	2.98082500	0.40976200	H 4.75337900	5.49512600	-1.51857200
H 5.16302800	4.84347500	-0.77789200	C -3.22943400	1.89493000	0.32985900
C -3.27530300	1.52988000	-0.05656900	C -4.56922700	1.91301200	0.72808600
C -4.57648100	1.71549200	0.41890600	C -2.62307200	3.09138300	-0.03963000
C -2.68865000	2.53005200	-0.82681700	C -5.27855800	3.10394800	0.76955100
C -5.27186300	2.88204400	0.13371500	H -5.06705200	0.98719200	0.99652600
H -5.05915700	0.94188400	1.00705900	C -3.33561400	4.28581600	-0.00518800
C -3.38913200	3.69464100	-1.12126600	H -1.58489300	3.07839400	-0.34858000
H -1.66909300	2.39241700	-1.16808800	C -4.66195800	4.29551000	0.40153900
C -4.67869600	3.87395600	-0.64027300	H -6.31674000	3.10252200	1.08358500
H -6.27917500	3.01620800	0.51272000	H -2.84927400	5.20999500	-0.29810000
H -2.92111700	4.46516600	-1.72403000	H -5.21730500	5.22669900	0.42986400
H -5.22283400	4.78472800	-0.86533400	H -1.34734400	-3.42865300	-0.88329800
H 0.05161800	-3.92276100	2.09984800	O 0.15346000	-4.50979000	0.06047800
TS-H₂/H₂O			KRu-O(H)CHOOCH₃		
P -2.32847100	-0.01769300	0.34167600	P -2.35997000	0.29949749	0.25304769
P 2.31610300	0.05381100	0.34939400	P 2.23901936	0.60405652	0.26952122
C -2.43546900	-0.25119400	2.18454300	C -2.43885381	-0.28692513	2.00468793
C 2.43576500	-0.03771600	2.20253000	C 2.38052860	0.65664094	2.12776075
H -2.38651900	-1.32626800	2.37036500	H -2.27847828	-1.36740733	1.96550760
H 2.46257000	-1.09805800	2.46202900	H 2.69449205	-0.33564198	2.46502617
H -3.37892100	0.12408500	2.58455000	H -3.40419921	-0.07739101	2.47038400
H 3.34315200	0.44700700	2.56595400	H 3.14121616	1.37032761	2.45071402
C -1.23730000	0.43286300	2.81917100	C -1.29155590	0.40908532	2.72648103
C 1.18228800	0.58214800	2.79479300	C 1.00096294	0.98542619	2.68692001
H -1.22989500	0.22977400	3.89999400	H -1.27899778	0.07182657	3.78052023
H 1.18576900	0.43384000	3.88433400	H 1.03077185	0.84446218	3.78426984
H -1.30655100	1.51980900	2.69322000	H -1.50778106	1.49390912	2.77300228
H 1.15070200	1.66173200	2.60852800	H 0.79875385	2.06198286	2.53570425
N -0.00086500	-0.05426600	2.20777600	N -0.01238287	0.14040814	2.08355711
O -0.00234000	0.26591100	-2.99623700	C -0.63097208	-3.46176144	0.03466564
H -0.01644500	-1.87406800	-0.29009200	Ru -0.03481650	0.26175429	-0.08003822
H 0.07862200	-2.00686900	0.51951200	C -0.07622994	0.45902323	-1.94053544
C -0.00336400	0.12005900	-1.85409900	O -0.11204679	0.65327303	-3.08165338
Ru -0.00827000	-0.03401400	0.01270100	O -1.39083628	-3.29196771	1.02198060
H -0.02442200	1.55997200	0.10925100	H -0.11457548	1.82057693	0.08083149
O 0.42661500	-2.53849300	2.16034600	K 0.65985494	-2.57466883	2.45788398
H 0.10164000	-1.17357500	2.35379000	C -3.59100414	-0.67085795	-0.72145717
C -3.35089600	-1.39033000	-0.34435600	C -3.79802514	-2.02970926	-0.47694338
C -3.02528300	-2.70139200	0.01532400	C -4.28115173	-0.05383778	-1.76801869
C -4.37471600	-1.17531000	-1.26548400	C -4.70375477	-2.74362932	-1.25343512
C -3.73393400	-3.76988300	-0.51390300	H -3.22175356	-2.54441271	0.28744588
H -2.20053100	-2.89311100	0.69506300	C -5.17624720	-0.77605969	-2.54503456
C -5.07527300	-2.24980300	-1.80169500	H -4.12712095	0.99877573	-1.97591337
H -4.62895900	-0.16768000	-1.57132600	C -5.39664745	-2.12298573	-2.28466898
C -4.76245800	-3.54754500	-1.42278300	H -4.86012287	-3.79754505	-1.04942314
H -3.47335000	-4.78144400	-0.22287800	H -5.70436815	-0.28231275	-3.35358873

H -5.86780700	-2.06756900	-2.51916100	H -6.10022971	-2.68663877	-2.88788638
H -5.31069300	-4.38466900	-1.84036800	C 3.49775695	-0.64063456	-0.27586690
C 3.35561300	-1.34297900	-0.25008800	C 4.47750299	-1.18579856	0.55412167
C 3.09845200	-2.62129600	0.25676000	C 3.44734523	-1.05410448	-1.60993044
C 4.31846000	-1.17804000	-1.24506300	C 5.38235500	-2.12270568	0.06462154
C 3.82640100	-3.70630300	-0.21248300	H 4.55578350	-0.87490669	1.58994804
H 2.31376100	-2.77448300	0.99947800	C 4.35577806	-1.98061029	-2.10131465
C 5.03525200	-2.27241900	-1.71445700	H 2.69281266	-0.63863690	-2.27017469
H 4.51369900	-0.19589000	-1.65906200	C 5.32389558	-2.52261045	-1.26304860
C 4.79623200	-3.53707100	-1.19431100	H 6.13945958	-2.53423835	0.72356223
H 3.62568000	-4.69371300	0.18899800	H 4.30490517	-2.28382491	-3.14130129
H 5.78172700	-2.13242500	-2.48871500	H 6.03067556	-3.25073945	-1.64492677
H 5.35769800	-4.39034800	-1.55904200	C 3.04085889	2.17506126	-0.29020002
C 3.26828500	1.56405500	-0.10415600	C 4.40089180	2.40485771	-0.06983131
C 2.68129100	2.55363200	-0.88820300	C 2.28665059	3.15252867	-0.93335319
C 4.58159000	1.74083000	0.34081800	C 4.98956771	3.59415261	-0.47396770
C 3.39193700	3.70076700	-1.22395100	H 5.01117555	1.64663400	0.40895949
H 1.65869600	2.42459500	-1.22110400	C 2.87781231	4.34271250	-1.34276112
C 5.28860400	2.88745600	0.00950900	H 1.23370364	2.97101131	-1.11011827
H 5.06109300	0.97483000	0.94090300	C 4.22766054	4.56697521	-1.11240849
C 4.69413200	3.87015200	-0.77524000	H 6.04668842	3.76003787	-0.29705829
H 2.92328700	4.46339600	-1.83601800	H 2.27916204	5.09372828	-1.84633100
H 6.30629300	3.01392300	0.36217800	H 4.68873050	5.49472519	-1.43295868
H 5.24760200	4.76584600	-1.03493100	C -3.19487441	1.95224438	0.31616374
C -3.32200100	1.49743200	0.01157500	C -4.46842728	2.06464810	0.88086697
C -4.62008700	1.63388500	0.51144000	C -2.59465161	3.09100094	-0.21294108
C -2.77445300	2.53280600	-0.74168700	C -5.11433480	3.29102722	0.93292934
C -5.35161800	2.78648000	0.26411300	H -4.96765861	1.18543142	1.27350627
H -5.06990100	0.83326900	1.08890000	C -3.24452499	4.32014548	-0.16939635
C -3.51012500	3.68530200	-0.99395200	H -1.60840327	3.00851724	-0.65259752
H -1.76189100	2.43430200	-1.11398500	C -4.50249845	4.42388322	0.40660191
C -4.79710400	3.81464000	-0.49091600	H -6.10016545	3.36240022	1.37949592
H -6.35687200	2.88225000	0.65944300	H -2.76301912	5.19756295	-0.58727768
H -3.07250300	4.48415000	-1.58221800	H -5.00814492	5.38260711	0.44431703
H -5.36949800	4.71510900	-0.68451000	H -1.06250467	-3.65870895	-0.96842559
H 0.02267200	-3.21969600	2.70223300	O 0.37476687	-4.48416268	0.28803062
			C 1.09887087	-4.91248724	-0.84020551
			H 0.43684701	-5.09226894	-1.69803606
			H 1.87530198	-4.19516702	-1.14239018
			H 1.58863911	-5.85385696	-0.58515516
			O 0.24068006	-2.16386617	-0.20336076
			H 0.72736731	-2.26718133	-1.02771265
Ru₂H₂O₂			KRu-HCO(OH)OCH₃		
P -2.31905900	0.01400700	0.35630200	P -2.39039005	0.38436131	0.34914702
P 2.31923200	0.01533000	0.35625200	P 2.21855007	0.39755332	0.25088892
C -2.44013900	-0.17937700	2.19822900	C -2.49312332	0.31319375	2.20671253
C 2.44066000	-0.17562600	2.19844000	C 2.40733265	-0.09825322	2.02428541
H -2.46488900	-1.25034200	2.40887600	H -2.72512826	-0.73165925	2.43579576
H 2.46712900	-1.24629900	2.41033300	H 2.38807478	-1.19162831	2.02793833
H -3.35459800	0.27304200	2.58598300	H -3.32457815	0.90358696	2.59827389
H 3.35444100	0.27873500	2.58551800	H 3.34529178	0.25352858	2.46032339
C -1.18606300	0.43343400	2.79730300	C -1.15032905	0.72238772	2.79529529
C 1.18568000	0.43582400	2.79695300	C 1.19654075	0.46387780	2.75722921
H -1.18473100	0.24114300	3.88381500	H -1.15753834	0.49708748	3.87929742
H 1.18456500	0.24432600	3.88360200	H 1.23896040	0.13758504	3.81379940
H -1.21818100	1.53144800	2.68057200	H -1.04976612	1.82182118	2.72972538
H 1.21606600	1.53378800	2.67935900	H 1.28368752	1.56664880	2.79240917
N 0.00030300	-0.14141900	2.18557900	N -0.04975655	0.04070211	2.13383409
O -0.00224200	0.49034600	-2.97568300	H 0.19304247	-1.87935200	-0.15549617
H 0.00931700	-1.87175000	-0.51965800	C 0.34174131	-3.04228265	-0.26666072
H -0.00724800	-1.95932000	0.26824700	Ru -0.09206017	0.17791521	-0.02071746
C -0.00111400	0.23662900	-1.85159900	C -0.16172393	0.32477630	-1.88853495
Ru 0.00005500	-0.04193600	0.01387600	O -0.20867098	0.48429289	-3.03164583
H 0.00005600	1.53189200	0.21386200	O -0.64897451	-3.75036726	0.07680867
O 0.00397200	-2.81754200	2.43297700	H -0.19342368	1.73912957	0.07714724
H 0.00244400	-1.79771100	2.42613400	K -0.48253833	-2.73627129	2.49707936
C -3.34731400	-1.35361700	-0.33311700	C -3.69256721	-0.80663973	-0.18394074
C -3.10664700	-2.65910000	0.10555900	C -5.04504035	-0.45575376	-0.20380944
C -4.28395400	-1.14157400	-1.34407700	C -3.31417410	-2.10717669	-0.51688762
C -3.81354800	-3.72232800	-0.43785200	C -6.00578129	-1.39488862	-0.55159539
H -2.35404400	-2.85602100	0.86339200	H -5.34847644	0.55634742	0.03993545
C -4.98363100	-2.21062900	-1.89137500	C -4.28322863	-3.04477156	-0.85963990
H -4.47187600	-0.13891300	-1.70916100	H -2.27298195	-2.42282876	-0.50358038
C -4.75551200	-3.50186700	-1.43626600	C -5.62553206	-2.69175859	-0.88154238
H -3.62013000	-4.72884600	-0.08358600	H -7.05286774	-1.11222527	-0.57055145
H -5.70892700	-2.02980700	-2.67714000	H -3.97118178	-4.05022833	-1.11866676

H -5.30322500	-4.33505300	-1.86245000	H -6.37711368	-3.42298676	-1.15925757
C 3.34746800	-1.35329600	-0.33123700	C 3.44154804	-0.59688562	-0.70423206
C 3.10598100	-2.65819900	0.10883200	C 4.40108338	-1.40845523	-0.10146559
C 4.28480100	-1.14271800	-1.34184700	C 3.39985062	-0.52015791	-2.09855964
C 3.81286900	-3.72226000	-0.43298500	C 5.30648877	-2.12280639	-0.87683803
H 2.35272400	-2.85400000	0.86633400	H 4.44123485	-1.49935982	0.97707203
C 4.98444000	-2.21265000	-1.88749400	C 4.30564003	-1.23374236	-2.87165805
H 4.47329700	-0.14053700	-1.70796000	H 2.65551891	0.10091317	-2.58487514
C 4.75555500	-3.50327800	-1.43105400	C 5.26197253	-2.03709107	-2.26195243
H 3.61886000	-4.72830500	-0.07769700	H 6.04576806	-2.75326673	-0.39490404
H 5.71030400	-2.03298500	-2.67300200	H 4.25838266	-1.16619963	-3.95275942
H 5.30323800	-4.33714600	-1.85594400	H 5.96588144	-2.59912284	-2.86544346
C 3.28950800	1.53468900	-0.02052600	C 2.99160448	2.07837339	0.16679238
C 2.70978300	2.57274800	-0.74488300	C 4.35383880	2.23612844	0.43480559
C 4.60710900	1.67112500	0.42551900	C 2.23563313	3.19990408	-0.16231845
C 3.43237500	3.72816400	-1.02143900	C 4.94109232	3.49187901	0.39117308
H 1.68398400	2.47462200	-1.07828800	H 4.96664166	1.37129888	0.66586197
C 5.32633100	2.82546100	0.15274800	C 2.82544408	4.45850178	-0.21125767
H 5.07979500	0.86847500	0.98150900	H 1.18122737	3.08013275	-0.38171940
C 4.73925300	3.85683100	-0.57294100	C 4.17643498	4.60775655	0.06740273
H 2.96915000	4.52922900	-1.58668700	H 5.99955197	3.59963359	0.60181710
H 6.34726800	2.92067900	0.50584700	H 2.22394158	5.32234625	-0.47212988
H 5.30195800	4.75897900	-0.78626000	H 4.63637890	5.58909823	0.02768546
C -3.28971700	1.53375500	-0.01802000	C -3.10399852	2.00978072	-0.14923880
C -4.60736300	1.66909800	0.42821700	C -3.32053669	2.24035328	-1.51022845
C -2.71024700	2.57315800	-0.74064900	C -3.37103464	3.03401509	0.75655823
C -5.32688100	2.82369900	0.15735900	C -3.81028675	3.46087870	-1.94977065
H -5.07985900	0.86539800	0.98285200	H -3.10651561	1.46016426	-2.23259539
C -3.43314400	3.72883700	-1.01530600	C -3.85569266	4.26048571	0.31393273
H -1.68440000	2.47584600	-1.07414700	H -3.19568942	2.89162039	1.81607920
C -4.74006300	3.85641800	-0.56661800	C -4.07963438	4.47607367	-1.03820452
H -6.34784800	2.91806500	0.51060500	H -3.97632901	3.62168415	-3.00919941
H -2.97012400	4.53095900	-1.57922100	H -4.05788977	5.04772867	1.03204972
H -5.30300000	4.75877200	-0.77845000	H -4.45891205	5.43169036	-1.38270907
H -0.00132800	-3.07584000	3.35728200	O 1.52801246	-3.16187548	0.67743550
			C 2.08231252	-4.46411108	0.66833370
			H 2.77470267	-4.53681943	1.51203594
			H 1.30266253	-5.22848414	0.76979141
			H 2.63543786	-4.66342525	-0.25497709
			O 0.80716508	-3.26066852	-1.57242780
			H 1.51998969	-2.63110303	-1.73718749
Ru_H₂O			TS-CH_κ		
H -0.07195947	1.35050216	-0.26912584	P -2.29220100	0.57896200	0.27873700
Ru -0.00178463	-0.17598016	0.07594882	P 2.25780200	0.25476100	0.38238000
C -0.01774165	-0.49780876	-1.76783311	C -2.43177000	0.84902200	2.12330800
O -0.03729283	-0.65426157	-2.91340078	C 2.33273500	-0.33299400	2.13220200
N 0.00239766	0.06838555	2.21098630	H -2.88439300	-0.06286400	2.52576500
P -2.31848613	-0.09318937	0.38702215	H 2.16553000	-1.41404000	2.10144600
P 2.29997703	0.09655446	0.37887709	H -3.12052600	1.66464400	2.35559800
C 2.44035183	0.26168411	2.23387428	H 3.29452300	-0.12256200	2.60683900
C -2.42445277	-0.23976117	2.23453246	C -1.04708300	1.06742800	2.70782900
H 3.28745570	0.88916445	2.51791235	C 1.18393800	0.36707700	2.83977100
H -3.37840267	0.10982673	2.63307796	H -1.12159200	0.99648700	3.80955100
H 2.61077802	-0.74565799	2.62408342	H 1.16513300	0.04523000	3.89740700
H -2.34298773	-1.30852181	2.44983158	H -0.72925400	2.10686500	2.49850300
C -1.23938619	0.50717688	2.82613886	H 1.40776400	1.45167600	2.86963500
C 1.12342766	0.79817378	2.77309908	N -0.09272100	0.10524600	2.19117800
H -1.39430641	1.59380914	2.69957688	H 0.19643500	-1.70159300	-0.12111500
H 1.05157875	1.88028584	2.56559828	C 0.72121900	-3.16181300	-0.14187400
H -1.21333097	0.32885980	3.91414822	Ru -0.03233200	0.13085800	-0.01994500
H 1.13401694	0.70310013	3.87203638	C 0.00107500	0.24682600	-1.88399400
H 0.13336750	-1.60766123	1.92913581	O 0.02750800	0.36451200	-3.03428400
C 3.46076720	-1.28305408	-0.01962877	O 1.16303600	-3.38033800	0.99660300
C -3.41704944	-1.43224426	-0.24593433	H -0.08448100	1.74173800	0.12099500
C 5.15351553	-3.40904699	-0.68097660	K -0.99984600	-2.51585600	2.19038200
C -4.96683692	-3.56167906	-1.17179290	C -3.72983100	-0.57282300	0.02784500
C 3.19602190	-2.08148765	-1.13329204	C -5.05125900	-0.17171700	0.24160200
C -2.94791112	-2.74488603	-0.14055008	C -3.47406900	-1.90252600	-0.29252700
C 4.58453971	-1.56660084	0.76103067	C -6.08881900	-1.08840400	0.14571200
C -4.65833837	-1.19654473	-0.83398717	H -5.27156700	0.86434700	0.47493700
C 5.42354942	-2.62405335	0.43361819	C -4.51334500	-2.82432100	-0.38655000
C -5.42801784	-2.25836133	-1.29574915	H -2.44949700	-2.20303800	-0.48387700
C 4.03994812	-3.13455788	-1.46436679	C -5.82213600	-2.41831000	-0.16591800
C -3.72545364	-3.80135341	-0.59314654	H -7.11079800	-0.76478600	0.31138000
H 2.32001377	-1.88107354	-1.73905291	H -4.30011300	-3.85611100	-0.64496700
H -1.96783581	-2.93088766	0.28785213	H -6.63511100	-3.13175600	-0.24399500

H 4.81287337	-0.95999554	1.63011120	C 3.53777500	-0.71348600	-0.53219700
H -5.02707755	-0.18365776	-0.94151173	C 4.27058600	-1.74782800	0.05275300
H 6.29062361	-2.83397106	1.05032444	C 3.77017000	-0.39733900	-1.87411200
H -6.39059791	-2.06241101	-1.75557493	C 5.22190200	-2.44479100	-0.68847300
H 3.82077771	-3.74479635	-2.33343116	H 4.09667600	-2.02628200	1.08477900
H -3.35425270	-4.81651468	-0.50354924	C 4.72099200	-1.08949500	-2.60790100
H 5.80846428	-4.23487299	-0.93572791	H 3.19915600	0.39347800	-2.34819700
H -5.56876534	-4.38861240	-1.53239467	C 5.45111100	-2.11579800	-2.01676300
C 3.15643105	1.59286251	-0.28464606	H 5.77978400	-3.24872200	-0.22115200
C -3.20686657	1.46158646	-0.04977762	H 4.88700000	-0.83325500	-3.64832000
C 4.39090345	3.92970762	-1.19769350	H 6.19015600	-2.66074300	-2.59327700
C -4.53055666	3.80497224	-0.80731490	C 3.10435200	1.90392500	0.42515600
C 2.46249178	2.80431034	-0.29590431	C 4.43590600	1.99590100	0.83876900
C -4.33291778	1.89902613	0.64996982	C 2.43648200	3.06210400	0.04042500
C 4.47096367	1.56401903	-0.74948976	C 5.07788300	3.22456100	0.88368700
C -2.75404140	2.21280319	-1.13415903	H 4.98178400	1.10112900	1.11906400
C 5.08215432	2.72585326	-1.20605376	C 3.08273600	4.29341600	0.07661800
C -3.41516191	3.37376419	-1.51391339	H 1.40339600	2.98715100	-0.28052300
C 3.07947448	3.96574895	-0.73927620	C 4.40126300	4.37809100	0.50053700
C -4.98751528	3.06607291	0.27688817	H 6.11045100	3.28218300	1.21076100
H 1.42810771	2.82793112	0.02781040	H 2.55056300	5.18753500	-0.22957100
H -4.71236350	1.32945268	1.49048837	H 4.90450100	5.33844500	0.52994900
H 5.02248306	0.63187293	-0.76595975	C -2.94023300	2.11567500	-0.51143200
H -1.86989777	1.88913097	-1.67034602	C -3.48572300	2.05455200	-1.79411700
H 6.10193668	2.68582852	-1.57310449	C -2.81412200	3.35834400	0.10770100
H -3.05185908	3.94591914	-2.36041199	C -3.91126000	3.20962800	-2.43628400
H 2.52786385	4.89948985	-0.73969093	H -3.58010500	1.09897600	-2.29826100
H -5.85692505	3.39699844	0.83436688	C -3.24439500	4.51335300	-0.53323100
H 4.86901048	4.83529145	-1.55443143	H -2.36292000	3.43446100	1.09049600
H -5.04205415	4.71565982	-1.09897536	C -3.79594900	4.44239100	-1.80604800
H 0.94553371	-2.75287943	1.15870587	H -4.33118400	3.14512600	-3.43405700
O 0.07343211	-2.35500458	1.23883291	H -3.14300900	5.47226100	-0.03659800
			H -4.12854600	5.34451400	-2.30738900
			O -0.47967400	-3.78354300	-0.47681000
			O 1.53640500	-3.12750400	-1.23796600
			C -0.88093400	-3.69486800	-1.84067200
			H -1.87455800	-4.13841500	-1.89766700
			H -0.91667100	-2.65134600	-2.16687900
			H -0.19533900	-4.24660600	-2.48422400
			H 2.39813900	-2.81290100	-0.93301800
TS-H₂O			TS-CH₃disCO_x		
H -0.06456945	1.31391046	-0.36021218	P -2.16353500	0.60363900	0.43804200
Ru -0.02061490	-0.19918554	0.08343885	P 2.33912200	0.05933400	0.47887100
C -0.04388403	-0.62155199	-1.73135739	C -2.26515700	1.16374100	2.21603900
O -0.06657677	-0.85195426	-2.86397353	C 2.46358800	-0.18701500	2.31473800
N -0.01736409	0.12937857	2.23202606	H -2.73065900	0.37964100	2.81848000
P -2.33712294	-0.09306218	0.39106540	H 2.28211600	-1.24317200	2.53751700
P 2.29075364	0.01713875	0.38603863	H -2.89234200	2.05226300	2.31117700
C 2.42425326	0.17736110	2.24331303	H 3.44334500	0.08848000	2.71303100
C -2.44408340	-0.14954001	2.24651788	C -0.84788500	1.41098000	2.70444600
H 3.30829821	0.74776414	2.53413654	C 1.35087300	0.67492900	2.88610100
H -3.39531765	0.23028138	2.62241896	H -0.87108700	1.54352300	3.80156900
H 2.52303490	-0.83721432	2.63882591	H 1.34839700	0.59245200	3.98756600
H -2.37348859	-1.20744983	2.51080575	H -0.49199200	2.36809300	2.28331600
C -1.25842671	0.61148272	2.82125752	H 1.60159100	1.73134600	2.66657000
C 1.14647110	0.80574295	2.77959949	N 0.04616800	0.32080500	2.34279800
H -1.38287600	1.68977191	2.63913913	H -0.03793600	-1.72217900	-0.07937700
H 1.12438070	1.87868081	2.53726360	C -0.06332500	-1.58789600	-1.71497200
H -1.24195072	0.47817726	3.91475590	O 0.04909100	-0.37916500	-2.02731300
H 1.15381595	0.73582883	3.87929327	H 0.14903800	1.68314300	0.18032000
H 0.05117299	-1.19137409	2.09170443	Ru 0.05762300	0.05763200	0.17290900
C 3.42422936	-1.38343124	-0.01360260	C 3.50066600	-1.18353600	-0.26471000
C -3.41417173	-1.47977448	-0.16720311	C 3.94034000	-2.32630700	0.40439100
C 5.08324201	-3.52468208	-0.71075864	C 3.88279800	-1.00956800	-1.60102200
C -4.91636421	-3.68116044	-0.99249097	C 4.74588000	-3.26160300	-0.23559800
C 3.22232921	-2.07929461	-1.20674749	H 3.66681200	-2.49038200	1.44010200
C -2.95377969	-2.77755801	0.07704241	C 4.68261100	-1.94676700	-2.24196600
C 4.46742665	-1.77744240	0.82735450	H 3.55836100	-0.12484400	-2.13980000
C -4.61877575	-1.29555089	-0.84303638	C 5.11820500	-3.07738000	-1.56039900
C 5.28930203	-2.84348420	0.48208205	H 5.08488100	-4.13845400	0.30598700
C -5.36520444	-2.39417319	-1.25451170	H 4.96657200	-1.79130500	-3.27703200
C 4.04981545	-3.13846619	-1.55522764	H 5.74351300	-3.80906400	-2.05945500
C -3.70976327	-3.86873964	-0.32697818	C 3.35878800	1.59140200	0.21557400
H 2.40808354	-1.79611018	-1.86311155	C 4.71776400	1.61523900	0.53948800
H -1.99627087	-2.91991351	0.57180257	C 2.77026900	2.73913700	-0.30645100
H 4.64809245	-1.25367655	1.75898030	C 5.46779900	2.76819700	0.35663600

H -4.97711870	-0.29613966	-1.05817779	H 5.19917400	0.72375800	0.92853500
H 6.09285406	-3.14027774	1.14723550	C 3.52309300	3.89319300	-0.49744100
H -6.29959075	-2.23969398	-1.78315238	H 1.71257500	2.71295200	-0.54706500
H 3.87905982	-3.66838268	-2.48563571	C 4.87047400	3.91145500	-0.16461800
H -3.34798050	-4.87227178	-0.13073343	H 6.52120000	2.77428900	0.61590400
H 5.72419321	-4.35699634	-0.97953421	H 3.05161600	4.78024000	-0.90674400
H -5.50030353	-4.53683252	-1.31361579	H 5.45698200	4.81202500	-0.31175100
C 3.19824583	1.49535284	-0.25403704	C -2.86419600	1.99974000	-0.55333400
C -3.24858891	1.42776879	-0.11157594	C -4.11834900	2.54910100	-0.28267000
C 4.52063851	3.80247919	-1.11661183	C -2.11404600	2.50060900	-1.61431900
C -4.60657226	3.72292005	-0.94958239	C -4.60635700	3.59834300	-1.04883400
C 2.49961720	2.69079326	-0.42474258	H -4.72353400	2.15230400	0.52634600
C -4.42624237	1.82792703	0.52367263	C -2.60965400	3.54370800	-2.38944400
C 4.56524336	1.46585376	-0.53304183	H -1.14399100	2.06130100	-1.81971600
C -2.76253263	2.19049634	-1.17254590	C -3.85082500	4.09734500	-2.10514600
C 5.22066805	2.61263256	-0.96333853	H -5.57886400	4.02441000	-0.82619200
C -3.44028312	3.32849350	-1.59199010	H -2.02096200	3.92430200	-3.21713900
C 3.15891309	3.83855858	-0.84479408	H -4.23385600	4.91430800	-2.70727900
C -5.09830054	2.97079679	0.11058813	C -3.58445300	-0.60364000	0.28243300
H 1.43102233	2.70867224	-0.24247291	C -4.23252200	-1.22277200	1.35481800
H -4.83302699	1.24499553	1.34233650	C -3.96279000	-0.98051400	-1.01145900
H 5.12310702	0.54327743	-0.42563017	C -5.22082700	-2.18326800	1.14657500
H -1.83968051	1.89361243	-1.65661951	H -4.01640300	-0.92948600	2.37687200
H 6.28171578	2.57272954	-1.18442794	C -4.95217800	-1.92828600	-1.22146100
H -3.05079486	3.91088993	-2.41966086	H -3.46807500	-0.52886800	-1.86279500
H 2.60232522	4.76057274	-0.97246471	C -5.58365700	-2.54106000	-0.14311600
H -6.00864629	3.27267263	0.61684793	H -5.72158000	-2.63258200	1.99828900
H 5.03341269	4.69637556	-1.45427757	H -5.23139300	-2.19279900	-2.23575300
H -5.13172061	4.61510614	-1.27252061	H -6.35934100	-3.28041400	-0.30919000
H 0.78015849	-2.66199313	1.36567929	O -1.27175800	-2.18786600	-1.94448400
O -0.03767882	-2.15894274	1.40939783	C -1.38556100	-3.55174100	-1.60091300
			H -2.44153000	-3.80470800	-1.68833400
			H -0.78867600	-4.18632800	-2.25885500
			H -1.05287500	-3.71757500	-0.56680300
			O 0.94876900	-2.48045800	-1.97549000
			H 1.78225200	-1.99758800	-1.88779100
			K -0.93961900	-2.20367400	2.30770100
Ru_2H₂O			TS-CH_disP_K		
P -2.31260000	0.03055700	0.32033600	N 0.04004800	0.64053500	-0.88277500
P 2.31115000	0.12153300	0.38271000	P 2.96682500	0.28685600	-0.34573000
C -2.44288500	-0.21587100	2.15896200	P -3.78282700	1.82146600	-0.66257900
C 2.44098600	0.14852700	2.23816500	C 2.20913800	0.26412500	-2.03062800
H -2.39415200	-1.29380000	2.33644200	C -2.15524900	1.36606000	0.13713600
H 2.58640800	-0.87774200	2.57844700	H 1.97649300	-0.78500500	-2.23859300
H -3.38578800	0.16512100	2.55730300	H -2.08105400	1.94172400	1.06242500
H 3.29818300	0.74278400	2.55940500	H 2.87840500	0.61968400	-2.81707600
C -1.23902800	0.46340200	2.79253700	H -2.15428000	0.31542600	0.42356200
C 1.12835200	0.69025300	2.78461400	C 0.94983100	1.10613300	-1.92114400
H -1.25194900	0.26738700	3.87866200	C -0.97653000	1.67821700	-0.79241900
H 1.13200600	0.57267500	3.88148200	H 0.44316500	1.12565200	-2.90690500
H -1.33756900	1.55699200	2.68259800	H -1.36773100	1.86951600	-1.81206600
H 1.06407200	1.77353300	2.58978700	H 1.26431000	2.15559700	-1.75005900
N -0.00095100	-0.02288600	2.20033900	H -0.54375400	2.64873200	-0.48856300
O 0.05261300	0.28670400	-2.98719300	O 0.35322200	-2.24468100	0.62667600
H 0.11665200	-2.66099800	0.98181700	H -0.39333800	-0.03964800	1.78340700
C 0.03721400	0.13035300	-1.84076800	C 2.03472500	-0.28752400	2.54028300
Ru 0.01178200	-0.00778200	0.02236100	O 2.66161900	-0.31508000	3.51095300
H 0.03322800	1.56617600	0.10721200	C -0.32762400	-1.71560400	1.55718600
O 0.47582200	-2.55171600	2.61017800	O -1.74976300	-1.65816500	1.32321000
H 0.22991200	-1.52986600	2.55504100	C -2.39187500	-2.91255600	1.53996000
C -3.37616500	-1.27887200	-0.41930000	H -1.91738400	-3.71526800	0.96245300
C -4.31029700	-2.00337800	0.32122400	H -2.37338500	-3.19692200	2.59410800
C -3.23496200	-1.55349000	-1.78016600	C -3.96844300	0.35676800	-1.80478500
C -5.09033600	-2.97968600	-0.28779900	C -3.49190600	0.48288400	-3.11449900
H -4.43767000	-1.81273100	1.38051700	C -4.54998900	-0.85866400	-1.43043300
C -4.01989300	-2.52195300	-2.38927000	C -3.55012800	-0.58362300	-4.00661300
H -2.50182900	-1.01106500	-2.36576500	H -3.07728400	1.43085200	-3.44044500
C -4.94803700	-3.23962200	-1.64409600	C -4.62720400	-1.92138100	-2.32540800
H -5.81028200	-3.53740800	0.30126300	H -4.95478700	-0.96968000	-0.43076500
H -3.89818600	-2.72377300	-3.44772200	C -4.12021400	-1.79107500	-3.61552100
H -5.55599400	-4.00169200	-2.11902100	H -3.17803400	-0.46015500	-5.01820000
C 3.36809200	-1.29237500	-0.16274200	H -5.10115400	-2.84869700	-2.02013600
C 3.29852800	-2.51868500	0.50645900	H -4.19378500	-2.61433000	-4.31788500
C 4.13854100	-1.20346000	-1.32393400	C -5.01931000	1.40427000	0.64889400
C 4.00877500	-3.61717400	0.03715100	C -6.32642900	1.86236500	0.45726600
H 2.68594100	-2.62833600	1.39551000	C -4.71965400	0.71560200	1.82644400

C 4.84371700	-2.30490800	-1.79117700	C -7.31313200	1.62058800	1.40286200
H 4.19495800	-0.26632500	-1.86547800	H -6.56834500	2.42202200	-0.44112000
C 4.78466300	-3.51440200	-1.11075100	C -5.70503300	0.48704100	2.78127400
H 3.95130900	-4.55817200	0.57345000	H -3.71498100	0.35026500	2.00401200
H 5.44097800	-2.21547700	-2.69200700	C -7.00299700	0.93376400	2.57112500
H 5.33746500	-4.37328500	-1.47468200	H -8.32212400	1.98119700	1.23473600
C 3.27230800	1.59436500	-0.16974500	H -5.45453800	-0.04302900	3.69403600
C 2.66894600	2.56794400	-0.96110900	H -7.76881500	0.75476800	3.31779200
C 4.60674000	1.75900400	0.21191800	C 4.21166200	-1.07413900	-0.36395700
C 3.38551300	3.68953800	-1.36504700	C 5.54913000	-0.89619800	-0.71508400
H 1.63208900	2.44442600	-1.24951200	C 3.75828600	-2.34935300	-0.01720100
C 5.31956500	2.87959300	-0.18808800	C 6.41772600	-1.98063500	-0.73781000
H 5.09653700	1.00328300	0.81705500	H 5.92225300	0.09181200	-0.95790900
C 4.70886300	3.84785300	-0.97877900	C 4.62901300	-3.43091800	-0.04865500
H 2.90480300	4.43987300	-1.98294800	H 2.72708700	-2.48475500	0.29763000
H 6.35402000	2.99766000	0.11546600	C 5.95878700	-3.25004000	-0.40963000
H 5.26686100	4.72326400	-1.29247500	H 7.45800400	-1.83010200	-1.00557800
C -3.28607900	1.57107600	0.00653200	H 4.26904100	-4.41577900	0.22845200
C -4.67826000	1.54553900	-0.09919400	H 6.63957600	-4.09427500	-0.42276200
C -2.62485300	2.79488600	-0.08435600	C 3.95930500	1.83546000	-0.26669400
C -5.39238900	2.72210400	-0.28098200	C 4.06074200	2.49078400	0.96050500
H -5.20948000	0.60181500	-0.05311800	C 4.61732900	2.37172100	-1.37493000
C -3.34135000	3.97225600	-0.26125300	C 4.81726300	3.64906400	1.08043000
H -1.54256100	2.81301400	-0.02650700	C 3.52993400	2.09701800	1.81902000
C -4.72582700	3.93909000	-0.36000900	C 5.36583900	3.53597500	-1.25657600
H -6.47296800	2.68669000	-0.36739100	H 4.54927300	1.88655500	-2.34196000
H -2.81297100	4.91680500	-0.33131300	C 5.46968400	4.17499200	-0.02736200
H -5.28458100	4.85715900	-0.50523200	H 4.88757300	4.14677500	2.04121500
H -0.04077300	-2.95265400	3.31283500	H 5.86693000	3.94481500	-2.12725800
H 0.64604500	-2.73382100	-0.48760600	H 6.05349800	5.08422300	0.06495700
O -0.06935200	-2.38020100	0.04833500	H -3.42631200	-2.79043400	1.21794300
			O -0.08400500	-2.19273900	2.83443400
			H -0.38879400	-1.53057200	3.46421100
			Ru 1.05691300	-0.02254500	0.97735000
			H 1.08812000	1.50283900	1.36054100
			K -1.21806800	-1.68877300	-1.50309800
TS-H₂O/H₂O			KRu-CH₃OCO₂H		
P -2.31337400	0.02927300	0.31497800	Ru-H-Ph-anion-K-CH ₃ OCHOHOH-TSFS-MH		
P 2.31374000	0.12422400	0.37802000	P -2.24213193	0.88280748	0.26051845
C -2.44070100	-0.22158300	2.15406600	P 2.31086324	0.69174553	0.60048068
C 2.44258400	0.16405700	2.23363000	C -2.54698989	0.98913719	2.10609777
H -2.38626000	-1.29953900	2.32869100	C 2.30013177	0.34141508	2.42693390
H 2.58448000	-0.86074700	2.57931800	H -2.86149971	-0.00066300	2.45306587
H -3.38541600	0.15316200	2.55381000	H 2.21973262	-0.74244808	2.55936769
H 3.29968800	0.75976700	2.55195500	H -3.35743318	1.68577991	2.33007770
C -1.24355600	0.46244900	2.79468400	H 3.21713352	0.68059239	2.91480197
C 1.13217200	0.70783300	2.78180600	C -1.24194342	1.39346992	2.77384423
H -1.25704000	0.26449000	3.87946100	C 1.06274731	1.02753478	2.98442102
H 1.13764600	0.59776900	3.87851700	H -1.37079571	1.30214490	3.86944760
H -1.33837400	1.55371500	2.68140200	H 1.00764482	0.82957657	4.07172320
H 1.05432100	1.78532800	2.57354100	H -1.06192718	2.46663431	2.57522449
N 0.00192700	-0.01703600	2.20537100	H 1.19957447	2.12249340	2.88568085
O 0.05595800	0.28279100	-2.98926200	N -0.13882332	0.57508991	2.31012228
H 0.11601300	-2.59953700	1.03373000	H 0.09711985	-0.93966601	-0.13128207
C 0.03882100	0.13623200	-1.84201600	C -0.14988425	-5.24187995	-0.09166491
Ru 0.01231100	-0.00201000	0.01865900	Ru 0.05797090	0.75858368	0.09152434
O 0.03446300	1.57496500	0.10095200	C 0.20535713	1.00297375	-1.74607752
H 0.48200900	-2.46148300	2.58783700	O 0.30138748	1.16891679	-2.89047334
H 0.20929400	-1.36651000	2.51900400	O -0.17226969	-4.51636576	0.87095465
C -3.37139000	-1.28535300	-0.42177400	H 0.05310419	2.39728386	0.41859574
C -4.31882600	-1.99582400	0.31547500	K -0.65053791	-2.10619116	1.95045522
C -3.21324400	-1.57816400	-1.77691900	C -3.29836639	-0.55597066	-0.25464289
C -5.09513300	-2.97643200	-0.29126600	C -4.44955403	-0.95210239	0.43120238
H -4.45911200	-1.79176000	1.37059500	C -2.90794153	-1.28481672	-1.37948732
C -3.99454600	-2.55090400	-2.38396000	C -5.19014688	-2.04987262	0.00470609
H -2.46956300	-1.04737600	-2.35977300	H -4.78236682	-0.39961597	1.30329101
C -4.93593300	-3.25456800	-1.64211300	C -3.65689964	-2.36962776	-1.81718842
H -5.82516100	-3.52343600	0.29534500	H -1.99774821	-1.00064405	-1.89609521
H -3.85941400	-2.76713200	-3.43789200	C -4.79781300	-2.75809983	-1.12389384
H -5.54086400	-4.02015400	-2.11517100	H -6.07990470	-2.34480350	0.55081865
C 3.36403500	-1.29958400	-0.15099100	H -3.34565543	-2.91654855	-2.70085787
C 3.27708900	-2.51998400	0.52702000	H -5.37846036	-3.60980255	-1.46108702
C 4.14686900	-1.22375100	-1.30476200	C 3.43683087	-0.58430890	-0.12854964
C 3.98445500	-3.62659400	0.07233600	C 4.21079222	-1.45737402	0.63571827
H 2.65091900	-2.61873300	1.40857300	C 3.51513251	-0.66726821	-1.52119640
C 4.84847600	-2.33377200	-1.75684200	C 5.04443686	-2.39021654	0.02507003

H 4.21562000	-0.29098500	-1.85235400	H 4.17773790	-1.41296041	1.71829788
C 4.77323400	-3.53764000	-1.06786500	C 4.35517831	-1.58809340	-2.13074842
H 3.91381500	-4.56338500	0.61434000	H 2.91147392	-0.00489672	-2.13176200
H 5.45562100	-2.25548900	-2.65205900	C 5.12185865	-2.45591769	-1.35924792
H 5.32331800	-4.40315000	-1.42008600	H 5.64187722	-3.05858246	0.63623046
C 3.27889800	1.59012600	-0.18476800	H 4.41081186	-1.62917719	-3.21334061
C 2.67765800	2.56179400	-0.98016600	H 5.77843596	-3.17567006	-1.83581371
C 4.61468100	1.75178600	0.19367600	C 3.39110808	2.19605030	0.46256375
C 3.39778800	3.67834200	-1.39171800	C 4.76717380	2.13441045	0.69455627
H 1.63960100	2.44115400	-1.26531400	C 2.81393751	3.42103570	0.14133358
C 5.33104300	2.86740900	-0.21395500	C 5.54661182	3.28013676	0.61849689
H 5.10267700	0.99758300	0.80210700	H 5.23949662	1.18544404	0.92475180
C 4.72258000	3.83355900	-1.00899000	C 3.59577481	4.56831150	0.06181735
H 2.91878200	4.42712000	-2.01277900	H 1.74375495	3.45434643	-0.03748719
H 6.36650400	2.98313800	0.08695300	C 4.96139819	4.50134894	0.30100198
H 5.28338900	4.70493700	-1.32876000	H 6.61433558	3.21925086	0.80052449
C -3.29290200	1.56663800	0.00511100	H 3.13369709	5.51640919	-0.19179068
C -4.68352500	1.53388600	-0.11821900	H 5.57154331	5.39589969	0.23657018
C -2.63783500	2.79518200	-0.06499800	C -3.18685367	2.31846488	-0.44112387
C -5.40234500	2.70819700	-0.29625500	C -4.53340844	2.24506834	-0.80079828
H -5.20956700	0.58665000	-0.08880100	C -2.51440588	3.53098204	-0.59150680
C -3.35920600	3.97023500	-0.23778500	C -5.19655163	3.36617132	-1.28440289
H -1.55625100	2.81866900	0.00401900	H -5.07166958	1.30862247	-0.71819361
C -4.74219900	3.92994100	-0.35373900	C -3.18080878	4.65237333	-1.06851840
H -6.48149100	2.66732600	-0.39663300	H -1.45970060	3.57160406	-0.33879226
H -2.83568500	4.91851700	-0.29167300	C -4.52329605	4.57409443	-1.41617335
H -5.30466000	4.84617400	-0.49599600	H -6.24172273	3.29173745	-1.56537243
H -0.01324900	-2.89589700	3.28559000	H -2.64334172	5.58794177	-1.18029182
H 0.62709500	-2.72403700	-0.45064800	H -5.04130625	5.44778182	-1.79672173
O -0.08372100	-2.35486100	0.08070400	O 0.47940484	-5.01443339	-1.23695740
			C 1.23659611	-3.78651437	-1.34050423
			H 1.57693093	-3.75083917	-2.37095761
			H 0.61652960	-2.91803050	-1.11208644
			H 2.09032990	-3.82068683	-0.66468007
			O -0.78721731	-6.41307286	-0.11374989
			H -0.64128991	-6.83350491	-0.97160865
HRu-OH_H₂O			KRu-O(CH₃)C(OH)HO		
P -2.34814600	-0.04971100	0.30018200	P -2.44860400	0.24583600	0.31810100
P 2.28271300	0.13026100	0.33711200	P 2.12893000	0.59216400	0.32328300
C -2.45325100	-0.37599400	2.13094600	C -2.59117500	0.13185200	2.16860000
C 2.41568100	0.08515800	2.19701200	C 2.32091300	0.20397800	2.12583700
H -2.34512700	-1.45765500	2.24793500	H -2.71214100	-0.93567800	2.37862600
H 2.53227900	-0.95695400	2.50009000	H 2.43470500	-0.88162400	2.20433000
H -3.41554100	-0.09127800	2.55951500	H -3.48686300	0.62762300	2.55039900
H 3.28550100	0.64680900	2.54139300	H 3.20206200	0.67990400	2.56300400
C -1.30326300	0.34392600	2.81541400	C -1.30886800	0.66470100	2.78796700
C 1.12997100	0.63763700	2.78999800	C 1.03589300	0.65929000	2.80132300
H -1.31957300	0.14485500	3.89552500	H -1.34099800	0.47733600	3.87889500
H 1.15401100	0.53847000	3.88363700	H 1.09517200	0.41224200	3.87883100
H -1.39091800	1.42488800	2.67531100	H -1.29490700	1.76676100	2.68158700
H 1.00972300	1.69663500	2.54857000	H 0.99686800	1.76541100	2.75947000
N -0.02339600	-0.09256000	2.23497900	N -0.13533700	0.05291900	2.19016600
O -0.00672500	0.10333900	-2.99166000	C -0.17055200	0.40064500	-1.85941400
H 0.48316500	-2.73001400	1.52963700	O -0.19735800	0.60002900	-3.00046100
C -0.01208100	0.01013900	-1.83997400	C 0.90363700	-2.92127800	-0.60781900
Ru -0.02024500	-0.08959600	0.00783200	C 2.62816500	-4.46092900	0.07745400
H -0.09524400	1.51120200	0.07525700	O 1.57401500	-3.61328300	0.48796600
O 0.76365800	-2.80412000	2.54297300	O -0.03773200	-2.14266200	-0.13484300
H 0.11278200	-1.08847000	2.47636800	H 3.16242300	-4.78293700	0.97439300
C -3.45998000	-1.31367800	-0.44656200	H 3.33157500	-3.92748900	-0.57334400
C -2.93095300	-2.59874100	-0.59965400	H -0.31532100	1.73417600	0.19115400
C -4.76308600	-1.04840300	-0.86626400	Ru -0.13859600	0.17314100	-0.01044600
C -3.71772500	-3.60748900	-1.14015100	C 3.50577000	-0.30389000	-0.52290700
H -1.89472900	-2.78212100	-0.31174600	C 3.54289600	-0.27071100	-1.91916400
C -5.53919400	-2.06271000	-1.41424500	C 4.51134400	-0.98690300	0.15930900
H -5.17468000	-0.05012900	-0.77932100	C 4.56755700	-0.89575000	-2.61412700
C -5.02085500	-3.34444300	-1.54627900	H 2.76223000	0.24616100	-2.46682900
H -3.30346200	-4.60320100	-1.25733500	C 5.53652900	-1.61731600	-0.53823500
H -6.55028900	-1.84703900	-1.74235700	H 4.50478300	-1.03464900	1.24187200
H -5.62834300	-4.13408400	-1.97523500	C 5.56840600	-1.57191400	-1.92502900
C 3.44165300	-1.17688100	-0.25347400	H 4.58089100	-0.86021100	-3.69782000
C 3.46729200	-2.43053900	0.36436900	H 6.31209300	-2.14466300	0.00685800
C 4.20802400	-0.97398700	-1.40321700	H 6.36772300	-2.06363200	-2.46829700
C 4.27158800	-3.44345600	-0.14348600	C 2.75685300	2.33241100	0.18475200
H 2.85060400	-2.63273500	1.23366300	C 1.92560200	3.36148100	-0.24811200
C 5.00481800	-1.99202500	-1.90956500	C 4.08356300	2.62723600	0.50905800

H 4.18858900	-0.01408200	-1.90607900	C 2.40683600	4.66290800	-0.34530500
C 5.04355300	-3.22858100	-1.27798300	H 0.89733100	3.13397900	-0.50286000
H 4.28711600	-4.40863400	0.35092600	C 4.56141200	3.92633900	0.42031500
H 5.59627400	-1.81624500	-2.80142400	H 4.75623900	1.83541700	0.82110000
H 5.66796000	-4.02283200	-1.67193100	C 3.72211500	4.94912300	-0.00880000
C 3.15142700	1.69284300	-0.11972400	H 1.74739900	5.45320700	-0.68710500
C 2.48206500	2.68546400	-0.82991300	H 5.59307700	4.14026200	0.67804900
C 4.48126500	1.90461100	0.25559000	H 4.09639800	5.96430000	-0.08423700
C 3.12863300	3.87200300	-1.15978700	C -3.64676000	-1.03927700	-0.25192800
H 1.44722100	2.52377900	-1.10740500	C -5.02576700	-0.82338300	-0.27752700
C 5.12371100	3.09022100	-0.06911500	C -3.13855200	-2.28729600	-0.61538900
H 5.02389200	1.13473700	0.79419000	C -5.88643200	-1.84560900	-0.65528400
C 4.44726400	4.07694500	-0.77942600	H -5.42909800	0.14820200	-0.01384500
H 2.59691400	4.63696700	-1.71481800	C -4.00639900	-3.30817900	-0.98963900
H 6.15509500	3.24397600	0.22884600	H -2.06045200	-2.44241700	-0.60173400
H 4.95053900	5.00290300	-1.03525900	C -5.37814700	-3.09018900	-1.01130700
C -3.24326400	1.54473100	0.05597500	H -6.95646300	-1.66866600	-0.67696400
C -4.36596700	1.90105000	0.80570700	H -3.60431500	-4.27452100	-1.27561800
C -2.79252500	2.41726000	-0.93421900	H -6.05207700	-3.88568100	-1.31081300
C -5.01934200	3.10510300	0.57362000	C -3.29247700	1.80885900	-0.17637200
H -4.74605000	1.23944900	1.57578600	C -3.70235500	2.77778900	0.73674300
C -3.45341000	3.61439700	-1.17580600	C -3.47094400	2.05192400	-1.54059100
H -1.90829600	2.15865500	-1.50381800	C -4.28955400	3.96004800	0.29780900
C -4.56544800	3.96321300	-0.41995800	H -3.55835300	2.62731600	1.79982500
H -5.88600200	3.37052600	1.16914100	C -4.06327000	3.22717600	-1.97734500
H -3.09208800	4.28018200	-1.95172800	H -3.14286500	1.31763300	-2.26825400
H -5.07619200	4.90222400	-0.60263400	C -4.47497900	4.18644400	-1.05840100
H 0.37645700	-3.60989600	2.89129300	H -4.60093600	4.70501800	1.02204400
H 0.65258800	-2.66620100	-0.46248000	H -4.19656500	3.39798900	-3.03991200
O 0.06209500	-2.33039400	0.21601900	H -4.93359000	5.10774800	-1.40009600
			H 2.25197800	-5.33795700	-0.45626900
			O 0.39221800	-3.98560500	-1.42918400
			K -0.14222600	-2.72770500	2.34097300
			H 1.70077200	-2.40522100	-1.17454100
			H -0.20248700	-3.55290100	-2.04937400
HRu-OH_MF			TS-CO_k		
P -2.41707674	0.16746371	0.16098063	P -2.34887100	0.42253000	0.31304600
P 2.19384931	0.55960245	0.17805487	P 2.26367000	0.37252800	0.34395700
C -2.48706087	-0.32837981	1.95674009	C -2.49622400	0.28489800	2.16331600
C 2.35147556	0.25616766	2.01106019	C 2.40523500	-0.13180600	2.12202800
H -2.33584580	-1.41076193	1.97161343	H -2.75223700	-0.76223800	2.35112100
H 2.45965074	-0.82138622	2.15540489	H 2.41705900	-1.22468900	2.14461000
H -3.45522961	-0.12314543	2.41574191	H -3.32755200	0.87547100	2.55470100
H 3.22682431	0.75505712	2.43046414	H 3.31976400	0.24279700	2.58773500
C -1.36076460	0.36452128	2.70635004	C -1.16434800	0.64637300	2.79534600
C 1.07453964	0.71255491	2.69871538	C 1.16060900	0.39531100	2.81596900
H -1.32605468	0.01204042	3.74504882	H -1.20897200	0.39983400	3.87315000
H 1.10507849	0.42562898	3.75731081	H 1.17761900	0.06396800	3.87082500
H -1.51433847	1.44698337	2.72063419	H -1.03620300	1.74494200	2.75293600
H 0.95993751	1.79796742	2.64089541	H 1.22376100	1.50018300	2.85696600
N -0.08206858	0.09366049	2.03493377	N -0.05848800	-0.04658900	2.15420100
O -0.15754546	0.65491330	-3.14178425	C -0.01202900	0.71992100	-1.82074700
C -0.13560639	0.50938047	-1.99398952	O 0.00871300	1.14233200	-2.89814100
H 0.85884306	-2.15614161	-0.43457148	C 0.71880900	-3.76567000	-0.26405600
O 0.15507224	-1.88632966	0.16112461	C -0.38082900	-2.38381700	-2.04930500
C 0.59064925	-3.49422447	2.45535636	O 0.05710400	-2.24486800	-0.71809200
H -0.31900671	-3.72329852	1.88371516	O -0.16581700	-4.50785500	0.19751900
O 0.63129085	-2.73226498	3.38358167	H -1.16041600	-1.65306800	-2.27432000
H 0.06967536	-0.92040486	2.00634538	H -0.80352200	-3.38360400	-2.21995900
Ru -0.10497057	0.31833178	-0.15435580	H -0.10311700	1.75181200	0.34044500
H -0.28150852	1.91101091	-0.02818910	Ru -0.03379300	0.22798100	-0.01845700
C 3.37197986	-0.62866734	-0.59983394	C 3.47228300	-0.69175900	-0.55954100
C 4.29043978	-1.39372294	0.11857744	C 3.38455600	-0.75412800	-1.95243900
C 3.32809783	-0.75839341	-1.99039539	C 4.47279800	-1.42270800	0.08533300
C 5.15088380	-2.26531347	-0.54022622	C 4.28282900	-1.51894900	-2.68200500
H 4.34233974	-1.32405509	1.19829996	H 2.60468400	-0.20455400	-2.46676100
C 4.19137325	-1.62357047	-2.64688601	C 5.36597900	-2.19753100	-0.64733700
H 2.61122631	-0.18124979	-2.56389841	H 4.55926600	-1.40043900	1.16570900
C 5.10558070	-2.38042852	-1.92279058	C 5.27491900	-2.24404100	-2.03132900
H 5.85853720	-2.85430308	0.03301982	H 4.20149600	-1.55670100	-3.76255800
H 4.14482118	-1.71090384	-3.72670367	H 6.13182800	-2.76611700	-0.13159000
H 5.77795435	-3.05952671	-2.43530254	H 5.97012000	-2.84926300	-2.60221100
C -3.39991990	-1.13054579	-0.69929394	C 3.09996500	2.02133700	0.26510100
C -2.74099091	-2.33971826	-0.94191733	C 2.37744000	3.16277200	-0.07241400
C -4.71519464	-0.96062525	-1.12803002	C 4.46303100	2.14144900	0.54617600
C -3.41378069	-3.37308085	-1.58036965	C 3.00275800	4.40399600	-0.11846300

H -1.69675647 -2.43961910 -0.63567494	H 1.32165600 3.07220600 -0.29767800
C -5.37674826 -1.99843152 -1.77441920	C 5.08532200 3.38040000 0.50507200
H -5.22537244 -0.01773615 -0.97196489	H 5.05005900 1.26182800 0.78694000
C -4.73028897 -3.20727033 -1.99604044	C 4.35494500 4.51610900 0.17177900
H -2.90130015 -4.31074010 -1.76844909	H 2.42781100 5.28370600 -0.38591500
H -6.39874815 -1.85746313 -2.10923576	H 6.14417200 3.45936900 0.72612000
H -5.24835568 -4.01501923 -2.50177629	H 4.84229100 5.48421600 0.13455600
C 3.05100409 2.17653256 -0.08232331	C -3.64592800 -0.78130400 -0.22469600
C 2.30552596 3.31266780 -0.38689855	C -4.98678100 -0.42528600 -0.37643200
C 4.43785461 2.28641313 0.04454241	C -3.27315600 -2.11649000 -0.38872300
C 2.93396489 4.54216292 -0.55110503	C -5.93740700 -1.39107300 -0.68219100
H 1.23063122 3.21816792 -0.49532953	H -5.29117200 0.60865600 -0.26159300
C 5.06325799 3.51409374 -0.11841696	C -4.22784600 -3.08138400 -0.68739100
H 5.03660079 1.40752316 0.25792336	H -2.22720200 -2.39995500 -0.31178200
C 4.31140462 4.64572010 -0.41619737	C -5.56109000 -2.72032800 -0.83544900
H 2.34297736 5.41935518 -0.79085520	H -6.97617900 -1.10267300 -0.80192600
H 6.14087676 3.58706399 -0.01993416	H -3.91861900 -4.11240700 -0.81872900
H 4.80158779 5.60412340 -0.54795356	H -6.30536900 -3.47140800 -1.07649800
C -3.45610149 1.68682685 0.04745797	C -3.07669000 2.04718000 -0.16107400
C -3.06623662 2.69922423 -0.82853633	C -3.39788600 3.03589100 0.76639700
C -4.62794812 1.85173976 0.78893787	C -3.24716500 2.31833000 -1.52099900
C -3.83536615 3.84735879 -0.96761051	C -3.89178700 4.26597600 0.34526100
H -2.14392443 2.58757451 -1.38584112	H -3.25645300 2.86307800 1.82636700
C -5.39081698 3.00541827 0.65894086	C -3.74792000 3.54191800 -1.93969000
H -4.96035626 1.07782106 1.47165792	H -2.98641100 1.56867700 -2.26001900
C -4.99675034 4.00475187 -0.22218219	C -4.07196600 4.52073400 -1.00675100
H -3.52028885 4.62458742 -1.65504889	H -4.13502700 5.02576500 1.07995100
H -6.29523656 3.12180281 1.24603962	H -3.87687000 3.73444000 -2.99894300
H -5.59265218 4.90497675 -0.32480723	H -4.45819500 5.47949800 -1.33431500
O 1.67355846 -4.15856733 2.04000673	H 0.43532800 -2.23128200 -2.77095800
C 1.49735478 -5.00551508 0.90118502	O 1.69832700 -3.34090300 0.67771500
H 1.22841702 -6.01476669 1.22167270	K -0.52358600 -2.80076700 2.16761700
H 0.73344342 -4.60045215 0.23446927	H 1.20118000 -4.00108600 -1.23010100
H 2.45233313 -5.03282235 0.38050372	H 2.31670100 -2.76487000 0.21019300
TS-MF-OH	
P -2.39806000 0.16730700 0.31555800	KRu-OCH₃-HCOOH
P 2.22957600 0.38732900 0.22940200	
C -2.49898500 -0.03903100 2.16500400	
C 2.40136900 -0.02766600 2.03703100	
H -2.52113000 -1.10814100 2.37913900	P -2.46265600 0.21058000 0.32570300
H 2.41490900 -1.11888800 2.11063500	P 2.10430200 0.66056200 0.29907900
H -3.40736800 0.41755100 2.56111600	C -2.57855200 -0.03442100 2.16815300
H 3.32455500 0.37128000 2.46257200	C 2.32872300 0.13048300 2.06286800
C -1.25540600 0.57166900 2.78926200	H -2.69716900 -1.11321100 2.31040000
C 1.18689200 0.51878700 2.76831400	H 2.46107500 -0.95521100 2.06181300
H -1.24928100 0.37266900 3.86939600	H -3.47056700 0.43344800 2.59136500
H 1.23316200 0.23892600 3.82915700	H 3.20643900 0.58840000 2.52553100
H -1.23781600 1.65528300 2.64527400	C -1.29251200 0.45877400 2.80840500
H 1.16420400 1.61129100 2.71377500	C 1.04460800 0.49879500 2.78804800
N -0.05007700 0.00694000 2.15935200	H -1.30101600 0.17412700 3.87790700
O -0.18740700 0.79049200 -3.00270600	H 1.12296200 0.15983600 3.83817100
C -0.14915100 0.54753400 -1.87306800	H -1.29307000 1.56587000 2.79752000
H -0.56854200 -2.30501000 -0.79982800	H 0.97882700 1.60333200 2.84051800
O 0.12596700 -2.01796600 -0.19926200	N -0.12065600 -0.07867700 2.13925000
C 0.03465900 -3.25972700 1.30901100	C -0.25330800 0.82817600 -1.82153900
H -0.40025800 -4.03331400 0.65587600	O -0.31507700 1.25230600 -2.89791600
O -0.61704600 -2.72026900 2.20410700	C 2.02984500 -4.44316000 0.18995100
H -0.09661200 -1.01995400 2.28674100	C 0.37854700 -2.24251300 -1.84187600
Ru -0.09271200 0.21690200 -0.05293800	O 0.24027300 -1.94668500 -0.49826600
H -0.21481700 1.79318300 0.20763500	O 1.23768500 -5.14073200 0.76328000
C 3.39908700 -0.74966900 -0.62247700	H -0.50191400 -1.96291300 -2.44999900
C 4.46621200 -1.36678600 0.03085100	H 0.52290200 -3.32904900 -2.01184900
C 3.21507900 -0.98280000 -1.98543600	H -0.40566900 1.81376500 0.39001000
C 5.33978700 -2.19111300 -0.66849800	Ru -0.16623400 0.29341000 -0.03887600
H 4.62103100 -1.21714600 1.09318700	C 3.42240200 -0.24746700 -0.63309300
C 4.09078100 -1.80227700 -2.68407900	C 3.41043700 -0.17515500 -2.02760200
H 2.37615600 -0.53009300 -2.50036700	C 4.43134600 -0.98948800 -0.01307100
C 5.15568000 -2.40786900 -2.02772900	C 4.37918500 -0.82387800 -2.78074300
H 6.16440300 -2.66566600 -0.14772200	H 2.63506300 0.39408900 -2.52806600
H 3.93462700 -1.97483300 -3.74314400	C 5.39660500 -1.65199900 -0.76970700
H 5.83710300 -3.05112200 -2.57346700	H 4.48755800 -1.03854000 1.06896600
C -3.42612400 -1.19924200 -0.37616100	C 5.37086700 -1.57143600 -2.15585800
C -3.33681100 -2.48878900 0.15497300	H 4.35268000 -0.75300700 -3.86244900
C -4.20897500 -0.98810200 -1.51320100	H 6.17506000 -2.21920200 -0.27028200
C -4.04657600 -3.53380300 -0.42422000	H 6.12405600 -2.08157900 -2.74578600
H -2.70218100 -2.68585600 1.01312400	C 2.79249600 2.37921800 0.25525700
	C 1.95650500 3.45625700 -0.02696600
	C 4.14529300 2.61912900 0.50830100
	C 2.46156200 4.75184900 -0.04803100
	H 0.90742300 3.26693200 -0.22353400

C -4.90973300	-2.03772900	-2.09202200	C 4.64755400	3.91215200	0.49230100
H -4.27943700	0.00237000	-1.94769500	H 4.81786100	1.79198900	0.70922100
C -4.83562200	-3.31284600	-1.54583900	C 3.80481400	4.98286400	0.21285900
H -3.97753600	-4.52727300	0.00544600	H 1.79950100	5.58112600	-0.27194500
H -5.51630900	-1.85605200	-2.97246600	H 5.69965600	4.08491900	0.69166300
H -5.38671200	-4.13143600	-1.99540900	H 4.19792500	5.99355800	0.19557800
C 3.08114100	2.02460000	0.06623300	C -3.56010700	-1.14027600	-0.29482900
C 2.32551900	3.18959500	-0.04994100	C -4.95326600	-1.05834300	-0.29217900
C 4.47453300	2.12370400	0.08508800	C -2.94121800	-2.31853000	-0.71363300
C 2.94786900	4.43007500	-0.13050600	C -5.71711100	-2.14516400	-0.69771400
H 1.24489400	3.11018800	-0.08369500	H -5.44358100	-0.14167200	0.01668600
C 5.09493600	3.36245600	0.00432300	C -3.71086600	-3.40570900	-1.11469300
H 5.08372500	1.22930000	0.14623400	H -1.85134600	-2.35759200	-0.72299400
C 4.33252600	4.52007200	-0.10219500	C -5.09754000	-3.32071700	-1.10813600
H 2.34572500	5.32732800	-0.22365500	H -6.79949500	-2.07310000	-0.69751500
H 6.17776100	3.42297500	0.01639200	H -3.22385200	-4.31559700	-1.44941000
H 4.81833600	5.48726600	-0.17037800	H -5.69682900	-4.16595200	-1.42907000
C -3.42919600	1.66078200	-0.01816700	C -3.43731500	1.72456000	-0.06664900
C -2.88395700	2.76059100	-0.67465700	C -3.79409700	2.66201800	0.90040400
C -4.76429800	1.70826200	0.39327900	C -3.76069300	1.97811000	-1.40159800
C -3.65767400	3.89103000	-0.91598000	C -4.47482100	3.82101800	0.54425100
H -1.84633900	2.72676800	-0.98394400	H -3.53300700	2.50399200	1.94003000
C -5.53346700	2.83826600	0.15814900	C -4.44395800	3.13214500	-1.75575300
H -5.21147200	0.85347100	0.88984900	H -3.47613000	1.26917900	-2.17151300
C -4.98041300	3.93288700	-0.49877900	C -4.80462700	4.05766600	-0.78293300
H -3.22196000	4.73986900	-1.43131200	H -4.74497700	4.54082600	1.30932100
H -6.56747600	2.86428000	0.48415000	H -4.68870900	3.31244100	-2.79669800
H -5.58283700	4.81518300	-0.68514900	H -5.33551800	4.96160200	-1.06030300
O 1.37373100	-3.43064600	1.49628000	H 1.23938800	-1.73999900	-2.31734400
C 2.03639400	-4.14438500	0.46068100	O 2.75538600	-3.53589500	0.84904000
H 3.04823300	-4.33858900	0.81223500	K -0.13656400	-2.82992900	1.82272900
H 1.53924600	-5.10186400	0.26591700	H 2.22264100	-4.49741200	-0.89050200
H 2.05871600	-3.54953400	-0.45301600	H 3.20979700	-2.93488200	0.23248500
HRu-O(H)CHOOCH₃			KRu-CH₃OCOOH'		
P -2.40757586	0.15071133	0.34013652	P 2.29812300	-0.70572100	0.36958900
P 2.23004878	0.33589465	0.24049304	P -2.29819900	-0.70540700	0.36963400
C -2.49921773	0.00426427	2.19344526	C 2.45250000	-0.79743200	2.22671300
C 2.39809966	-0.09980952	2.03848667	C -2.45250700	-0.79642000	2.22679100
H -2.53829231	-1.05894667	2.43236607	H 2.56273300	0.22608300	2.60022400
H 2.37703979	-1.19226649	2.09626713	H -2.56229700	0.22727300	2.59993800
H -3.39470473	0.49117780	2.58244693	H 3.33827500	-1.36035500	2.52914500
H 3.33201382	0.27220239	2.46523641	H -3.33848100	-1.35889400	2.52948600
C -1.23618770	0.60573591	2.78745920	C 1.17045500	-1.41707800	2.75710600
C 1.19687603	0.47257646	2.77240083	C -1.17070000	-1.41646400	2.75727600
H -1.22057036	0.42404321	3.87076004	H 1.20829900	-1.41000700	3.86294700
H 1.23212244	0.17299513	3.82823879	H -1.20850300	-1.40916700	3.86311600
H -1.20673296	1.68827081	2.63017002	H 1.14974300	-2.48425900	2.46379400
H 1.21217032	1.56729300	2.74023025	H -1.15046800	-2.48372100	2.46418700
N -0.05161985	0.00596411	2.15624632	N 0.00002800	-0.70796900	2.27373700
O -0.18133786	0.62115366	-3.02117790	O 0.00001200	-0.85305700	-2.96376400
C -0.14802874	0.40964208	-1.88612353	H -0.00003400	1.11492800	0.06408200
H -0.74779709	-2.42171419	-0.71998342	H -0.00005300	2.17179000	-0.77387300
O 0.03756783	-2.17672041	-0.21914871	O -0.00009700	3.03672500	-1.33182700
C 0.02532647	-3.10569976	1.06139371	C -0.00000900	-0.72976800	-1.81249900
H -0.37519993	-4.05085043	0.63282452	K 0.00088700	2.04441800	2.38414400
O -0.62093394	-2.58336072	2.02444110	H -0.00006300	-2.25846000	0.19098900
H -0.14612652	-1.04589095	2.24928437	Ru -0.00002300	-0.61850100	0.04876800
Ru -0.09605393	0.14538916	-0.04805412	C -0.00002700	4.08226500	-0.55566900
H -0.19745007	1.71286824	0.14605732	C -3.38143300	0.71813800	-0.10167900
C 3.43433093	-0.74348242	-0.63662872	C -3.17297200	1.32111700	-1.34292900
C 4.45249446	-1.43181549	0.02240059	C -4.39109100	1.21696600	0.72414500
C 3.33543662	-0.84754766	-2.02474787	C -3.96050200	2.38771200	-1.75354900
C 5.36082345	-2.20131502	-0.69498152	H -2.37923000	0.95928700	-1.98619500
H 4.53948457	-1.38319292	1.10135282	C -5.17390700	2.29222400	0.31756500
C 4.24499900	-1.61341049	-2.74001550	H -4.58087200	0.76522500	1.69157000
H 2.54036280	-0.33123203	-2.55018702	C -4.96148300	2.87836300	-0.92328400
C 5.26069160	-2.29188260	-2.07676519	H -3.78196800	2.84374500	-2.72090400
H 6.14627222	-2.73366694	-0.16970055	H -5.95417200	2.66755900	0.97123300
H 4.15499922	-1.68581033	-3.81815883	H -5.57277900	3.71554200	-1.24204800
H 5.96900987	-2.89336728	-2.63561512	C 3.38146200	0.71791100	-0.10124600
C -3.46835847	-1.21335310	-0.30627125	C 4.39112900	1.21645900	0.72473100
C -3.37444531	-2.49388859	0.24769635	C 3.17303600	1.32127000	-1.34232500
C -4.28604559	-1.01262353	-1.42049788	C 5.17399000	2.29181200	0.31847600
C -4.11332973	-3.54097574	-0.29060179	H 4.58090400	0.76440500	1.69201200
H -2.70581320	-2.67928748	1.08515244	C 3.96061800	2.38794500	-1.75262600
C -5.01618161	-2.06520750	-1.95628888	H 2.37927700	0.95967300	-1.98570100

H -4.36118128 -0.02933308 -1.87007575	C 4.96160800 2.87831900 -0.92220200
C -4.93676100 -3.33107789 -1.38952342	H 5.95426200 2.66692400 0.97226400
H -4.03893053 -4.52748620 0.15383112	H 3.78212200 2.84425800 -2.71985600
H -5.64993236 -1.89304047 -2.81933277	H 5.57294300 3.71556600 -1.24071300
H -5.51045942 -4.15151506 -1.80628289	C -3.29694200 -2.14935700 -0.23051500
C 3.04491771 1.99445024 0.10531883	C -4.69111700 -2.10909000 -0.30069700
C 2.28291620 3.14413689 -0.08810774	C -2.63744500 -3.32101100 -0.59569400
C 4.43195580 2.11666439 0.22201477	C -5.40881200 -3.22366500 -0.71329900
C 2.89129306 4.39280774 -0.15188398	H -5.22435800 -1.20032200 -0.04700600
H 1.20843460 3.05031319 -0.19168351	C -3.35697800 -4.43671100 -1.00686700
C 5.03850946 3.36289527 0.16029024	H -1.55371100 -3.33988700 -0.55603200
H 5.04765879 1.23292126 0.34621507	C -4.74322900 -4.39180600 -1.06616200
C 4.26861107 4.50561557 -0.02642680	H -6.49119300 -3.17625300 -0.76716000
H 2.28416668 5.27820554 -0.30580936	H -2.82899000 -5.34075800 -1.29046200
H 6.11643785 3.44145345 0.25038229	H -5.30446700 -5.26039900 -1.39323000
H 4.74362016 5.47904705 -0.07975853	C 3.29672800 -2.14950500 -0.23116400
C -3.39812132 1.65891343 -0.04258280	C 4.69092000 -2.10938800 -0.30115900
C -2.84192108 2.70414073 -0.77489790	C 2.63711400 -3.32088800 -0.59700000
C -4.71787229 1.77043676 0.40447190	C 5.40851400 -3.22385300 -0.71422400
C -3.58870239 3.84367068 -1.05485599	H 5.22424600 -1.20081200 -0.04695200
H -1.81720050 2.62266085 -1.11586697	C 3.35655000 -4.43647900 -1.00864300
C -5.46028965 2.90942119 0.13017489	H 1.55337300 -3.33963800 -0.55746400
H -5.17479505 0.95826855 0.96003144	C 4.74281200 -4.39173000 -1.06774700
C -4.89584535 3.94936563 -0.60146554	H 6.49090700 -3.17656800 -0.76793400
H -3.14429135 4.64935939 -1.62863179	H 2.82847700 -5.34031500 -1.29275300
H -6.48239111 2.98507889 0.48460543	H 5.30397600 -5.26023500 -1.39517600
H -5.47724924 4.83884969 -0.81775610	O 0.00023700 4.08799100 0.66788200
O 1.40104431 -3.28516780 1.32107896	O -0.00027000 5.19857200 -1.28852100
C 2.05944790 -4.11994497 0.39062837	C -0.00017600 6.42284200 -0.55604700
H 3.06617342 -4.29557763 0.76974648	H 0.88906600 6.50134500 0.07130000
H 1.54839358 -5.08798622 0.29850061	H -0.00023100 7.20982700 -1.30691200
H 2.12089899 -3.65656600 -0.59821944	H -0.88930800 6.50137800 0.07145400
HRu-HCO(OH)OCH ₃	TS-H ₂ /CH ₃ COOH _K
P -2.29392601 0.29784932 0.27570982	P 2.45358600 0.00873400 0.34977300
P 2.34366458 0.34332611 0.30432498	P -1.97429000 -1.24225600 0.29900200
C -2.43259440 0.00773744 2.10260400	C 2.44239100 0.44737100 2.15039000
C 2.45969223 0.17891542 2.14884878	C -2.05926800 -1.54314900 2.14602000
H -2.41226820 -1.07508357 2.25180008	H 2.10261200 1.48677800 2.19060200
H 2.52428436 -0.88974323 2.36382677	H -2.66324900 -0.73608800 2.57262600
H -3.36087399 0.41398459 2.50950558	H 3.43249000 0.41363900 2.61054900
H 3.35388213 0.66147375 2.54626093	H -2.57639600 -2.47937400 2.36539600
C -1.20654188 0.63144230 2.75304183	C 1.44788800 -0.48243300 2.82675500
C 1.18506757 0.74658488 2.75179635	C -0.64906000 -1.52875800 2.71629100
H -1.18021394 0.33192431 3.81225037	H 1.38776400 -0.22595800 3.90094900
H 1.15910118 0.49557115 3.82372726	H -0.72353100 -1.47936700 3.81903000
H -1.29543626 1.73019514 2.74751285	H 1.86087500 -1.50953700 2.79488500
H 1.19883689 1.84694809 2.69267718	H -0.16709700 -2.50003600 2.49838100
N 0.01278311 0.19492708 2.07897859	N 0.13456800 -0.41867000 2.20189300
O 0.09848116 -0.20962047 -3.04338697	O 0.28095300 -0.72781500 -3.00715500
H -0.08975424 -2.09858972 0.33367351	H -0.05311300 1.39818400 0.17151900
H 0.11839576 -1.39798702 2.31301931	H -0.45489400 1.92837200 -0.37458900
C -0.18016007 -2.88590260 1.14925956	O -0.95344000 3.09932000 -1.13190900
O 0.22013279 -2.42756807 2.34232525	C 0.23007500 -0.56269000 -1.86694600
H 0.03386145 1.66655589 -0.31570043	K -1.27583300 2.01852400 2.35759500
C 0.06894862 -0.09402804 -1.89392395	H 0.58234300 -1.95835600 0.09806800
Ru 0.02849259 0.13879170 -0.03236209	Ru 0.18415500 -0.42083100 0.00411600
C 3.56383196 -0.87251673 -0.35503756	C -1.29253300 4.07366000 -0.40760600
C 3.49733891 -2.20080253 0.07333107	C -3.47865000 -0.21786000 -0.01553000
C 4.50559577 -0.51770417 -1.32108548	C -3.39494200 0.85656300 -0.89955700
C 4.37844559 -3.14458009 -0.43629130	C -4.69651400 -0.48016700 0.62236900
H 2.75100291 -2.51878144 0.79327779	C -4.50748900 1.65638200 -1.14219300
C 5.37822543 -1.46871360 -1.83559498	H -2.45525100 1.09045800 -1.38601800
H 4.56424708 0.50474536 -1.67423157	C -5.80418400 0.32015000 0.38088800
C 5.32232054 -2.78227958 -1.38981697	H -4.78622700 -1.32056900 1.30263800
H 4.32058028 -4.16905123 -0.08588899	C -5.71054700 1.39052200 -0.50394900
H 6.10555093 -1.17775115 -2.58559137	H -4.42003400 2.49298900 -1.82579200
H 6.00742907 -3.52265601 -1.78782401	H -6.74327600 0.10636300 0.87989700
C 3.12587906 1.96921435 -0.08617948	H -6.57638700 2.01605000 -0.69169500
C 4.32293268 2.35432841 0.52255179	C 3.37312700 1.38937400 -0.45876500
C 2.54314660 2.81994260 -1.02343386	C 4.76417500 1.48472500 -0.37756600
C 4.91310473 3.57133644 0.21214252	C 2.66167500 2.37524200 -1.14151800
H 4.80923589 1.69858815 1.23614005	C 5.42893200 2.55653700 -0.95663900
C 3.13838147 4.03570953 -1.34022200	H 5.33432800 0.71262800 0.12684300
H 1.61508270 2.52806155 -1.50010397	C 3.33074700 3.44756800 -1.72043700
C 4.32075160 4.41559021 -0.72034912	H 1.58413000 2.31029600 -1.23006400
H 5.83935754 3.85960122 0.69684542	C 4.71266900 3.54088200 -1.62869100

H 2.67337324	4.68631459	-2.07257184	H 6.50974500	2.61887000	-0.89009300
H 4.78263169	5.36612983	-0.96340484	H 2.76281900	4.20402600	-2.25013600
C -3.12775749	1.92952112	0.02589895	H 5.23372800	4.37498700	-2.08591700
C -4.50037220	2.01721449	-0.21198978	C -2.41210500	-2.86953600	-0.45855400
C -2.38715134	3.10582699	0.14169213	C -3.52790000	-3.04070700	-1.27572000
C -5.11731740	3.25590219	-0.32990469	C -1.57296700	-3.96112000	-0.22361000
H -5.09291669	1.11573682	-0.31473694	C -3.80594300	-4.28228400	-1.83714900
C -3.00714824	4.34387248	0.03252777	H -4.18316000	-2.20404500	-1.48442900
H -1.31756762	3.04669140	0.30729533	C -1.86148200	-5.20241800	-0.77096000
C -4.37302806	4.42227908	-0.20630453	H -0.67732300	-3.83145500	0.37362800
H -6.18337818	3.30798469	-0.52214241	C -2.97941500	-5.36684900	-1.58126100
H -2.41743060	5.24926463	0.12506134	H -4.67312400	-4.39721700	-2.47820300
H -4.85564994	5.38881387	-0.29995165	H -1.20224400	-6.04114200	-0.57575000
C -3.46632969	-0.88076490	-0.51818104	H -3.19836000	-6.33482900	-2.01822900
C -4.38366612	-1.64169300	0.20781469	C 3.61834000	-1.41051100	0.17395300
C -3.42072151	-1.02111818	-1.90791420	C 3.58079400	-2.13265200	-1.02063200
C -5.24002398	-2.52218733	-0.44418483	C 4.53140000	-1.78577400	1.15790700
H -4.43137379	-1.56052157	1.28671950	C 4.44713500	-3.19509200	-1.23060200
C -4.28333648	-1.89287842	-2.55731727	H 2.86062100	-1.86755900	-1.78622300
H -2.70588405	-0.44666740	-2.48607568	C 5.39034900	-2.86043400	0.95264900
C -5.19411142	-2.64734242	-1.82631188	H 4.57754400	-1.25220100	2.09965000
H -5.94356935	-3.11131969	0.13348976	C 5.35355900	-3.56400700	-0.24280200
H -4.23715885	-1.98903193	-3.63632542	H 4.40738500	-3.74280900	-2.16562800
H -5.86268566	-3.33444571	-2.33283335	H 6.08962900	-3.14506200	1.73133500
O 0.64989113	-3.95212021	0.79343846	H 6.02498300	-4.40016600	-0.40380500
C 0.35469700	-4.52698394	-0.46057544	O -1.43263700	4.09455400	0.83049100
H 1.15824547	-5.22685767	-0.68593543	O -1.52512400	5.21500800	-1.12020100
H -0.59239239	-5.07760079	-0.44276527	C -1.91208200	6.35527000	-0.36834000
H 0.31940165	-3.76826916	-1.25483571	H -1.14071000	6.64004800	0.35099500
O -1.54128635	-3.26953649	1.20872077	H -2.05338700	7.15548500	-1.09450300
H -1.92173295	-3.23195214	0.32466000	H -2.84373400	6.17935200	0.17476800
TS-CH			KRu-OCOOCH₃-H₂		
P -2.29519190	0.12476215	0.32783017	P 2.58856400	0.59205000	0.22387700
P 2.32838174	0.29658919	0.30776868	P -1.56820700	-1.47185100	0.09767600
C -2.41588727	-0.02079413	2.17900305	C 2.38175700	1.21553100	1.96800500
C 2.46773383	0.29432784	2.16549734	C -2.14433500	-0.70562500	1.67741700
H -2.34112021	-1.08464991	2.41910201	H 2.08236000	2.26530000	1.89070600
H 2.54045776	-0.74631018	2.48724207	H -2.64477800	0.23680600	1.43955100
H -3.36157096	0.36933373	2.56059151	H 3.32143200	1.17298800	2.52224700
H 3.36150779	0.82401014	2.49840125	H -2.86347400	-1.34998000	2.18702100
C -1.23450277	0.72021111	2.78472787	C 1.28694900	0.39460300	2.63195400
C 1.20788351	0.91386727	2.74528989	C -0.89784400	-0.47134500	2.51787900
H -1.23632086	0.59601574	3.87561459	H 1.06396800	0.84677600	3.61659800
H 1.23022214	0.84665533	3.84125212	H -1.19914400	0.02113200	3.46047100
H -1.29654821	1.79058681	2.57046380	H 1.68447900	-0.61245200	2.86120000
H 1.12880405	1.96941159	2.47303305	H -0.48030400	-1.45080800	2.82068700
N 0.02548491	0.21136943	2.21699185	N 0.09084300	0.33617200	1.81158100
O 0.04426113	-0.11574651	-2.98987973	O 1.17942400	-1.67864300	-2.86280300
H 0.06670596	-1.67501914	0.35364741	O 0.06052600	1.29704000	-0.91095500
H 0.12521734	-0.79026792	2.47483091	H -0.65941800	0.92064800	-0.90015300
C 0.06186308	-2.87802946	1.33666524	O -3.59575800	2.27432000	0.91514300
O 0.51933017	-2.51125924	2.41970738	C 0.90296000	-1.14538900	-1.87988100
H -0.00459410	1.69714319	-0.03945582	K -1.12772300	2.89836400	1.64704700
C 0.03325417	-0.05305148	-1.83524888	H 1.13479600	-1.65254200	0.49588900
Ru 0.01708785	0.06959893	0.01596559	Ru 0.49781800	-0.38149700	-0.20470500
C 3.55073047	-0.96523994	-0.25452964	C -3.93504700	3.48120500	0.88952300
C 3.64282962	-2.19680733	0.39572246	C -2.91527500	-1.28898000	-1.14257700
C 4.33381889	-0.73659213	-1.38783872	C -3.80083000	-0.21029100	-1.10854100
C 4.52725036	-3.16469089	-0.06220406	C -2.99025500	-2.20762400	-2.19337200
H 3.00547096	-2.42654895	1.24068434	C -4.75991400	-0.07467000	-2.10722600
C 5.20940939	-1.71112682	-1.84774653	H -3.76812400	0.54455500	-0.32646800
H 4.26673867	0.20861659	-1.91360365	C -3.94677100	-2.06087400	-3.18704700
C 5.31498224	-2.92510962	-1.18088344	H -2.30531800	-3.04750500	-2.23325400
H 4.58951936	-4.11453653	0.45705838	C -4.83743500	-0.99406600	-3.14414600
H 5.81185904	-1.51779981	-2.72856577	H -5.44661000	0.76311900	-2.06113000
H 6.00314886	-3.68421383	-1.53634195	H -3.99618500	-2.78231300	-3.99530200
C 3.15551374	1.87628135	-0.18226841	H -5.58787900	-0.88074200	-3.91895500
C 4.45431166	2.15953846	0.24990757	C 3.14396300	2.07088200	-0.72601900
C 2.49817299	2.79703401	-0.99283608	C 3.89579900	3.09240100	-0.14022900
C 5.07402801	3.34697471	-0.11073182	C 2.79403600	2.17779100	-2.07220700
H 4.99380354	1.44344225	0.86082820	C 4.28141900	4.19971000	-0.88500600
C 3.12320564	3.98335202	-1.36269067	H 4.18990100	3.02654300	0.90142900
H 1.48750150	2.58038853	-1.31786793	C 3.18826300	3.28093200	-2.81900100
C 4.40839676	4.26213728	-0.91989091	H 2.20455000	1.39472900	-2.53593400
H 6.08020411	3.55683223	0.23528184	C 3.92859400	4.29541600	-2.22585400
H 2.60064775	4.69054618	-1.99743428	H 4.86076100	4.98799300	-0.41704200

H 4.89420174	5.18894389	-1.20477399	H 2.90899000	3.34974100	-3.86433100
C -3.27747333	1.64873796	-0.05519588	H 4.22952300	5.16025000	-2.80640200
C -4.66423073	1.66331337	0.11594251	C -1.58044200	-3.28692200	0.42750500
C -2.64005271	2.80258414	-0.50217139	C -0.42809500	-4.05778300	0.30856400
C -5.39345859	2.81509594	-0.14108165	C -2.77707400	-3.90650800	0.79924500
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C -3.37211581	3.95586009	-0.76313827	H 0.49990300	-3.58135300	0.01648000
H -1.56464347	2.78308613	-0.64005812	C -2.81207000	-5.26750200	1.06227900
C -4.74787210	3.96541535	-0.58211911	H -3.69005200	-3.32519700	0.87274800
H -6.46939877	2.81307516	-0.00475872	C -1.65449200	-6.03017900	0.94497100
H -2.86293822	4.84703435	-1.11357627	H 0.43869600	-6.01468300	0.46477900
H -5.31906995	4.86393852	-0.78828921	H -3.74575500	-5.73590500	1.35343000
C -3.40994658	-1.18590761	-0.33936939	H -1.68327900	-7.09536800	1.14637200
C -4.27310864	-1.94155670	0.45452433	C 4.09615500	-0.47399800	0.28069300
C -3.38400375	-1.41731654	-1.71735774	C 5.32093200	-0.06319700	-0.24481300
C -5.09560053	-2.90542084	-0.11825241	C 4.00848700	-1.72895700	0.88667400
H -4.30164609	-1.79673193	1.52758728	C 6.43704200	-0.88706600	-0.15638100
C -4.21143040	-2.37399193	-2.28816866	H 5.40945500	0.89908300	-0.73360400
H -2.71159316	-0.84695402	-2.34858584	C 5.12783100	-2.54254500	0.98783100
C -5.06955543	-3.12135792	-1.48938786	H 3.05401800	-2.07420400	1.26684000
H -5.75605181	-3.48961949	0.51292443	C 6.34557400	-2.12508200	0.46400300
H -4.18062310	-2.53981270	-3.35929301	H 7.38006900	-0.55730100	-0.57821800
H -5.71164127	-3.87326407	-1.93433675	H 5.04428200	-3.51257600	1.46531500
O 0.84630458	-3.70783767	0.56865190	H 7.21720700	-2.76632100	0.53282400
C 0.39581710	-4.03590813	-0.72963647	O -3.22545500	4.47056700	1.17715100
H 1.22291943	-4.53991944	-1.22649544	O -5.23431200	3.69614300	0.49424400
H -0.46514318	-4.71345502	-0.70179912	C -5.65736600	5.04939500	0.46122400
H 0.14469867	-3.12585387	-1.28834995	H -5.05875300	5.64047900	-0.23640900
O -1.29621542	-3.16574629	1.29178374	H -6.69704600	5.03062500	0.13218700
H -1.60853088	-3.14859417	0.37953897	H -5.59023700	5.51464000	1.44776100
TS-CH_disCO			KRu-H_H₂O		
P -2.23493100	0.16623400	0.51147300	P -2.27942622	-0.03707225	0.32349335
P 2.34322400	0.24643200	0.50618600	P 2.35902685	0.27553535	0.16410466
C -2.39164100	0.23072300	2.36973400	C -2.32911453	-0.53868752	2.09784155
C 2.52251000	0.60222800	2.33282300	C 2.57849417	-0.11560036	1.96969040
H -2.37216800	-0.79408900	2.75073800	H -2.37702042	-1.64333718	2.17533865
H 2.72910700	-0.35231900	2.82465600	H 2.76098736	-1.19249947	2.04151188
H -3.32285900	0.70047400	2.69343400	H -3.22657280	-0.14003965	2.57647496
H 3.36104100	1.26618700	2.54945100	H 3.43653118	0.40827026	2.39597031
C -1.19180400	0.99510000	2.88840500	C -1.06638379	0.01598944	2.74155009
C 1.22356000	1.19884000	2.83258200	C 1.27626228	0.24190662	2.66865627
H -1.19852500	1.04365800	3.98552000	H -1.02944424	-0.33922564	3.78704973
H 1.23842200	1.30307100	3.92620900	H 1.35129483	-0.07191832	3.72634823
H -1.20300600	2.01782700	2.50431600	H -1.13805272	1.11869500	2.80562582
H 1.07180000	2.18719000	2.39465800	H 1.17874387	1.34449165	2.69947159
N 0.06642900	0.37687600	2.41537500	N 0.14053609	-0.39248921	2.02634907
H 0.02293900	-1.78105100	0.32023700	O -0.16819153	0.94537688	-2.99008428
H 0.15086500	-0.53685600	2.85328200	H 0.50347925	-1.75246510	-0.50117437
C 0.09169000	-1.79206500	-1.37631400	H -0.30908291	-1.78156640	-0.47348593
O 0.10126900	-0.60491900	-1.81736200	O -2.31173787	-3.69414107	2.37414034
H 0.11862200	1.60097500	0.16872300	C -0.08639718	0.54422413	-1.91215042
Ru 0.07177400	-0.04607400	0.28132800	H -3.12866143	-4.07409235	2.69864745
C 3.60911600	-1.10078400	0.28897400	K 0.03291591	-3.18894436	2.31612154
C 3.35045400	-2.33272100	0.89876900	Ru 0.03903326	0.02025404	-0.10658335
C 4.76619100	-0.96634400	-0.47963600	H -0.06195652	1.54288054	0.32192497
C 4.24341000	-3.38702200	0.77842500	C 3.15336469	1.93123251	-0.04951050
H 2.42051300	-2.47251300	1.44164800	C 4.50704913	2.06351070	-0.36400726
C 5.65388900	-2.02899500	-0.61233500	C 2.39122575	3.08233308	0.14841772
H 4.97793400	-0.02910500	-0.97963600	C 5.08625337	3.32161681	-0.46679304
C 5.40153700	-3.23653300	0.02366500	H 5.11422970	1.18412084	-0.54202717
H 4.02596300	-4.33443800	1.25919800	C 2.97451812	4.33913780	0.05429508
H 6.54674900	-1.90827600	-1.21613700	H 1.33396237	2.98643536	0.36608143
H 6.09546100	-4.06323700	-0.08028700	C 4.32273960	4.46247255	-0.25493973
C 3.13301600	1.66679800	-0.36690900	H 6.13736888	3.40884064	-0.71919256
C 4.26962400	2.32920500	0.09762000	H 2.36855560	5.22449061	0.21204300
C 2.55273900	2.07191200	-1.56926000	H 4.77580109	5.44416395	-0.33780862
C 4.81061300	3.38859200	-0.62072200	C -3.23818173	1.53703257	0.23093445
H 4.74872600	2.01923800	1.02034200	C -4.57814954	1.54458735	0.62922800
C 3.10509300	3.11979400	-2.29505900	C -2.66221760	2.71966798	-0.22283125
H 1.65917300	1.56458200	-1.91766700	C -5.31893905	2.71597866	0.58536014
C 4.22958600	3.78354500	-1.81986800	H -5.04857644	0.62695982	0.96620643
H 5.68854600	3.90302200	-0.24509200	C -3.40727388	3.89344170	-0.27234294
H 2.64871900	3.42410000	-3.23058900	H -1.62504108	2.71712955	-0.53491454
H 4.65335300	4.60851900	-2.38216600	C -4.73397822	3.89461680	0.13344797
C -3.09156800	1.73400100	-0.00230200	H -6.35687476	2.70892627	0.89965775
C -4.45201400	1.92754600	0.25182100	H -2.94666936	4.80733570	-0.63127914

C -2.37795200	2.73442200	-0.65567300	H -5.31469094	4.80977017	0.09577706
C -5.07854000	3.10806200	-0.12053100	C -3.33211065	-1.20479823	-0.63362656
H -5.03200900	1.14567200	0.73116500	C -3.90903080	-0.77146825	-1.83079787
C -3.00852500	3.91395100	-1.03844600	C -3.46896572	-2.53775773	-0.23792507
H -1.32240400	2.57437200	-0.84881300	C -4.63351048	-1.65326587	-2.61958436
C -4.35646800	4.10494200	-0.76903100	H -3.80184975	0.26071068	-2.14642649
H -6.13434100	3.24723100	0.08587400	C -4.20247663	-3.40947902	-1.03809645
H -2.44161400	4.68365500	-1.55107600	H -3.02775213	-2.92807945	0.69505934
H -4.84767500	5.02492700	-1.06722400	C -4.78339767	-2.97750192	-2.22287125
C -3.52715700	-1.05714300	0.00615900	H -5.08022580	-1.30489334	-3.54455733
C -4.23912700	-1.85488000	0.90044700	H -4.31440967	-4.44073281	-0.71964512
C -3.78460200	-1.18869100	-1.36090200	H -5.35187064	-3.66771380	-2.83733775
C -5.19677300	-2.75473800	0.44203000	C 3.52207476	-0.85918943	-0.70897333
H -4.06541500	-1.78137100	1.96730500	C 4.62565261	-1.43894268	-0.07965531
C -4.74104000	-2.08183200	-1.81731000	C 3.27963250	-1.15659538	-2.05123616
H -3.21990100	-0.59716100	-2.07229100	C 5.46512263	-2.29985248	-0.77711349
C -5.45191900	-2.86883400	-0.91681200	H 4.84141565	-1.21903372	0.95983036
H -5.74473500	-3.36390500	1.15296700	C 4.12428897	-2.00850417	-2.75000582
H -4.92629700	-2.17071600	-2.88209600	H 2.42035443	-0.72261282	-2.55011133
H -6.19994700	-3.56775800	-1.27472300	C 5.21681042	-2.58517287	-2.11354436
O -1.03222900	-2.51937900	-1.59227200	H 6.31716080	-2.74459018	-0.27459044
C -1.09565600	-3.79923100	-0.98727600	H 3.92308534	-2.22771797	-3.79263519
H -2.11100700	-4.15854000	-1.14637400	H 5.87235824	-3.25594800	-2.65756281
H -0.37668600	-4.48870900	-1.43378800			
H -0.89784300	-3.71318200	0.08786100			
O 1.20146500	-2.59176000	-1.51193700			
H 1.97757200	-2.03297400	-1.38641700			
TS-CH₄disP			TS-H₂/H₂O_K		
N -0.03469300	0.53507400	-0.80953600	P -2.30650700	-0.08496000	0.22499800
H -0.33131100	-0.08998100	-1.55797100	P 2.29295000	0.30839000	0.23015000
P 2.92619500	0.45481400	-0.13969900	C -2.33365800	-0.90605100	1.87800700
P -3.77344200	1.03958700	0.95754000	C 2.41605400	0.33685000	2.09669600
C 2.21662900	1.14474200	-1.71166500	H -2.11917500	-1.97022200	1.69095600
C -2.30447700	0.16752100	0.20035500	H 2.83796500	-0.62582100	2.40066900
H 2.20075900	0.33006300	-2.44022800	H -3.30481100	-0.81514900	2.36978000
H -1.88968300	-0.49916600	0.95975100	H 3.10226600	1.11724200	2.43140200
H 2.80595700	1.97242900	-2.11427100	C -1.22202800	-0.24383300	2.68074700
H -2.61181000	-0.44488800	-0.64982800	C 1.01711400	0.51040100	2.67359700
C 0.80439800	1.60688300	-1.40052500	H -1.18762000	-0.70247900	3.68708200
C -1.24027300	1.16198100	-0.21377200	H 1.06477400	0.29418200	3.75762800
H 0.32364800	2.00983700	-2.30053700	H -1.49050000	0.81645800	2.85535500
H -1.66098200	1.87562800	-0.93512100	H 0.72407000	1.57490200	2.60082100
H 0.84282800	2.41968700	-0.67025900	N 0.06992000	-0.36552200	2.01612000
H -0.90280100	1.73185000	0.65440600	O -0.10972600	0.72326400	-3.07250900
O 1.03729400	-2.18493800	-1.46671800	H 0.39690000	-1.81782600	-0.56849300
H -0.23070100	-1.88599000	0.61312200	H -0.32187100	-1.99101400	-0.24289300
C 2.09045900	-2.02325100	1.60138600	O -1.15691300	-3.80117400	0.82838100
O 2.66124500	-2.65838200	2.37645300	C -0.05421900	0.38680900	-1.97167400
C 0.13645900	-2.70558500	-0.76810500	H -1.58271900	-4.58539800	0.47740800
O -1.20695100	-2.57365100	-1.17007700	K 0.74653500	-3.06371200	2.14250100
C -1.43074600	-3.11552700	-2.47480500	Ru 0.01500900	-0.04086100	-0.13921600
H -0.80563000	-2.61504400	-3.21835700	H -0.05206700	1.51154900	0.18973400
H -1.22533700	-4.18986000	-2.49726400	C 3.06588000	1.89644300	-0.31044300
C -4.54137900	1.78654900	-0.56070000	C 4.23252700	1.94742500	-1.07114000
C -4.49894700	3.17493400	-0.69485800	C 2.44064700	3.09295100	0.04823600
C -5.13804500	1.03289300	-1.57366000	C 4.76873400	3.17099200	-1.45757000
C -5.02558500	3.79762200	-1.82158600	H 4.72742700	1.03220900	-1.37193200
H -4.05559300	3.77265800	0.09543000	C 2.98631900	4.31239900	-0.32436100
C -5.66921100	1.65281600	-2.69628800	H 1.51249800	3.06639400	0.60822000
H -5.20121100	-0.04572800	-1.47563500	C 4.15212300	4.35538100	-1.08093300
C -5.61146900	3.03695000	-2.82416800	H 5.67248100	3.19378900	-2.05663000
H -4.98545500	4.87789000	-1.91032200	H 2.49168800	5.23276300	-0.03388400
H -6.13495200	1.05534600	-3.47280800	H 4.57219500	5.30881000	-1.38134900
H -6.02978200	3.51996000	-3.70042600	C -3.18511300	1.52081200	0.46592100
C -4.91825700	-0.37764300	1.27434600	C -4.42265900	1.55200000	1.11381400
C -4.59421800	-1.71935700	1.06941000	C -2.64818600	2.71123700	-0.01728700
C -6.16934100	-0.06881200	1.81876000	C -5.09792100	2.75139000	1.28915500
C -5.50304100	-2.72298600	1.39093300	H -4.86955800	0.63311300	1.47707700
H -3.63183500	-1.99666600	0.65606400	C -3.32903400	3.91223700	0.14975300
C -7.07936500	-1.06870800	2.12599200	H -1.68709100	2.69194500	-0.51702700
H -6.43176500	0.96837900	2.00368000	C -4.55163100	3.93559300	0.80633300
C -6.74724200	-2.40276100	1.91488400	H -6.05491100	2.76130500	1.79938700
H -5.23341000	-3.76092800	1.22733200	H -2.89966000	4.83109400	-0.23441500
H -8.04657400	-0.80755200	2.54149200	H -5.08053400	4.87282700	0.94084300
H -7.45352500	-3.18703200	2.16361000	C -3.45038000	-1.01952600	-0.86947900
C 4.55442300	-0.25717000	-0.60964200	C -4.35874200	-0.36673700	-1.70383000

C 5.04362500	-0.24708200	-1.91476300	C -3.34515800	-2.41205500	-0.91012000
C 5.31774800	-0.85681100	0.39507500	C -5.16819900	-1.09909700	-2.56304900
C 6.27635000	-0.81928800	-2.20876400	H -4.44002300	0.71375200	-1.68642000
H 4.46900600	0.20144300	-2.71598500	C -4.16714300	-3.13347200	-1.76703400
C 6.54927100	-1.42147700	0.10081100	H -2.60916600	-2.92719900	-0.27896300
H 4.94621700	-0.88711400	1.41345600	C -5.07823600	-2.48484400	-2.59235100
C 7.03176300	-1.40517300	-1.20312500	H -5.87087100	-0.58332300	-3.20861400
H 6.64321400	-0.80745300	-3.22920500	H -4.08865800	-4.21547400	-1.79132800
H 7.12935100	-1.88506200	0.89079200	H -5.71296700	-3.05656600	-3.26110100
H 7.99176700	-1.85314900	-1.43400700	C 3.55218600	-0.95282700	-0.26274600
C 3.40298700	1.95960200	0.81734500	C 4.75653200	-1.11218900	0.42903300
C 4.46173500	2.77558700	0.41219400	C 3.28961900	-1.78031700	-1.35408200
C 2.67842100	2.29882900	1.95771700	C 5.66959000	-2.08490200	0.04310500
C 4.77827300	3.92001700	1.12953100	H 4.99126400	-0.46830500	1.26973600
H 5.05177800	2.50835500	-0.45816500	C 4.20699000	-2.74873200	-1.74594700
C 2.99849700	3.44530700	2.67696400	H 2.35729800	-1.66630200	-1.89637300
H 1.87090500	1.64890700	2.27809200	C 5.39586900	-2.90545600	-1.04579300
C 4.04544600	4.25725300	2.26312000	H 6.59936200	-2.19855900	0.58992600
H 5.60334300	4.54680200	0.80919200	H 3.98751300	-3.38326000	-2.59730100
H 2.43124000	3.69846700	3.56585000	H 6.10968700	-3.66383700	-1.34772100
H 4.29735100	5.14930200	2.82604300			
H -2.48240200	-2.94363400	-2.69974600			
O 0.38544200	-3.95096000	-0.25093300			
H -0.37547400	-4.20679100	0.28306500			
Ru 1.15373800	-0.93936400	0.44115800			
H 0.79439800	-0.11418500	1.74275400			
HRu_CH₃COOH			KRu-OH_H₂		
P -2.21262041	0.44407342	0.19064380	P -2.24267707	0.03416662	0.35627268
P 2.39578763	0.56172311	0.09151827	P 2.31000582	0.44416001	0.22133697
C -2.31788336	0.21448989	2.04404087	C -2.25777332	-0.67903865	2.07290467
C 2.57740644	0.09748656	1.88984640	C 2.55162100	0.30840428	2.07769219
H -2.37703949	-0.85924874	2.23850979	H -2.12202256	-1.76068369	1.97517958
H 2.58255826	-0.99333800	1.95174141	H 2.96225698	-0.68470707	2.28780562
H -3.20928297	0.69026061	2.45690069	H -3.20228870	-0.49109352	2.58946986
H 3.51697084	0.46155520	2.30891147	H 3.28233000	1.03978853	2.42877337
C -1.05721490	0.77142718	2.68231092	C -1.07513481	-0.06365007	2.80322434
C 1.38573977	0.65989235	2.64493861	C 1.19899904	0.48566813	2.74994392
H -1.05557090	0.54875798	3.75794563	H -1.04044664	-0.47393869	3.83019374
H 1.43204205	0.36310737	3.70116533	H 1.30343264	0.20479795	3.81555045
H -1.00403754	1.85535158	2.55670745	H -1.26846310	1.02082045	2.92229234
H 1.38743860	1.75217360	2.59964602	H 0.94102571	1.56113677	2.74291397
N 0.13067711	0.18724770	2.03656639	N 0.17203803	-0.30730812	2.10151363
O 0.03103518	0.94459307	-3.13807289	O -0.13413073	1.28323191	-2.89068672
H 0.17938872	-1.22272284	-0.37867056	H 0.06444630	-1.36585473	-0.59163218
H 0.08117183	-0.83069521	2.16127318	H -0.74800028	-2.73821880	-0.72642850
C -0.39195141	-3.55779358	1.60509785	O -0.88822597	-3.67713265	-0.45348196
O -0.17887117	-2.69511922	2.43407946	C -0.07245104	0.87600457	-1.80802481
H 0.06306862	2.09667562	0.17621946	H -1.77795602	-3.89426501	-0.74462661
C 0.05243341	0.76070125	-1.99760811	K 0.94548986	-2.83988053	1.32573198
Ru 0.08756349	0.47571210	-0.16672436	Ru 0.02464792	0.26742275	-0.04992474
C 3.51553070	-0.61247641	-0.79229547	H -0.02373008	1.81345542	0.55751343
C 3.29404944	-1.98345580	-0.64659843	C 3.21402102	1.99014982	-0.25134989
C 4.51823823	-0.18252108	-1.66010984	C 4.45551515	1.99670119	-0.88596305
C 4.08214369	-2.90234401	-1.32293980	C 2.60102839	3.20954798	0.04368417
H 2.48219581	-2.33482673	-0.02041561	C 5.07948352	3.19839288	-1.20254436
C 5.29735913	-1.10482181	-2.34990488	H 4.94040151	1.06465330	-1.14849514
H 4.69419232	0.87601290	-1.80633553	C 3.23254227	4.40730465	-0.25930823
C 5.08852942	-2.46549913	-2.17710351	H 1.61166930	3.20385682	0.48908725
H 3.90044523	-3.96351183	-1.19298398	C 4.47435193	4.40611780	-0.88396163
H 6.06992845	-0.75343250	-3.02505375	H 6.04104215	3.18650946	-1.70445792
H 5.69880682	-3.18388451	-2.71312018	H 2.74402893	5.34608916	-0.02150613
C 3.30079584	2.16854835	-0.02233554	H 4.96208359	5.34263394	-1.13149491
C 4.59464782	2.31582703	0.48534570	C -3.37279272	1.50027016	0.47310556
C 2.68330271	3.26127383	-0.62504342	C -4.75260596	1.35423841	0.63301122
C 5.25200233	3.53483928	0.39767032	C -2.83034280	2.78107983	0.41718191
H 5.10189618	1.47295545	0.94292179	C -5.57028009	2.46955775	0.74910084
C 3.34600064	4.47982839	-0.72218402	H -5.19808890	0.36566556	0.65484597
H 1.67050799	3.14981315	-0.99458677	C -3.65039124	3.89828194	0.53046195
C 4.62810721	4.61975917	-0.20916435	H -1.75758870	2.88180533	0.28654127
H 6.25384731	3.63764664	0.80013424	C -5.01981969	3.74576629	0.69788763
H 2.85437365	5.32227687	-1.19611220	H -6.64063340	2.34302493	0.87197594
H 5.14261705	5.57185259	-0.27979781	H -3.21523989	4.89071715	0.48226144
C -3.25109648	1.94733958	-0.12926310	H -5.65983418	4.61736781	0.78303480
C -4.64450289	1.88169937	-0.19851875	C -3.27781772	-1.12917003	-0.64425069
C -2.62610913	3.18392014	-0.27789473	C -3.20679389	-1.04426457	-2.03652183
C -5.39500481	3.03319945	-0.39443730	C -4.10488390	-2.09853398	-0.07478915

H -5.15106225 0.92747115 -0.11440852	C -3.94882023 -1.90103878 -2.83777501
C -3.37894534 4.33592916 -0.47183098	H -2.55462745 -0.31003740 -2.49563684
H -1.54231513 3.22437044 -0.24699572	C -4.83992231 -2.96584085 -0.87747953
C -4.76415654 4.26426789 -0.52964138	H -4.17911024 -2.18913015 1.00286272
H -6.47614287 2.96640498 -0.45037155	C -4.76497126 -2.86802810 -2.26096881
H -2.87792480 5.29086458 -0.58826643	H -3.88173376 -1.81879562 -3.91702650
H -5.35149771 5.16220939 -0.68772509	H -5.47706192 -3.71427735 -0.41815240
C -3.27028558 -0.90946599 -0.48239214	H -5.33970000 -3.54150241 -2.88717166
C -4.26865188 -1.54035529 0.26135975	C 3.43388907 -0.89304559 -0.41472627
C -3.05705867 -1.31166013 -1.80116728	C 4.66410880 -1.19461406 0.17840466
C -5.03998426 -2.54933125 -0.30384632	C 3.01606301 -1.64783660 -1.51129336
H -4.45289640 -1.25322872 1.29040807	C 5.45324153 -2.22892088 -0.31076506
C -3.83542978 -2.31056118 -2.36896082	H 5.01625655 -0.61482406 1.02505664
H -2.26621559 -0.85000129 -2.38082583	C 3.81028857 -2.67597066 -2.00825744
C -4.82783700 -2.93314557 -1.62140192	H 2.04656609 -1.43436021 -1.94965032
H -5.80898235 -3.03365228 0.28819952	C 5.02812559 -2.97056571 -1.40767713
H -3.65756828 -2.61068494 -3.39564125	H 6.40449459 -2.45113000 0.16101303
H -5.43114787 -3.71852778 -2.06327004	H 3.47265178 -3.24956155 -2.86465633
O -0.66407023 -4.80384482 2.00315944	H 5.64570891 -3.77486246 -1.79241663
C -0.92803838 -5.80481831 1.01536979	
H -1.13354325 -6.71361957 1.57724197	
H -1.79183895 -5.53542914 0.40695309	
H -0.06303613 -5.95349201 0.36789058	
O -0.38410848 -3.40599722 0.30023508	
H -0.18749272 -2.42786346 0.04799588	
HRu-O(CH₃)C(OH)HO	KRu-OCOCH₃
P -2.37200200 0.22420600 0.33814800	P -2.16851290 0.76233296 0.00844184
P 2.27430800 0.22858400 0.31668600	P 2.46147074 0.63672027 -0.01624346
C -2.48716500 0.13704700 2.19390300	C -2.28774979 0.03497134 1.69921361
C 2.40023100 -0.10801800 2.13633400	C 2.55395583 -0.07681701 1.69149685
H -2.54554100 -0.91834500 2.46314500	H -2.25859232 -1.05548209 1.59816561
H 2.32692100 -1.19177300 2.26016200	H 2.46998131 -1.16156081 1.58293464
H -3.38005300 0.64772300 2.55765200	H -3.21557679 0.31916712 2.20022131
H 3.34393200 0.24855800 2.55409600	H 3.49503131 0.16174382 2.19229230
C -1.22262000 0.73645900 2.78538900	C -1.05771843 0.49156272 2.47004423
C 1.20861300 0.55214100 2.81086900	C 1.34807499 0.43728930 2.46477000
H -1.22838600 0.60014200 3.87540200	H -0.94856903 -0.14674639 3.35736263
H 1.21676300 0.31809400 3.88366200	H 1.21146739 -0.18653953 3.35933061
H -1.16614000 1.81065400 2.58392000	H -1.19909213 1.51899242 2.84252845
H 1.25968900 1.64146800 2.71029700	H 1.54901420 1.45652010 2.83274862
N -0.04222200 0.08363700 2.20097900	N 0.14436088 0.40032324 1.64601564
C -0.06025700 0.33764600 -1.85192400	O 0.03329286 -0.48440553 -3.14999920
O -0.06145800 0.53958600 -2.98947700	C 0.08991283 0.01787680 -2.10082845
C -0.01014100 -3.07139900 1.25633300	C -1.62541612 -4.26732333 1.67100156
C 0.24858500 -2.89813500 -1.21398800	C 0.02632708 -6.01586950 1.35554057
O -0.14268900 -2.22288600 -0.04069700	O -0.55762897 -4.82833563 0.85071195
O -0.62360500 -2.49948500 2.20761100	O -2.07933786 -3.23609243 1.12477153
H -0.26882700 -2.45736200 -2.06713400	H 0.80357647 -6.31449196 0.64771794
H -0.03947000 -3.95675600 -1.15592300	H 0.47032929 -5.85522793 2.34119751
H -0.06593900 1.69336000 0.12324800	C -3.36318219 -0.14305633 -1.06123168
Ru -0.04907500 0.11863700 -0.00755400	C -3.70800393 0.42337428 -2.29248644
C 3.45589600 -0.92799900 -0.49729800	C -3.87808235 -1.39461831 -0.71738228
C 3.60655300 -0.82989700 -1.88311400	C -4.56255640 -0.24129315 -3.15863781
C 4.18535700 -1.89388700 0.19429800	H -3.31134626 1.39361534 -2.57217428
C 4.47559600 -1.67227000 -2.56024300	C -4.73329885 -2.05725722 -1.59456278
H 3.04116800 -0.08843400 -2.43775100	H -3.60820120 -1.88173165 0.21398211
C 5.05415500 -2.73999900 -0.48738700	C -5.07974131 -1.48498097 -2.81060011
H 4.07647800 -2.00140200 1.26599100	H -4.82474884 0.21209794 -4.10819631
C 5.20194600 -2.63176100 -1.86330300	H -5.13139587 -3.02554771 -1.31140131
H 4.58196000 -1.58272600 -3.63562600	H -5.75045994 -2.00383378 -3.48661757
H 5.61695000 -3.48565100 0.06361000	C -2.95169995 2.42788968 0.15073952
H 5.87966600 -3.29252600 -2.39224600	C -4.29857630 2.54344990 0.50381636
C 3.16038700 1.83863400 0.10055700	C -2.20463573 3.58252572 -0.06379013
C 2.47699700 2.98657100 -0.29043000	C -4.88171706 3.79377186 0.64606931
C 4.53399700 1.91877600 0.34567900	H -4.89846064 1.65286564 0.65886176
C 3.15026900 4.19603000 -0.42657500	C -2.79090062 4.83597295 0.07593219
H 1.41311600 2.92409900 -0.48546400	H -1.16295099 3.48860903 -0.34963090
C 5.20415500 3.12590700 0.21480300	C -4.12770097 4.94334196 0.43258297
H 5.08821700 1.02996600 0.62805700	H -5.92789616 3.87240345 0.92051733
C 4.51234100 4.26884400 -0.17263400	H -2.20046040 5.72898847 -0.09745189
H 2.60586700 5.08183600 -0.73492600	H -4.58551315 5.92037035 0.54134801
H 6.27008600 3.17435400 0.40868300	C 3.61691072 -0.35742647 -1.04507742
H 5.03731000 5.21168800 -0.27974800	C 3.59806080 -0.16484279 -2.42868061
C -3.48729300 -1.10789000 -0.27096700	C 4.49297996 -1.29966529 -0.50550128
C -4.33009200 -0.89634500 -1.36319800	C 4.44453869 -0.89229539 -3.25267944
C -3.42090600 -2.37914000 0.30504500	H 2.91472515 0.55690255 -2.86238060

C -5.11460900	-1.93104500	-1.85632300	C 5.33420355	-2.03437018	-1.33399853
H -4.38234100	0.08028200	-1.83016200	H 4.52942004	-1.46650660	0.56451126
C -4.21561700	-3.40617900	-0.18710500	C 5.31279483	-1.83150487	-2.70723560
H -2.73143400	-2.57297500	1.12146000	H 4.42014651	-0.73075759	-4.32454399
C -5.06470500	-3.18673600	-1.26503100	H 6.00939223	-2.76451493	-0.90157288
H -5.76773000	-1.75203600	-2.70344100	H 5.97018009	-2.40406901	-3.35193139
H -4.16371500	-4.38663200	0.27368500	C 3.31945212	2.26332683	0.14189783
H -5.68138600	-3.99314600	-1.64662600	C 2.56047736	3.38583189	0.47210695
C -3.28445300	1.76928100	-0.09050300	C 4.70116314	2.39360621	-0.00067185
C -4.59695800	1.96289600	0.35001400	C 3.17431725	4.61613930	0.66842416
C -2.67571200	2.76194800	-0.85370200	H 1.48392500	3.28797213	0.56158129
C -5.27952500	3.12986900	0.03992600	C 5.31178536	3.62678074	0.18723988
H -5.09577900	1.19267000	0.92865400	H 5.30413214	1.53364825	-0.26929238
C -3.36215700	3.92964000	-1.16947900	C 4.55040183	4.73931548	0.52422610
H -1.65662200	2.61799100	-1.19054000	H 2.57446519	5.48206718	0.92598137
C -4.66216400	4.11665000	-0.72186300	H 6.38562775	3.71876352	0.06677045
H -6.29656100	3.26865500	0.38985200	H 5.02898409	5.70146284	0.66945448
H -2.87655500	4.69345900	-1.76671600	H 0.19250060	2.01548296	-1.12639100
H -5.19670800	5.02807800	-0.96596100	Ru 0.14544702	0.63866065	-0.34901896
H 1.32989100	-2.83420800	-1.39247000	H -0.71229538	-6.81633079	1.44569833
O 1.39595600	-3.20614400	1.49702100	K -0.60344705	-2.85054896	-0.97133603
H -0.39810800	-4.05263500	0.90602500	O -1.89449770	-4.85275903	2.70225951
H 1.78006400	-3.74716200	0.79801300			
H -0.15639700	-0.96103800	2.34799400			
TS-CO			TS-CO_{2,K}		
P -2.34899500	0.22777600	0.33067800	P -2.23093900	0.38257500	0.34361500
P 2.29027600	0.26203400	0.29430600	P 2.35030400	0.31097900	0.32166700
C -2.46640200	0.09013000	2.18569900	C -2.39219200	-0.08857800	2.12402200
C 2.43064000	-0.06131600	2.12071300	C 2.50464900	0.28891400	2.17851700
H -2.52277900	-0.97015000	2.43495000	H -2.40759100	-1.18156600	2.13291400
H 2.39475300	-1.14477800	2.26010600	H 2.72038000	-0.73733900	2.49190100
H -3.36442100	0.58536900	2.55824000	H -3.32051100	0.25758100	2.58466600
H 3.36505900	0.32639800	2.53141100	H 3.33581200	0.91213300	2.51505200
C -1.21187800	0.68653600	2.79865400	C -1.15393400	0.44632300	2.82769000
C 1.22683900	0.56530500	2.80374400	C 1.17239400	0.73919000	2.75781000
H -1.22126600	0.53205400	3.88592900	H -1.18548200	0.14160900	3.89089600
H 1.25140300	0.34168300	3.87840300	H 1.21215700	0.61565500	3.85678200
H -1.15785400	1.76213900	2.61087900	H -1.21000100	1.55202100	2.84006600
H 1.23743000	1.65319800	2.68989500	H 1.06105800	1.82630200	2.58662100
N -0.01859900	0.05797100	2.20611200	N 0.06935800	-0.01597900	2.19029000
C -0.04867100	0.48869500	-1.84047800	O 0.05578000	0.63719200	-2.98015100
O -0.05742400	0.73703100	-2.96892400	C 0.05163600	0.36225500	-1.85461800
C 0.04907100	-3.18404700	1.44258900	C -1.79188700	-3.89598200	0.23099400
C -0.14824800	-2.70715800	-1.29394000	C 0.46271900	-2.73955300	-1.42186600
O 0.11445500	-2.06819700	-0.08313500	O -0.06689500	-2.30031100	-0.21162300
O -0.65675200	-2.66150900	2.30497600	O -1.82973600	-3.72655500	1.39339600
H -1.11712100	-2.42033700	-1.72599900	H 1.44756300	-2.30068000	-1.63540900
H -0.17309100	-3.80371800	-1.16224000	H 0.59714700	-3.83563300	-1.44063000
H -0.08960200	1.76669500	0.19615700	C -3.58047400	-0.51694300	-0.53311800
Ru -0.03028700	0.18268700	-0.01398800	C -4.92582100	-0.30293200	-0.22368000
C 3.39455700	-0.97449400	-0.50868100	C -3.24692800	-1.40941000	-1.54752100
C 3.39385900	-1.03314500	-1.90403800	C -5.91921200	-0.98102500	-0.91404500
C 4.22029700	-1.84519000	0.20196400	H -5.20140100	0.40831100	0.54763400
C 4.20837700	-1.93479900	-2.57317600	C -4.24476900	-2.08466900	-2.24277200
H 2.75100300	-0.36988700	-2.47235100	H -2.20212000	-1.58123600	-1.77812600
C 5.03073200	-2.75448900	-0.47031400	C -5.57908400	-1.87215700	-1.92756200
H 4.23898800	-1.82579600	1.28492100	H -6.96151500	-0.80893400	-0.66795000
C 5.02752700	-2.80073500	-1.85760900	H -3.97258700	-2.78080800	-3.02783000
H 4.19628600	-1.96717400	-3.65693200	H -6.35688600	-2.39738800	-2.47121100
H 5.66638900	-3.42645200	0.09596900	C -2.84490500	2.12216900	0.22304900
H 5.65983800	-3.50959300	-2.38044000	C -3.48409300	2.79042600	1.26491400
C 3.23368200	1.83239100	0.04847700	C -2.66747300	2.78712200	-0.99237200
C 2.55579900	3.02133300	-0.20972300	C -3.93620000	4.09571700	1.09761900
C 4.62725800	1.85309700	0.14679000	H -3.62660900	2.30694300	2.22382100
C 3.25643700	4.21340100	-0.35660600	C -3.12926800	4.08329500	-1.16338100
H 1.47547300	2.99983200	-0.29671300	H -2.15710300	2.28833900	-1.80879600
C 5.32505800	3.04326700	0.00098300	C -3.76398500	4.74371900	-0.11674600
H 5.17376200	0.93324600	0.32438000	H -4.42456800	4.60409700	1.92203000
C 4.64013700	4.22727000	-0.25057800	H -2.98675400	4.58257300	-2.11555500
H 2.71692100	5.13183500	-0.56047500	H -4.11866900	5.76006700	-0.24794800
H 6.40691000	3.04608200	0.07708400	C 3.63202400	-0.89193800	-0.27010400
H 5.18666900	5.15644700	-0.36889800	C 3.76672900	-1.05070300	-1.65276500
C -3.44934000	-1.10904200	-0.30160500	C 4.44742900	-1.65317200	0.56709700
C -4.26612200	-0.89394000	-1.41324300	C 4.69308500	-1.93699800	-2.18029000
C -3.39443900	-2.38479700	0.26506400	H 3.14124100	-0.47054200	-2.32300800
C -5.03500200	-1.92712800	-1.93265200	C 5.37086500	-2.55107300	0.03859900

H -4.30977300	0.08565000	-1.87489200	H 4.39404800	-1.53741600	1.64355100
C -4.17274900	-3.41162400	-0.25339900	C 5.49553400	-2.69610800	-1.33525600
H -2.72649200	-2.58828200	1.09593500	H 4.78257800	-2.04219900	-3.25578600
C -4.99589100	-3.18727000	-1.34987500	H 6.00044300	-3.12962800	0.70637800
H -5.66680600	-1.74403700	-2.79490200	H 6.21620300	-3.39348800	-1.74748500
H -4.12754200	-4.39540200	0.20087200	C 3.17232700	1.90367000	-0.15254200
H -5.59973300	-3.99292700	-1.75276400	C 2.43008000	2.95685700	-0.67955400
C -3.30436700	1.76058600	-0.05047100	C 4.54693900	2.07178200	0.03440300
C -4.63093100	1.89249600	0.37032400	C 3.04808400	4.15874100	-1.00789600
C -2.71156200	2.80608500	-0.75294700	H 1.36443300	2.82835500	-0.82539400
C -5.34390200	3.05114100	0.10014700	C 5.16187700	3.27262300	-0.28807500
H -5.11632900	1.08062100	0.90164300	H 5.14645500	1.25529100	0.42252100
C -3.42892200	3.96520700	-1.02963800	C 4.41208500	4.32055300	-0.81158500
H -1.68066200	2.70936800	-1.07044400	H 2.45707700	4.96892400	-1.42065800
C -4.74305500	4.09082900	-0.60232100	H 6.22968500	3.38893000	-0.13727700
H -6.37163200	3.14207200	0.43424600	H 4.89305100	5.25800600	-1.06874200
H -2.95598200	4.77071000	-1.58049000	H 0.07451700	1.65107800	0.20945400
H -5.30147700	4.99557600	-0.81602800	Ru 0.05208600	0.08118400	-0.01141700
O 0.62998700	-2.49686000	-2.04212300	H -0.17734000	-2.50059400	-2.28977400
O 1.40546700	-3.25412500	1.69854200	K 0.56411900	-2.69091900	-2.20355300
H -0.31232800	-4.02238700	0.82579100	O -1.94666200	-4.29501900	-0.84699200
H 1.84582700	-3.46975000	0.86760900			
H -0.09690100	-0.95981500	2.38439200			
HRu-O(H)CH₃_HCOO			KRu-OCH₃_CO₂		
P -2.25031000	0.35381700	0.22367700	P -2.13482782	0.57731016	0.18609407
P 2.40033100	0.09250000	0.28378100	P 2.44375676	0.37039686	0.22538385
C -2.42379400	-0.00723700	2.03833800	C -2.31206056	0.45778975	2.04326993
C 2.45978400	-0.39674800	2.07956500	C 2.52476478	-0.36658370	1.92424125
H -2.52565000	-1.08944300	2.16905900	H -2.67053017	-0.55572211	2.24925076
H 2.37261200	-1.48368100	2.13885100	H 2.40807749	-1.44762935	1.80450708
H -3.31052700	0.47736400	2.45033300	H -3.07539338	1.14244594	2.42024953
H 3.40399600	-0.10258300	2.54087000	H 3.47812784	-0.16726642	2.41969467
C -1.16332000	0.45809800	2.74525900	C -0.95180408	0.69017824	2.68423066
C 1.27498200	0.24094100	2.78382900	C 1.34354556	0.20586353	2.69215621
H -1.21041200	0.17769300	3.80523100	H -1.02012478	0.41428079	3.75428510
H 1.25297700	-0.07125400	3.83562200	H 1.34670092	-0.21276875	3.71678028
H -1.05209800	1.54414100	2.68822300	H -0.73246161	1.77498209	2.67194257
H 1.34698600	1.33160500	2.75879900	H 1.50972116	1.29342221	2.82207102
N 0.02259500	-0.15158400	2.11227400	N 0.08722225	-0.07106827	2.01657527
C 0.11874300	0.60624800	-1.88586900	O 0.16917830	1.33748142	-3.00847895
O 0.14833800	0.91709300	-2.99640500	C 0.15788079	0.91107261	-1.93245672
C -0.97146600	-3.56507400	2.71963700	C -3.93539456	-4.83989083	2.17979280
C -0.29173300	-2.90127400	-1.33610400	C 0.65120056	-2.27189258	-1.86085376
O 0.12137600	-2.10490500	-0.24130700	O 0.29739170	-1.88803225	-0.57834403
O -2.15463400	-3.24713300	2.58598100	O -2.86482663	-4.39364826	2.26802382
H -1.37117200	-2.83735500	-1.50142200	H 1.59022235	-1.81753812	-2.21420207
H -0.01914400	-3.94714500	-1.16604300	H 0.79608818	-3.36757528	-1.92782585
H 0.12971500	1.73435900	0.23331200	C -3.36081269	-0.68525459	-0.39220546
Ru 0.07558200	0.18291900	-0.07772900	C -4.73782891	-0.56471285	-0.18857585
C 3.45176100	-1.14329600	-0.58645400	C -2.85677023	-1.82833363	-1.01269000
C 4.26808900	-0.74759400	-1.64789000	C -5.59765555	-1.57540091	-0.59658988
C 3.36766700	-2.50052800	-0.26713300	H -5.14186958	0.32817538	0.27686237
C 5.00282600	-1.68580900	-2.36037200	C -3.72321704	-2.83965373	-1.42184408
H 4.33689100	0.29948200	-1.91914000	H -1.77726806	-1.91334323	-1.14308179
C 4.11068800	-3.43426300	-0.97727200	C -5.09140106	-2.71456135	-1.21667944
H 2.71067800	-2.84212400	0.52301300	H -6.66629498	-1.47138906	-0.44151659
C 4.93079700	-3.03125000	-2.02347200	H -3.32634195	-3.71777293	-1.92101006
H 5.63387400	-1.36181100	-3.18056700	H -5.76677454	-3.49668234	-1.54692680
H 4.04131900	-4.48348000	-0.71236700	C -2.95338831	2.15791695	-0.29387324
H 5.50768500	-3.76362300	-2.57714400	C -2.93675692	3.26431472	0.55480427
C 3.41446400	1.63023000	0.21813600	C -3.51344658	2.29293858	-1.56479646
C 2.86940900	2.80840100	-0.28511300	C -3.48911462	4.47309527	0.15066023
C 4.73515600	1.63318100	0.67626000	H -2.47642177	3.19335705	1.53378527
C 3.62825500	3.97322400	-0.32720300	C -4.06269083	3.50222523	-1.96924929
H 1.84367200	2.80648500	-0.63364200	H -3.52054222	1.44940679	-2.24609527
C 5.48939700	2.79642800	0.63908800	C -4.05663587	4.59489651	-1.11122732
H 5.18346600	0.71955500	1.05217300	H -3.47088398	5.32338785	0.82382541
C 4.93613800	3.96976000	0.13616800	H -4.49310544	3.59070697	-2.96072693
H 3.19323700	4.88411300	-0.72319900	H -4.48530479	5.53935434	-1.42764960
H 6.51230400	2.78754700	0.99898700	C 3.65608425	-0.58132824	-0.78977708
H 5.52721400	4.87837700	0.10518100	C 3.89035612	-0.14947715	-2.09804430
C -3.41885300	-0.78849200	-0.62614300	C 4.32569391	-1.71253448	-0.32816826
C -3.94260300	-0.41410700	-1.86678600	C 4.78110792	-0.82523830	-2.91773966
C -3.71848100	-2.05165600	-0.11164400	H 3.36937845	0.72248781	-2.47904113
C -4.77076500	-1.27616400	-2.57052800	C 5.21527751	-2.39403146	-1.15253460
H -3.71154600	0.56026300	-2.28310800	H 4.16352608	-2.07215977	0.68070002

C -4.55473500	-2.90751800	-0.82085000	C 5.44619433	-1.95252592	-2.44740822
H -3.29856800	-2.39407200	0.82934900	H 4.95044549	-0.47552524	-3.93015972
C -5.08311600	-2.52532800	-2.04631200	H 5.72932520	-3.27271952	-0.77765246
H -5.17275100	-0.97048600	-3.53023400	H 6.13942858	-2.48435123	-3.08970616
H -4.78603100	-3.88222900	-0.40578000	C 3.35444903	1.97242556	0.41345094
H -5.73376300	-3.19823900	-2.59397500	C 2.68965039	3.18475561	0.25285219
C -3.07865800	1.98968900	0.01077100	C 4.71696169	1.98246302	0.72316942
C -4.43053100	2.13429800	0.33600200	C 3.37129438	4.38733755	0.40794954
C -2.37503100	3.09341900	-0.46238600	H 1.63318091	3.17200994	0.00898257
C -5.05899500	3.36295200	0.20030700	C 5.39504944	3.18177561	0.88450716
H -4.99960800	1.27929700	0.68548700	H 5.25694752	1.04701928	0.82649584
C -3.00756200	4.32423100	-0.60396400	C 4.72201838	4.38897937	0.72622988
H -1.32712700	2.98211500	-0.71271500	H 2.84176248	5.32468877	0.27597579
C -4.34748100	4.46161100	-0.27134800	H 6.45250032	3.17564576	1.12622031
H -6.10770800	3.46312700	0.45753200	H 5.25309590	5.32707022	0.84654181
H -2.44904300	5.17567600	-0.97690800	H 0.09282561	1.89831376	0.28806480
H -4.84046000	5.42125700	-0.38113800	Ru 0.14156119	0.35780529	-0.15187431
H 0.22499200	-2.54802400	-2.22954300	H -0.11274098	-2.01362725	-2.62159180
O 0.04109600	-3.03127100	2.14896600	K -0.52639250	-2.71496675	1.59285049
H -0.72524400	-4.39844700	3.41291400	O -4.99404772	-5.29163696	2.10248194
H -0.03073800	-2.55849500	0.64455500			
H -0.05969700	-1.18056800	2.20272600			
TS-H₂/CH₃COOH			KRu-OCH₃		
P -2.27037000	-0.52187800	-0.15907900	P -2.26076200	0.41319500	0.28389500
P 2.35160000	-0.11569000	-0.16203900	P 2.29855100	-0.05272400	0.33334500
C -2.45329400	-0.03329400	-1.95153200	C -2.39924100	0.71374600	2.13179500
C 2.38236000	0.74214000	-1.81342900	C 2.30727700	-0.68406000	2.07436100
H -2.63940200	1.04316100	-1.97471500	H -2.90767300	-0.15284200	2.56600700
H 2.21901600	1.80599100	-1.62692000	H 2.05574100	-1.74689100	2.01665000
H -3.29011600	-0.55016200	-2.42431400	H -3.02463800	1.58539300	2.33485500
H 3.34423000	0.62663800	-2.31587600	H 3.28092600	-0.56953200	2.55730100
C -1.14762500	-0.32115400	-2.67386800	C -1.00021300	0.86713400	2.71284100
C 1.25051700	0.17259900	-2.65324700	C 1.20849000	0.07546500	2.80103100
H -1.20468600	0.06052300	-3.70184400	H -1.07061200	0.75835100	3.81199300
H 1.21194900	0.67760100	-3.62701700	H 1.17594700	-0.26022600	3.85478000
H -0.94745900	-1.39437800	-2.71896900	H -0.65299800	1.90224000	2.53857600
H 1.41237700	-0.89369100	-2.83561600	H 1.49855800	1.14362300	2.84533400
N -0.03704400	0.32801100	-1.95357300	N -0.08006900	-0.10455300	2.15217300
O 0.17561000	-1.37447700	2.97870000	O 0.06470900	0.70020800	-3.00257200
H -0.22795200	1.33928900	0.81027300	C 0.03513500	0.40636500	-1.88389000
H -0.27075600	1.33930200	-1.93520800	C 0.38519400	-2.77728100	-1.40201900
H 0.06635300	2.05459100	0.27630000	O 0.07212100	-2.20199200	-0.18448200
O 0.38667400	3.26764100	-0.17083100	H 1.33674400	-2.42301900	-1.82905600
C 0.12044300	-0.95034800	1.90854500	H 0.47808500	-3.87691900	-1.31511400
C -0.29642400	3.68711600	-1.15942400	C -3.48332100	-0.95837000	0.02712300
O -0.88969500	3.00041200	-2.00325300	C -4.73311000	-0.99846400	0.65454000
Ru 0.03919200	-0.30413000	0.16553100	C -3.10823700	-2.01636200	-0.80157400
H 0.18001000	-1.80892900	-0.40603100	C -5.58831600	-2.07452500	0.45665300
C 3.44512200	0.88163200	0.93768600	H -5.04790100	-0.17891400	1.29220400
C 3.22316000	2.25491200	1.06791300	C -3.96747000	-3.09420700	-1.00045800
C 4.43476100	0.27645300	1.71362400	H -2.12348900	-1.99869100	-1.25547400
C 4.00304200	3.00748500	1.93538300	C -5.20647400	-3.12451900	-0.37382600
H 2.42890900	2.74523500	0.51583500	H -6.55803800	-2.09055700	0.94264700
C 5.20378300	1.03362700	2.58857600	H -3.66591000	-3.90703100	-1.65232700
H 4.61014300	-0.78986400	1.63984400	H -5.87721600	-3.96211500	-0.53222800
C 4.99551200	2.40182900	2.69633800	C -3.10554200	1.86205700	-0.48876200
H 3.82136600	4.07293100	2.02208900	C -2.57049700	3.13219900	-0.26274500
H 5.96754300	0.54871300	3.18664600	C -4.22117000	1.73821000	-1.31434700
H 5.59759000	2.99285000	3.37767700	C -3.15673400	4.25483700	-0.82815500
C -3.44781200	0.56843800	0.74199700	H -1.67636300	3.23458900	0.34248300
C -4.52856400	1.19522500	0.12057100	C -4.79823800	2.86348100	-1.89306700
C -3.24382500	0.76878200	2.10752300	H -4.64248500	0.76103200	-1.51690200
C -5.39024000	2.00312200	0.85263900	C -4.27352400	4.12404600	-1.64631400
H -4.70471800	1.06505700	-0.94093000	H -2.73194000	5.23492800	-0.64015900
C -4.11044700	1.56822600	2.83935300	H -5.66139800	2.74988000	-2.53995800
H -2.39404400	0.30855100	2.59813700	H -4.72537300	5.00098300	-2.09661100
C -5.18459400	2.18862700	2.21327700	C 3.43796600	-1.15566000	-0.60774800
H -6.22184100	2.49048100	0.35568500	C 3.73080900	-0.81775600	-1.93161200
H -3.93724700	1.71713300	3.89921200	C 3.99637000	-2.31402600	-0.07176100
H -5.85564500	2.82135600	2.78341000	C 4.57115400	-1.61334200	-2.69516200
C 3.34935100	-1.64199600	-0.45837400	H 3.29529000	0.07421000	-2.36932400
C 4.61305700	-1.56553800	-1.05067800	C 4.83594900	-3.11443400	-0.83941400
C 2.85610600	-2.88802200	-0.08051000	H 3.78152900	-2.60355000	0.94954900
C 5.35859200	-2.71437700	-1.27283200	C 5.12632700	-2.76654200	-2.15085000
H 5.02851400	-0.60291000	-1.32885100	H 4.78729300	-1.33643700	-3.72111500
C 3.60771400	-4.03844400	-0.29353900	H 5.26320600	-4.01328500	-0.40776900

H 1.87191800	-2.94929800	0.36798800	H 5.78016000	-3.39159300	-2.74900200
C 4.85647400	-3.95460700	-0.89321800	C 3.32664400	1.48459500	0.42940800
H 6.33552100	-2.64138200	-1.73794500	C 2.75739800	2.72893200	0.17484600
H 3.21237400	-5.00194200	0.00864600	C 4.68204800	1.41449500	0.76133400
H 5.44043000	-4.85226900	-1.06416300	C 3.52560500	3.88545900	0.25901700
C -3.08371900	-2.18153000	-0.05757200	H 1.70615000	2.77584800	-0.08717500
C -4.46562700	-2.31058100	0.09707800	C 5.44655300	2.56839700	0.85230500
C -2.30766500	-3.33359700	-0.17435800	H 5.14830000	0.45074400	0.93767000
C -5.05719000	-3.56648800	0.11831200	C 4.86856600	3.80846700	0.60021000
H -5.08512600	-1.42947000	0.21540200	H 3.07071900	4.84856300	0.05396200
C -2.90192600	-4.58943200	-0.15739400	H 6.49745400	2.50054700	1.11237900
H -1.23205800	-3.23388700	-0.26683600	H 5.46744000	4.71045600	0.66549500
C -4.27740000	-4.70933200	-0.01149800	H 0.04072400	1.65456100	0.19863200
H -6.13099700	-3.65154200	0.24449200	Ru -0.00108300	0.06871600	-0.04943800
H -2.28460300	-5.47660100	-0.24732200	H -0.37610700	-2.59502300	-2.18922700
H -4.74065500	-5.68961800	0.00959400	K -1.09220300	-2.65651500	1.93506600
O -0.31932900	5.03888400	-1.24205200			
C -1.04145800	5.58586700	-2.33934200			
H -0.94004700	6.66640700	-2.24878100			
H -0.62802200	5.25064500	-3.29284100			
H -2.09563200	5.30497800	-2.29716600			
HRu-OCOOCH₃			KRu-OCH₃H		
P -2.32198900	0.22873600	0.31106900	P -2.32623802	0.27753379	0.32003003
P 2.30137100	0.28780800	0.32708400	P 2.27568905	0.07267218	0.08682911
C -2.45435400	-0.05820900	2.14168200	C -2.37196469	0.52175518	2.17689287
C 2.43176500	0.09174900	2.16923300	C 2.42499282	-0.45928997	1.85364463
H -2.41443300	-1.14243200	2.27647100	H -2.71748313	-0.41991798	2.61503871
H 2.46102700	-0.98685300	2.34553500	H 2.25153739	-1.54082266	1.84974994
H -3.39723100	0.29044200	2.56602400	H -3.09372530	1.29266438	2.45360078
H 3.34916700	0.51629200	2.58094200	H 3.41676297	-0.26252567	2.26621781
C -1.25524300	0.58973700	2.81515300	C -0.96494273	0.85313183	2.65757495
C 1.18741000	0.68115000	2.81468500	C 1.32494256	0.26628412	2.61287973
H -1.27233900	0.37841800	3.89266500	H -0.94511912	0.75673815	3.76036113
H 1.20656200	0.49559700	3.89704200	H 1.36609778	-0.03051803	3.67913186
H -1.28153600	1.67651400	2.68860300	H -0.75562010	1.91962067	2.45550484
H 1.14405200	1.76391600	2.66268300	H 1.54770721	1.35049154	2.60774385
N -0.01308300	0.07730800	2.21825600	N 0.01699671	-0.02027017	2.04335754
C 0.00803000	0.06615400	-1.85044700	Ru -0.06437543	0.02903663	-0.12860073
O 0.01794900	0.13993100	-3.00284400	C -0.14549581	0.14516735	-1.99760001
C 0.06606500	-3.00443400	1.20872200	O -0.19098421	0.27566819	-3.14437446
O 0.10046800	-2.61061800	2.38538100	O 0.94030746	-3.58720082	0.78234039
O 0.01095200	-2.31072100	0.15257500	H -0.04574260	1.61015673	-0.04124342
H 0.02698000	-0.95869400	2.39062500	K -0.53569315	-2.68401251	2.59979846
H -0.01643000	1.60283800	-0.01761800	C -3.51236192	-1.11298772	0.04396927
Ru -0.00463200	0.02232900	0.00408800	C -4.65662993	-1.29689609	0.82590517
C 3.57624300	-0.85694900	-0.34346600	C -3.24433888	-2.01951589	-0.98151627
C 4.93785400	-0.55186000	-0.30962100	C -5.50914042	-2.36767077	0.58901292
C 3.15509800	-2.07061100	-0.88433300	H -4.89529494	-0.59433696	1.61726502
C 5.86750000	-1.45755000	-0.80099800	C -4.10268463	-3.08584791	-1.22455091
H 5.27385500	0.39957800	0.08783300	H -2.35174030	-1.88919270	-1.58299464
C 4.09028300	-2.97375900	-1.37598700	C -5.23335407	-3.26382019	-0.43817511
H 2.09437600	-2.29862500	-0.90896300	H -6.39451223	-2.49812192	1.20197984
C 5.44447100	-2.66975200	-1.33501800	H -3.88080519	-3.78166007	-2.02588881
H 6.92398400	-1.21417100	-0.77341800	H -5.90034679	-4.09830264	-0.62462477
H 3.75824000	-3.91607600	-1.79744400	C 3.44699871	-1.00141612	-0.84997768
H 6.17190800	-3.37454400	-1.72257700	C 3.48786625	-2.37701531	-0.60327076
C 3.00290000	1.94692800	-0.06592100	C 4.25439271	-0.46289071	-1.85421877
C 2.90609600	2.39335000	-1.38611100	C 4.35113477	-3.18365034	-1.33537218
C 3.61085400	2.77095000	0.87871100	H 2.82633141	-2.84040819	0.13119546
C 3.41917200	3.62777000	-1.75309200	C 5.10659435	-1.27876100	-2.58635691
H 2.42216200	1.77261100	-2.13188400	H 4.22495931	0.59953627	-2.06571235
C 4.11413700	4.01537000	0.51256000	C 5.16342377	-2.64140911	-2.32301477
H 3.69693300	2.45765700	1.91216700	H 4.37464151	-4.24914682	-1.13365376
C 4.02294200	4.44481700	-0.80319000	H 5.72794641	-0.84563220	-3.36275108
H 3.33975300	3.95716900	-2.78312300	H 5.83178223	-3.27875543	-2.89200239
H 4.57984100	4.64694800	1.26115100	C 3.12685319	1.71297375	0.03547266
H 4.41724400	5.41358600	-1.08893100	C 4.40256294	1.86969485	0.58330109
C -3.55765400	-0.91612600	-0.43187100	C 2.51551919	2.80707151	-0.57109897
C -4.91854400	-0.61496000	-0.49733300	C 5.04318456	3.09960043	0.54066593
C -3.09683600	-2.13194900	-0.93661200	H 4.90759851	1.02373605	1.03678195
C -5.80926600	-1.52657300	-1.04772700	C 3.16159103	4.03754982	-0.62373699
H -5.28539200	0.33763900	-0.13257800	H 1.52445367	2.68831356	-0.99312460
C -3.99304700	-3.04091800	-1.48554900	C 4.42295219	4.18750970	-0.06459550
H -2.03568800	-2.35574200	-0.89090700	H 6.03101376	3.20835061	0.97509117
C -5.34790100	-2.74105800	-1.54187900	H 2.67459025	4.87995322	-1.10273638
H -6.86519800	-1.28431800	-1.09771800	H 4.92506796	5.14814209	-0.10128794

H -3.62941900	-3.98406600	-1.87823700	C -3.24019573	1.73867256	-0.34999478
H -6.04451100	-3.45000800	-1.97573000	C -4.47968843	1.63502278	-0.97881949
C -3.05613300	1.89442800	0.01216700	C -2.65056757	2.99871746	-0.22514960
C -3.92666000	2.51993000	0.90410500	C -5.12118937	2.76954070	-1.46397122
C -2.73438500	2.54468700	-1.18067000	H -4.94917841	0.66668925	-1.10097094
C -4.46395200	3.76865800	0.61079100	C -3.29948871	4.13102841	-0.69505853
H -4.19433500	2.04487800	1.84039400	H -1.66848409	3.08648455	0.22637006
C -3.28188900	3.78355300	-1.47972300	C -4.53736705	4.01979691	-1.31830652
H -2.04131900	2.08217100	-1.87331200	H -6.08099796	2.67093585	-1.95928204
C -4.14608200	4.40104000	-0.58287900	H -2.82989329	5.10264897	-0.58696305
H -5.13343600	4.24483200	1.31874400	H -5.03916044	4.90376288	-1.69602178
H -3.02372700	4.27312900	-2.41212200	C 0.34831735	-3.08347740	-0.28476936
H -4.56646100	5.37377100	-0.81269400	H -0.01745385	-1.93692875	-0.14846024
O 0.09195100	-4.36289600	1.06007100	H 0.96470924	-2.99061632	-1.19884411
C 0.04571200	-4.88534300	-0.25702100	H -0.61728171	-3.55151584	-0.58475058
H 0.88702200	-4.53880800	-0.86089700			
H 0.09636800	-5.96850600	-0.14765600			
H -0.88145000	-4.61380400	-0.76669500			
HRu-OCOOCH₃'			TS-CH₃OH-H⁻_κ		
P -2.28113100	0.31919000	0.25871900	P -2.30396600	0.10854800	0.35285700
P 2.35005200	0.13806900	0.22976200	P 2.27157800	0.42575700	0.29827900
C -2.42029400	-0.01284100	2.08536200	C -2.37390500	-0.32160400	2.15830200
C 2.46089700	-0.40524600	2.00693100	C 2.44684900	0.60314300	2.15746900
H -2.52407000	-1.09772600	2.16987600	H -2.24363700	-1.40451300	2.24798600
H 2.37256500	-1.49479800	1.99071900	H 2.82030500	-0.34641100	2.55455900
H -3.31050300	0.43483300	2.53128500	H -3.33134600	-0.04749100	2.60776900
H 3.41659400	-0.16018700	2.47270500	H 3.18530400	1.36757600	2.40691000
C -1.14672700	0.43925200	2.78361200	C -1.20778400	0.40336800	2.81004500
C 1.29662000	0.20537900	2.77056200	C 1.07666300	0.92031800	2.73650500
H -1.17969500	0.15627000	3.84477700	H -1.20511200	0.17317200	3.89189400
H 1.30910100	-0.13245200	3.81565200	H 1.13689300	0.82960900	3.83751000
H -1.03663600	1.52555000	2.73236100	H -1.39553200	1.49268000	2.73886900
H 1.37024900	1.29648300	2.77426700	H 0.84384900	1.98145000	2.53156400
N 0.02456400	-0.16638800	2.12804200	N 0.05701300	0.03933600	2.19764400
C 0.00975200	0.35800100	-1.90668600	H -0.04516100	-1.51846300	-0.26645100
O -0.00020900	0.58039300	-3.03850700	C -0.42459800	-3.32435200	-0.86466800
C -0.18067800	-3.26322500	0.52254700	Ru -0.01433700	0.22301700	-0.01886600
C -0.48039200	-4.08642000	2.76423800	C -0.05083600	0.50121600	-1.86127800
O -0.30219100	-2.96279900	1.91067800	O -0.07574400	0.70312700	-3.00157700
O -0.02063700	-2.22576500	-0.17496000	O -0.07363000	-4.12516500	0.00106900
H -0.55805400	-3.69432100	3.77971900	H -0.05790900	1.83889800	0.30092500
H 0.36636400	-4.77181900	2.69429400	K 0.90682600	-2.55979300	1.87305100
H -0.07474400	-1.19108600	2.18333800	C -3.37149900	-1.13700900	-0.49592900
H 0.06270500	1.64483300	0.09824700	C -4.14132300	-2.07959400	0.18468600
Ru 0.02121700	0.07270100	-0.07402700	C -3.40025900	-1.12849100	-1.89316000
C 3.50997700	-0.96885300	-0.67446400	C -4.92212000	-2.99456800	-0.51477800
C 4.86469100	-0.67676700	-0.83853600	H -4.14029000	-2.10947900	1.26796500
C 2.98866600	-2.14926400	-1.20848900	C -4.18602200	-2.03506600	-2.58958700
C 5.69260300	-1.56542300	-1.51177300	H -2.79913300	-0.40993500	-2.43916000
H 5.27620000	0.24956000	-0.45550100	C -4.94803400	-2.97384000	-1.90201900
C 3.82489900	-3.03639900	-1.87462700	H -5.51225200	-3.72385800	0.02992500
H 1.93013400	-2.36792000	-1.10061900	H -4.19783300	-2.01285100	-3.67376100
C 5.17491900	-2.74763000	-2.02741500	H -5.55687300	-3.68648200	-2.44657900
H 6.74345300	-1.32915500	-1.63923300	C 3.40634800	-0.99272200	-0.08523000
H 3.41129100	-3.95229500	-2.28143300	C 4.53617300	-1.30133200	0.67897200
H 5.82321700	-3.43914600	-2.55452100	C 3.10394400	-1.79653300	-1.18544500
C 3.16880300	1.79001100	0.18303100	C 5.33707800	-2.39070000	0.35368800
C 2.75760500	2.70294000	-0.78896000	H 4.80598500	-0.68400900	1.52917100
C 4.19311200	2.15566100	1.05769700	C 3.91091500	-2.87689000	-1.51920200
C 3.36473600	3.94679500	-0.89166700	H 2.21678900	-1.57243300	-1.76726700
H 1.94665900	2.44089700	-1.45757200	C 5.02690700	-3.17919900	-0.74806100
C 4.79162300	3.40659100	0.96365300	H 6.20970600	-2.61703200	0.95708400
H 4.53774200	1.46912900	1.82226200	H 3.66227300	-3.48919500	-2.37894100
C 4.38083700	4.30334100	-0.01354300	H 5.65216000	-4.02760300	-1.00323600
H 3.03474400	4.64309700	-1.65449200	C 3.20663400	1.87091400	-0.38990400
H 5.58189700	3.67774000	1.65508600	C 4.54398600	1.80007200	-0.78235500
H 4.84882200	5.27862700	-0.08845200	C 2.53371000	3.08845400	-0.50278000
C -3.54158000	-0.78982300	-0.49073000	C 5.19869600	2.92871600	-1.26055200
C -4.90751100	-0.50980100	-0.41131000	H 5.08167500	0.86102600	-0.72728300
C -3.10928700	-1.95208600	-1.12852400	C 3.19268000	4.21725800	-0.97111300
C -5.83096400	-1.39110200	-0.95502100	H 1.48263300	3.13015100	-0.23589600
H -5.25108500	0.40320800	0.06297500	C 4.52705600	4.14125800	-1.35160900
C -4.04009900	-2.83241700	-1.66872600	H 6.23660100	2.85598300	-1.56881200
H -2.04753300	-2.16867200	-1.19006400	H 2.65546800	5.15631700	-1.05232800
C -5.39745900	-2.55394300	-1.58369700	H 5.03880800	5.02056500	-1.72700800
H -6.89056200	-1.16808800	-0.89311100	C -3.38184200	1.61287700	0.22526200

H -3.69582600 -3.73661700 -2.15761600	C -4.76771600 1.52638300 0.37756100
H -6.12077000 -3.24078100 -2.00958500	C -2.80355000 2.85788400 -0.00478400
C -2.99314700 1.99598800 -0.01622900	C -5.55591700 2.66651300 0.31318300
C -3.43757400 2.82312100 1.01258300	H -5.23949700 0.56218000 0.53423700
C -3.04975600 2.46596200 -1.33079600	C -3.59402900 3.99987400 -0.07213100
C -3.93440000 4.09266500 0.73484300	H -1.72706600 2.91301400 -0.12838100
H -3.40128100 2.49193400 2.04350900	C -4.96952100 3.90760300 0.08798300
C -3.55367300 3.72726400 -1.60776700	H -6.63106900 2.58604700 0.43209400
H -2.69880400 1.84089100 -2.14466800	H -3.13085400 4.96364500 -0.25517500
C -3.99607900 4.54644600 -0.57442300	H -5.58656400 4.79810300 0.03251900
H -4.27501500 4.72500100 1.54742900	H 0.22322100 -3.08309000 -1.72200700
H -3.59521800 4.07475400 -2.63404100	H -1.46075000 -2.97157000 -0.94745400
H -4.38519700 5.53500600 -0.79097700	
H -1.38858000 -4.63441500 2.50683900	
O -0.23924000 -4.43063100 0.18655800	
HRu-O(CH₃)COO	KRu-H CH₂O
P -2.34590226 0.33427598 0.33083880	P -2.36533651 0.42883757 0.33892942
P 2.30394319 0.23421717 0.39996912	P 2.19430503 0.18539129 0.25669211
C -2.49839760 0.05995642 2.16639372	C -2.49599363 0.61522820 2.20152559
C 2.38978654 -0.04536989 2.23902012	C 2.33730516 -0.20592011 2.06887401
H -2.53135438 -1.01697688 2.34099255	H -2.83578087 -0.34061593 2.61368625
H 2.37086868 -1.12262775 2.41371453	H 2.23222553 -1.28941497 2.18465977
H -3.41804706 0.49868756 2.55662086	H -3.24442470 1.36518000 2.46513456
H 3.31549848 0.35342539 2.65679829	H 3.30435547 0.09427112 2.47975372
C -1.27101947 0.64604170 2.84195254	C -1.11799997 0.96792468 2.74019045
C 1.16928010 0.59354098 2.87815709	C 1.17812128 0.50575834 2.74865935
H -1.29375808 0.41549502 3.91530795	H -1.14767609 0.88741554 3.84375198
H 1.15020528 0.36298247 3.95158272	H 1.21770917 0.29130907 3.83334902
H -1.25265419 1.73497137 2.73606362	H -0.91328905 2.03115121 2.51559274
H 1.20096272 1.68217848 2.77240294	H 1.33937960 1.59784118 2.65382336
N -0.05280846 0.09625912 2.23092249	N -0.09574108 0.10356822 2.18274952
O 0.03921164 0.79821742 -2.92225279	H -0.05700295 -1.41239298 -0.26529360
C 0.01668363 0.53403148 -1.79994003	C 1.16475514 -4.25460912 -0.50281174
C -0.10340937 -3.13109603 0.98365913	Ru -0.09378954 0.28722281 -0.04355523
C -0.05752932 -2.64867587 -1.43960439	C -0.11770902 0.53861512 -1.88722345
O -0.06594146 -2.13900847 -0.10568345	O -0.13008594 0.71363363 -3.03348424
O -0.10673062 -2.56647653 2.09547463	O 0.62752639 -4.55619899 0.53825812
H 0.85011661 -2.31078789 -1.94374759	H -0.07006386 1.92770942 0.27451493
H -0.07630129 -0.95317501 2.30160809	K -0.80518078 -2.54004654 1.84651743
H -0.08157913 -3.73653528 -1.40344098	C -3.45548652 -1.04206783 0.00684752
C -3.44831849 -0.92689498 -0.43307079	C -4.57712019 -1.35928154 0.77905231
C -3.43022775 -2.24652526 0.02399891	C -3.11471539 -1.88500174 -1.05257578
C -4.22455436 -0.60773641 -1.54906346	C -5.33532951 -2.49185555 0.50110804
C -4.19439779 -3.21867067 -0.60704321	H -4.87116332 -0.71687533 1.60223102
H -2.80993095 -2.53457589 0.86401284	C -3.88070881 -3.00835281 -1.34099197
C -4.98495022 -1.58371014 -2.17927788	H -2.22446954 -1.65948500 -1.63017840
H -4.24162992 0.40768043 -1.92744017	C -4.99046514 -3.31690979 -0.56271642
C -4.97510980 -2.89029603 -1.70789419	H -6.20167396 -2.72372721 1.11150934
H -4.16472623 -4.23811550 -0.24001800	H -3.60684250 -3.64704769 -2.17389702
H -5.58509626 -1.32014105 -3.04318792	H -5.58444429 -4.19704022 -0.78359990
H -5.56822081 -3.65209453 -2.20135001	C 3.21487037 -1.10166897 -0.59641500
C -3.24569627 1.91723920 0.04565488	C 4.04140894 -2.00042512 0.07848440
C -2.60780128 2.98696389 -0.57650367	C 3.13856430 -1.18089689 -1.98943127
C -4.57448173 2.06259962 0.45458648	C 4.77609773 -2.95452301 -0.62068558
C -3.28301458 4.18495030 -0.78428337	H 4.12536746 -1.96089484 1.15847212
H -1.57624265 2.87696267 -0.88789305	C 3.87763020 -2.12525497 -2.68775321
C -5.24547057 3.25933479 0.25197228	H 2.48972308 -0.50093125 -2.53006227
H -5.09453568 1.23311031 0.92197725	C 4.69815386 -3.01801896 -2.00517288
C -4.59969911 4.32365591 -0.36910519	H 5.41618175 -3.64292880 -0.07895370
H -2.77598273 5.01005201 -1.27200341	H 3.81009459 -2.16622168 -3.76951020
H -6.27561035 3.36119172 0.57497986	H 5.27553258 -3.75608722 -2.55115858
H -5.12566223 5.25827130 -0.52955424	C 3.28479816 1.67248352 0.04864313
C 3.37316847 -1.07366886 -0.33183657	C 4.67519202 1.58436597 0.14828699
C 4.19482577 -0.78892232 -1.42438073	C 2.70071407 2.91246363 -0.19301941
C 3.28514396 -2.39095139 0.12388399	C 5.46359079 2.71935811 0.02072192
C 4.93088581 -1.79706396 -2.03245349	H 5.15063041 0.62365981 0.31457542
H 4.26650074 0.22454251 -1.80158883	C 3.49125521 4.04899136 -0.32344964
C 4.02518010 -3.39542746 -0.48490120	H 1.61915928 2.96537485 -0.27147069
H 2.62868137 -2.65147695 0.94519353	C 4.87203260 3.95576053 -0.21597235
C 4.85123710 -3.10165903 -1.56218612	H 6.54253179 2.63836184 0.09918269
H 5.56689553 -1.56011819 -2.87822888	H 3.02401105 5.00922321 -0.51401397
H 3.94112744 -4.41237261 -0.11936417	H 5.48879662 4.84189367 -0.32075498
H 5.42540499 -3.88854911 -2.03836986	C -3.37670161 1.82814219 -0.33794368
C 3.27910812 1.77681942 0.14277013	C -4.72631640 1.71343937 -0.67234855
C 2.70645910 2.87275522 -0.49702007	C -2.74319969 3.06035110 -0.50357312
C 4.60027145 1.86500311 0.59080737	C -5.43164585 2.81373457 -1.14516768

C 3.43845991	4.04046157	-0.68379842	H -5.23473592	0.76171851	-0.57844501
H 1.68074460	2.80713516	-0.83874701	C -3.45227631	4.16053765	-0.96663504
C 5.32784884	3.03165001	0.40905537	H -1.68371793	3.13262397	-0.27964583
H 5.07011371	1.01409206	1.07264359	C -4.79854323	4.04133259	-1.28868546
C 4.74709055	4.12251387	-0.22989314	H -6.47876093	2.70694787	-1.40771027
H 2.98201939	4.88642166	-1.18555841	H -2.94538873	5.11157106	-1.08982351
H 6.35144701	3.08919118	0.76236901	H -5.34967914	4.89863120	-1.65971389
H 5.31730747	5.03354467	-0.37399689	H 1.76736734	-4.99248972	-1.06240272
H 0.01341807	1.79595343	0.22693812	H 1.06929284	-3.23848000	-0.92428433
Ru -0.01728071	0.23039791	0.03636976			
H -0.93465459	-2.27225539	-1.96980010			
O -0.12455159	-4.29840116	0.65294211			
TS-CO₂			KRu-OH_CH₃O		
P -2.28508900	0.23964300	0.28165700	P -2.22473443	-0.08464112	0.11340702
P 2.35223100	0.25251100	0.24130400	P 2.29161871	0.68890333	0.42239264
C -2.39265900	-0.15687100	2.09670800	C -2.35663540	-0.77152466	1.82965803
C 2.49093500	-0.05543700	2.07688200	C 2.32325664	0.65867386	2.29139733
H -2.34036600	-1.24367200	2.19447200	H -2.11211687	-1.83557279	1.76423836
H 2.52570200	-1.14038000	2.20222500	H 2.79260460	-0.28861361	2.57491308
H -3.32828500	0.19235200	2.53714200	H -3.36083221	-0.66423529	2.24697374
H 3.40949400	0.35480200	2.49866800	H 2.95734269	1.45208989	2.69345233
C -1.18848900	0.46122900	2.78739400	C -1.31624714	-0.03744534	2.66150122
C 1.26672100	0.51285500	2.77262800	C 0.89489469	0.73577635	2.81132418
H -1.19211900	0.20330000	3.85467200	H -1.33889906	-0.43729416	3.69215678
H 1.28954300	0.26224600	3.84162700	H 0.90442266	0.48993276	3.89003860
H -1.20885200	1.55108400	2.70595000	H -1.62845653	1.02174415	2.75159277
H 1.24075700	1.60175800	2.68262100	H 0.54916977	1.78565524	2.75179477
N 0.04616700	-0.02064500	2.14696700	N 0.01294217	-0.15907098	2.08498389
O 0.01109300	0.51829500	-3.03535500	Ru 0.08501846	0.18748114	-0.07907237
C 0.02189400	0.34487700	-1.89330100	C 0.16459926	0.65485843	-1.88395119
C 0.13146100	-3.71913200	1.92174300	O 0.20638277	1.01886567	-2.98305858
C -0.38733300	-2.76289400	-1.02338200	H -0.08040637	1.72852510	0.27504474
O -0.09110100	-2.10673700	0.17336800	K 1.07623336	-2.70907682	1.78261602
O 0.22837600	-2.94542500	2.79644600	C -3.17647658	-1.24616873	-0.95906455
H 0.39942400	-2.62868700	-1.78595900	C -4.01707813	-2.23627050	-0.45036531
H 0.06524000	-1.03932700	2.22642400	C -3.05435670	-1.11354347	-2.34365340
H -0.49318000	-3.84569900	-0.86297200	C -4.72394498	-3.07332841	-1.30728348
C -3.47372300	-0.90154900	-0.54055300	H -4.12428101	-2.36713190	0.62028587
C -4.11241200	-1.95558700	0.10893600	C -3.76323975	-1.94581994	-3.19839903
C -3.70782000	-0.70750200	-1.90478300	H -2.39907659	-0.35401071	-2.75563124
C -4.97425300	-2.79453200	-0.58943400	C -4.59932302	-2.92973954	-2.68242116
H -3.94578300	-2.13873100	1.16293900	H -5.37157879	-3.84005985	-0.89598501
C -4.57066600	-1.54156900	-2.59824300	H -3.65809164	-1.82855341	-4.27138853
H -3.20996300	0.10073400	-2.42998200	H -5.15015523	-3.58250173	-3.35052903
C -5.20630000	-2.58984100	-1.94166300	C 3.70213847	-0.42994263	-0.00633773
H -5.46177400	-3.61269600	-0.07088300	C 5.02551978	-0.14029925	0.33679027
H -4.74028800	-1.37834600	-3.65663100	C 3.40908382	-1.63463130	-0.64640920
H -5.87616400	-3.24678600	-2.48503500	C 6.03842373	-1.04377789	0.04727103
C 3.18811300	1.84969000	0.15492100	H 5.26784906	0.80021959	0.82020386
C -2.50556600	3.02221200	-0.15710500	C 4.42891075	-2.53884949	-0.93371284
C -4.56460300	1.90720100	0.39064100	H 2.37222549	-1.85875873	-0.89845185
C -3.18403600	4.23468400	-0.22393100	C 5.74148838	-2.24543424	-0.58916829
H -1.43907800	2.97192800	-0.34580800	H 7.06345697	-0.80913868	0.31352160
C -5.23930300	3.11739900	0.32848100	H 4.19490335	-3.47034774	-1.43843041
H -5.11668900	0.99923200	0.60933800	H 6.53560517	-2.94742130	-0.81947466
C -4.54898400	4.28529300	0.02045700	C 2.94244973	2.34466464	-0.05930711
H -2.64144700	5.14040200	-0.47184400	C 3.62458667	2.50571165	-1.26559891
H -6.30758100	3.14909000	0.51285700	C 2.67596140	3.47066876	0.71940527
H -5.07786700	5.23054900	-0.03355300	C 4.04727935	3.76370551	-1.67421207
C 3.49362400	-0.99795100	-0.48241900	H 3.82884322	1.64465654	-1.89204365
C 4.73663100	-0.69890000	-1.03738700	C 3.10232726	4.72795951	0.31163289
C 3.03827100	-2.31920200	-0.48050000	H 2.11918052	3.37432440	1.64471745
C 5.52735300	-1.71508500	-1.56177100	C 3.79166748	4.87793129	-0.88500417
H 5.09015300	0.32437900	-1.07187300	H 4.57603949	3.87230411	-2.61477536
C 3.83770000	-3.32968100	-0.99609400	H 2.89067712	5.59333114	0.93024247
H 2.03941800	-2.52855200	-0.09973000	H 4.12221412	5.85999833	-1.20447073
C 5.08434400	-3.03081200	-1.53456900	C -3.34820828	1.38669551	0.13167170
H 6.49197500	-1.47403500	-1.99513400	C -4.72452501	1.23550113	0.31689764
H 3.47681000	-4.35227000	-0.99156000	C -2.82643347	2.66643018	-0.03783035
H 5.70410100	-3.82101300	-1.94417900	C -5.55822719	2.34386846	0.34735334
C 3.21172700	1.86267300	-0.02702400	H -5.15417320	0.24545338	0.42575452
C 2.68655900	2.76474000	-0.95104800	C -3.66307236	3.77705048	-0.01218700
C 4.38802800	2.19797800	0.64757700	H -1.75892732	2.78085783	-0.18815191
C 3.32488900	3.97329000	-1.19971400	C -5.02800712	3.61909940	0.18227651
H 1.76383500	2.52038700	-1.46249300	H -6.62507903	2.21244126	0.49243441
C 5.01987800	3.41132800	0.40788500	H -3.24335927	4.76776609	-0.14864596

H 4.82806400	1.50972300	1.36064600	H -5.68028339	4.48543850	0.20081592
C 4.48975900	4.30108800	-0.51850600	C -0.71984295	-4.23824310	-0.28715912
H 2.90531800	4.66261500	-1.92403100	O -0.41451076	-4.67416260	0.81371244
H 5.92943500	3.65970600	0.94373100	H -1.69025682	-3.75986211	-0.47234449
H 4.98380400	5.24779100	-0.70732000	O 0.20327594	-2.14126730	-0.51648986
H 0.08922600	1.73621300	0.07211000	H 0.05400313	-2.09418079	-1.46283182
Ru 0.03210900	0.13703700	-0.05349400	H -0.12219002	-4.47673607	-1.18161552
H -1.32721300	-2.41503900	-1.47794700			
O 0.06390300	-4.67118600	1.26242900			
HRu_OCH₃_CO₂			TS-CH₂O-OH⁻_K		
P -2.29501066	0.26920935	0.19555578	P -2.39364000	0.16727500	0.31133700
P 2.33897970	0.26234304	0.17307346	P 2.22350500	0.32081600	0.29795600
C -2.41306559	-0.16083773	2.00439409	C -2.53327200	-0.07396900	2.15182700
C 2.46415676	-0.16074226	1.98577919	C 2.37668800	0.11416800	2.13969500
H -2.38176825	-1.25145705	2.07055940	H -2.57692400	-1.15503700	2.32860500
H 2.46048546	-1.25199919	2.03519519	H 2.52061100	-0.95289000	2.33499000
H -3.34330651	0.19481320	2.45127004	H -3.44436300	0.37886400	2.55076500
H 3.39577861	0.19085515	2.43127480	H 3.24711000	0.64329100	2.53729300
C -1.20256302	0.41536724	2.72120653	C -1.27660600	0.52518400	2.77378200
C 1.25717870	0.39834027	2.71973547	C 1.07736000	0.61981600	2.75616300
H -1.20574267	0.09901949	3.77288393	H -1.28898700	0.31730900	3.86233500
H 1.26568245	0.06416987	3.76583774	H 1.11006800	0.43257200	3.84757300
H -1.22061368	1.50838937	2.70144507	H -1.33331300	1.62886800	2.68961500
H 1.27570312	1.49161672	2.71796512	H 1.04796300	1.72374400	2.65272500
N 0.02387994	-0.03719878	2.05218907	N -0.08329600	-0.01840000	2.15617700
O 0.03130870	0.41310970	-3.13495559	Ru -0.08165100	0.09321000	-0.02555200
C 0.02823671	0.29902975	-1.98461535	C -0.04344300	0.35385200	-1.87471000
C 0.49274745	-3.96421519	2.73924313	O -0.00667000	0.57398700	-3.01257500
C -0.42343094	-2.92926277	-0.62027747	H -0.08479300	1.65938500	0.19188600
O 0.04151668	-2.02307808	0.32847905	K 0.16638900	-2.73472900	2.29238900
O 0.27748653	-3.08039242	3.46169644	C -3.46878400	-1.13291300	-0.43315500
H 0.18927359	-2.93690307	-1.53931611	C -4.45062500	-1.81989300	0.28251200
H 0.00818560	-1.06455362	1.97491298	C -3.29589500	-1.42269200	-1.78687800
H -0.40903364	-3.95881716	-0.22654263	C -5.23838400	-2.77899200	-0.34178400
C -3.49031175	-0.86116172	-0.63552020	H -4.60176800	-1.61620900	1.33828800
C -4.32842601	-1.74009417	0.04877625	C -4.08913200	-2.37640600	-2.41338900
C -3.54471597	-0.82429152	-2.03095314	H -2.54123300	-0.89244300	-2.35737700
C -5.20446097	-2.56519196	-0.64807525	C -5.06025100	-3.05805000	-1.69080000
H -4.30550187	-1.79556364	1.13045870	H -5.99940500	-3.30553000	0.22635500
C -4.42403827	-1.64220607	-2.72397585	H -3.94008200	-2.58797200	-3.46613600
H -2.88880600	-0.15781130	-2.58033765	H -5.67888200	-3.80591900	-2.17872100
C -5.25552676	-2.51731650	-2.03393093	C 3.51126100	-0.77624900	-0.44092100
H -5.84705122	-3.24767046	-0.10262682	C 4.46652700	-1.45517200	0.31839500
H -4.45216469	-1.60373904	-3.80717994	C 3.54377400	-0.89556100	-1.83320700
H -5.93726446	-3.16280989	-2.57634086	C 5.43509900	-2.23574900	-0.30108500
C -3.19917754	1.88324041	0.08917649	H 4.45941200	-1.39056000	1.40060000
C -2.50964476	3.06587953	-0.16393864	C 4.51543300	-1.67227100	-2.45197500
C -4.58209079	1.93365974	0.28418184	H 2.80712900	-0.37645900	-2.43854100
C -3.18672476	4.27983856	-0.21065941	C 5.46334800	-2.34491200	-1.68685000
H -1.43844070	3.02102158	-0.32559446	H 6.16792000	-2.76441800	0.30211200
C -5.25610866	3.14534260	0.24100038	H 4.52649000	-1.75606400	-3.53341100
H -5.14101732	1.01993612	0.45523708	H 6.21900700	-2.95666000	-2.16856300
C -4.55861007	4.32294352	-0.00660110	C 2.99301400	1.98143400	-0.00944500
H -2.63743115	5.19301031	-0.41236614	C 4.33390000	2.20697800	0.32076500
H -6.32978688	3.17010706	0.39232179	C 2.26242600	3.01643000	-0.58649700
H -5.08663426	5.26942024	-0.04592073	C 4.91849600	3.44512100	0.09994000
C 3.47305791	-0.94794547	-0.62566269	H 4.93217800	1.40448000	0.73881400
C 4.65614337	-0.59526567	-1.27232879	C 2.85070400	4.25560700	-0.81564500
C 3.07008693	-2.28642041	-0.60514217	H 1.22698000	2.84533800	-0.85233800
C 5.44140035	-1.57425906	-1.87092961	C 4.17627300	4.47387000	-0.47031300
H 4.96766156	0.44109657	-1.31884473	H 5.95780600	3.60325100	0.36604000
C 3.86446837	-3.25875040	-1.19575819	H 2.26857000	5.05030700	-1.27139700
H 2.11446019	-2.53586082	-0.14675540	H 4.63543700	5.44094700	-0.64979200
C 5.05262013	-2.90627777	-1.82678394	C -3.37066800	1.70787700	-0.01193000
H 6.35938152	-1.29097445	-2.37438899	C -4.76635800	1.69449100	-0.04708600
H 3.54584731	-4.29516345	-1.17468274	C -2.70216300	2.91891900	-0.18366300
H 5.66813856	-3.66761781	-2.29351956	C -5.47697700	2.87068800	-0.24227400
C 3.21509864	1.87744684	0.01080171	H -5.30628300	0.75920900	0.06069900
C 2.68012307	2.86139699	-0.81868855	C -3.41451500	4.09617500	-0.37633000
C 4.41518155	2.13603318	0.67759543	H -1.61851000	2.92256400	-0.17513900
C 3.33127780	4.07826651	-0.98070223	C -4.80260700	4.07617800	-0.40482900
H 1.73946372	2.67089039	-1.32125307	H -6.56107800	2.84608100	-0.27434800
C 5.06006918	3.35612687	0.52449139	H -2.88279000	5.03183100	-0.51088300
H 4.86277500	1.38074521	1.31422202	H -5.36101400	4.99338700	-0.56058600
C 4.51905750	4.32976078	-0.30699670	C 1.01229400	-3.53917900	-0.55089600
H 2.90427203	4.83317259	-1.63163500	O 1.65364100	-3.83193200	0.48604400

H 5.98831088	3.54486288	1.05259909	H 0.28413400	-4.27831300	-0.97150000
H 5.02340733	5.28213378	-0.42815094	O -0.27304800	-2.30354700	-0.18199200
H 0.05146949	1.76900446	-0.07749122	H -0.76353200	-2.35178300	-1.01418500
Ru 0.02128255	0.16546177	-0.13769472	H 1.50559200	-2.94388800	-1.35580300
H -1.45772079	-2.72913370	-0.94276547			
O 0.71715266	-4.87566104	2.06349735			
TS-CO₂'			KRu-OCH₂OH_{OH}		
P -2.30489600	0.24754500	0.23591200	P -2.37653138	0.09545523	0.42497098
P 2.33681900	0.26673000	0.28102600	P 2.22334701	0.30782751	0.11435823
C -2.43206900	-0.27060700	2.01577500	C -2.40468155	-0.02798788	2.28194056
C 2.46017500	-0.00868000	2.11609000	C 2.48565568	-0.16973324	1.88574588
H -2.39221700	-1.36286900	2.03737300	H -2.50988274	-1.08702214	2.53614087
H 2.57343800	-1.08174400	2.27520800	H 2.53008294	-1.26206674	1.89880356
H -3.36844800	0.05710600	2.47214700	H -3.25332769	0.50906306	2.71087896
H 3.33238800	0.49833800	2.53187800	H 3.42730134	0.21270752	2.28406104
C -1.21914400	0.29287200	2.73803000	C -1.06810294	0.49744506	2.78923854
C 1.16558500	0.46879200	2.75343800	C 1.28248614	0.35005672	2.65926467
H -1.22800500	-0.05738000	3.78213100	H -1.01536767	0.31657989	3.87992020
H 1.16721500	0.18166700	3.81696600	H 1.38594287	0.05430284	3.72136797
H -1.28912500	1.39056900	2.77919000	H -1.04882236	1.59767232	2.67421922
H 1.11242800	1.56678400	2.72483500	H 1.32181425	1.45645283	2.66290599
N 0.01351100	-0.12201200	2.07191600	N 0.03518439	-0.14846076	2.10257564
C 0.05016000	0.60024400	-1.90802900	Ru -0.10499825	0.00226758	-0.06560465
O 0.06826100	0.90054800	-3.02275400	C -0.21486728	0.24793355	-1.91565797
C -0.21511000	-3.24795000	0.09557400	O -0.28435787	0.47408489	-3.04910909
C 0.11022000	-3.36932900	3.17464500	H -0.12067219	1.56140133	0.14601676
O 0.39581200	-2.59792100	2.04275100	K 0.04555225	-2.91213837	2.39350015
O -0.09186700	-2.20929000	-0.44453200	C -3.52173673	-1.23107346	-0.16805995
H 0.94374900	-3.36898500	3.89223300	C -4.37672574	-1.95307801	0.66491718
H -0.06943300	-4.40878700	2.87765400	C -3.50793458	-1.52951006	-1.53362087
H 0.17552700	-1.47029200	2.12812200	C -5.19678647	-2.94998043	0.14672295
H 0.05765600	1.74720200	0.21481700	H -4.41920779	-1.73794941	1.72660069
Ru 0.02166800	0.21434600	-0.07736900	C -4.33068458	-2.52003163	-2.05149858
C 3.41184900	-1.02948200	-0.46831700	H -2.85020738	-0.97743185	-2.19716331
C 4.25486800	-0.73974000	-1.54166800	C -5.17489830	-3.23695014	-1.21120815
C 3.30362200	-2.35110900	-0.02747400	H -5.85713419	-3.50058277	0.80813895
C 4.99476700	-1.74742500	-2.14712700	H -4.30776847	-2.73585245	-3.11392291
H 4.34049700	0.27696400	-1.90686400	H -5.81360922	-4.01477627	-1.61438515
C 4.04986600	-3.35358200	-0.63215600	C 3.54741185	-0.56252321	-0.83695786
H 2.62356900	-2.60630900	0.77927700	C 3.77453445	-1.92577321	-0.63194258
C 4.89888800	-3.05544100	-1.69096000	C 4.29204587	0.11434076	-1.80564805
H 5.64796600	-1.50658100	-2.97866500	C 4.75682708	-2.58160736	-1.36435276
H 3.95967000	-4.37418700	-0.27685800	H 3.16523320	-2.50572938	0.06387561
H 5.47805500	-3.84122700	-2.16310800	C 5.26355609	-0.55200817	-2.54098307
C 3.27482300	1.82530900	-0.01697500	H 4.12036542	1.16832364	-1.98789488
C 2.68300800	2.88515100	-0.69908300	C 5.50586754	-1.90085658	-2.31560008
C 4.58809200	1.96229100	0.44141800	H 4.92175007	-3.63991593	-1.19342225
C 3.38810200	4.06382400	-0.91777200	H 5.83286868	-0.01186851	-3.28977601
H 1.66394200	2.78458300	-1.05160000	H 6.26795506	-2.42059381	-2.88639503
C 5.28943500	3.13958400	0.22706000	C 2.82603911	2.05836697	0.04390095
H 5.07220000	1.14094200	0.95900600	C 4.03492882	2.41919338	0.64376261
C 4.68941600	4.19379800	-0.45397000	C 2.10720411	3.02954782	-0.64873189
H 2.91603400	4.88067400	-1.45230900	C 4.49934156	3.72501936	0.57337153
H 6.30723200	3.23435600	0.58920100	H 4.63047911	1.67519440	1.16087082
H 5.23855000	5.11353700	-0.62283800	C 2.57756797	4.33541898	-0.73155640
C -3.39611500	-0.91161000	-0.69004500	H 1.16966970	2.75690005	-1.11683020
C -4.28074200	-1.78876500	-0.06257800	C 3.77042298	4.68774115	-0.11575513
C -3.32205700	-0.90911500	-2.08459500	H 5.43594162	3.99001433	1.05179529
C -5.07811700	-2.64376600	-0.81507900	H 2.00670131	5.07820072	-1.27802001
H -4.35471800	-1.81670300	1.01810300	H 4.13446610	5.70766915	-0.17413457
C -4.12420900	-1.75689300	-2.83401000	C -3.36105236	1.61796665	0.05899020
H -2.62831300	-0.24523900	-2.58785200	C -4.74230769	1.64798225	0.26511711
C -5.00305300	-2.62822600	-2.20081900	C -2.72256198	2.76446608	-0.40647477
H -5.75713400	-3.32452800	-0.31363900	C -5.46613479	2.80601259	0.02033414
H -4.05421100	-1.74456000	-3.91592000	H -5.26177158	0.75893558	0.60565533
H -5.62306900	-3.29737400	-2.78683600	C -3.44866483	3.92421789	-0.65289563
C -3.24685100	1.83485300	0.15749600	H -1.65247776	2.73692246	-0.57344592
C -2.56747300	3.04808400	0.07436700	C -4.81971961	3.94817464	-0.43958183
C -4.64251400	1.84172900	0.21336000	H -6.53856935	2.81536736	0.18196120
C -3.26847000	4.24844100	0.05959900	H -2.93893503	4.80915422	-1.01770243
H -1.48546300	3.04356700	0.01496900	H -5.38635587	4.85189639	-0.63528106
C -5.34117000	3.04037800	0.19791100	C 0.87843667	-3.44984403	-0.55082069
H -5.18960900	0.90639100	0.25433400	O 1.55165254	-3.72266695	0.51162619
C -4.65497400	4.24735400	0.12201100	H 0.27080770	-4.27478392	-0.98596954
H -2.72709400	5.18568500	-0.00758500	O -0.29456337	-2.39566463	-0.19948298
H -6.42488900	3.03208900	0.23812400	H -0.97788731	-2.50214266	-0.87001378

H -5.20203700 5.18353200 0.10560300	H 1.41043968 -2.91168700 -1.35864246
H -0.78726400 -3.01978000 3.70750300	
O -0.43229700 -4.37766300 0.27896400	
Ru-CH₃OH	KRu-OCH₂OH_H
H -0.07955900 1.33615000 -0.29197200	P -2.34045074 0.01761331 0.19039977
Ru -0.02705800 -0.18888200 0.04912700	P 2.24067711 0.38573382 0.32398548
C -0.05650400 -0.51216700 -1.79335600	C -2.47761333 -0.54332452 1.94512030
O -0.08277300 -0.67754200 -2.93777600	C 2.32043856 0.49412652 2.18291148
N -0.00996300 0.02024600 2.18887100	H -2.30219618 -1.62492524 1.92252326
P -2.34109800 -0.04131400 0.37188200	H 2.68725968 -0.48385899 2.51056728
P 2.27480300 0.12917500 0.33413800	H -3.46063163 -0.33756521 2.37426210
C 2.43567800 0.14129200 2.19125700	H 3.05629059 1.22649451 2.52246151
C -2.44737200 -0.19893300 2.21825700	C -1.35953590 0.15929941 2.70042184
H 3.30305200 0.71847600 2.51829500	C 0.92371253 0.76212579 2.72422174
H -3.38599200 0.18386200 2.62248100	H -1.37480840 -0.17732136 3.75424760
H 2.57194600 -0.89885100 2.50047900	H 0.93796628 0.60810157 3.82033528
H -2.40610100 -1.27188600 2.42250000	H -1.57933133 1.24325194 2.74001785
C -1.23311400 0.49593900 2.81462200	H 0.68181114 1.83234385 2.58515231
C 1.14017300 0.68162600 2.77682300	N -0.05956575 -0.10087345 2.09415928
H -1.34822700 1.58928300 2.70463600	H -0.23473622 -2.11049560 -0.05033787
H 1.10057200 1.77577700 2.63233200	C -0.61853521 -3.24481839 0.04454310
H -1.21023300 0.30162100 3.90005800	Ru -0.00880139 -0.07334195 -0.06402834
H 1.15877400 0.52533100 3.86861400	C 0.04694006 -0.06162940 -1.93805821
H 0.02270100 -1.65686400 1.90784100	O 0.07984627 -0.00918816 -3.09213527
C 3.53028500 -1.10212500 -0.22453100	O -1.30519928 -3.46896370 1.10598313
C -3.50670900 -1.31983200 -0.26804800	H -0.02210095 1.50038407 -0.06268459
C 5.37910300 -2.98440100 -1.15128100	K 0.68809055 -2.80530226 2.58760120
C -5.16112400 -3.36176700 -1.21158100	C -3.54465350 -0.98138940 -0.78737822
C 3.36554600 -1.70356500 -1.47307100	C -3.78331269 -2.32463340 -0.48808448
C -3.12099500 -2.65728900 -0.14059100	C -4.18189252 -0.40539788 -1.88936674
C 4.63367100 -1.45687600 0.55441800	C -4.66674094 -3.06254191 -1.26788481
C -4.71780500 -1.01599900 -0.88714000	H -3.25287632 -2.81118776 0.32630880
C 5.54971700 -2.39546300 0.09532200	C -5.05620887 -1.15106985 -2.66746390
C -5.53946500 -2.03434200 -1.35744000	H -4.00274528 0.63421066 -2.13902131
C 4.28714100 -2.63375800 -1.93556400	C -5.30688807 -2.48155207 -2.35453939
C -3.94986300 -3.66977700 -0.60208100	H -4.84617596 -4.10381670 -1.02268743
H 2.50742900 -1.44832100 -2.08368600	H -5.54377474 -0.68909218 -3.51906172
H -2.16346900 -2.89238900 0.31357500	H -5.99322574 -3.06363946 -2.95999198
H 4.78690400 -1.00059400 1.52561300	C 3.68155155 -0.71477748 -0.04447882
H -5.02300500 0.01589800 -1.01117400	C 5.00147984 -0.26055534 -0.01576267
H 6.39972000 -2.66424000 0.71300800	C 3.43256566 -2.06340965 -0.28993047
H -6.47795500 -1.78535500 -1.84080100	C 6.05164786 -1.14480778 -0.22339986
H 4.14539600 -3.09132100 -2.90835300	H 5.21026900 0.78917110 0.15827523
H -3.64332300 -4.70470500 -0.49505300	C 4.48557408 -2.94936678 -0.49107642
H 6.09428500 -3.71665100 -1.50934000	H 2.40745495 -2.41975768 -0.32490444
H -5.80372900 -4.15449400 -1.57872900	C 5.79614494 -2.49118086 -0.46043455
C 3.02567900 1.74167800 -0.17944200	H 7.07334781 -0.78117750 -0.20393613
C -3.16649500 1.55403900 -0.04591000	H 4.27873168 -3.99679619 -0.68263956
C 4.12007900 4.22993000 -0.84307100	C 6.61803034 -3.17902052 -0.62625670
C -4.40333800 3.95453400 -0.77272600	C 2.83398094 2.00934323 -0.31899458
C 2.26417000 2.90641100 -0.06622100	C 3.11508843 2.11588445 -1.68325755
C -4.26941300 2.02910700 0.66602400	C 2.93861127 3.14649422 0.47919842
C 4.33910400 1.83945100 -0.63909800	C 3.51168459 3.32720384 -2.22984101
C -2.69398700 2.29615300 -1.12820300	H 3.02172469 1.24647609 -2.32508386
C 4.88026800 3.07557900 -0.97219300	C 3.33042241 4.36237472 -0.07084199
C -3.31179400 3.48570000 -1.49245700	H 2.70337324 3.10010921 1.53574250
C 2.81070700 4.14149300 -0.38642300	C 3.62164389 4.45538012 -1.42433601
C -4.88042600 3.22433800 0.30868700	H 3.72843446 3.39185256 -3.29036781
H 1.23202800 2.83809700 0.25733900	H 3.40577996 5.23843841 0.56408173
H -4.66537300 1.46667700 1.50366300	H 3.92762878 5.40337855 -1.85256872
H 4.94525400 0.94838100 -0.74751100	C -3.15433358 1.67941152 0.17810569
H -1.82838200 1.94252000 -1.67556400	C -4.44893604 1.82211717 0.68488240
H 5.89994200 3.13269500 -1.33736400	C -2.50998905 2.79672673 -0.34507342
H -2.93327700 4.05008200 -2.33751300	C -5.07555782 3.05952755 0.68394760
H 2.20545700 5.03635500 -0.29090900	H -4.97831322 0.95869551 1.07330862
H -5.73188300 3.58390600 0.87605600	C -3.14093595 4.03646362 -0.35392891
H 4.54331500 5.19378300 -1.10357700	H -1.50637026 2.69019541 -0.73979908
H -4.88082900 4.88720700 -1.05233400	C -4.42147504 4.17130411 0.16314388
O -0.10617400 -2.37935300 1.20502600	H -6.07865162 3.15617093 1.08498091
C 0.87104300 -3.39805100 1.27132300	H -2.62637749 4.89726254 -0.76681069
H 0.75507300 -4.03969500 0.39650700	H -4.91231553 5.13844561 0.15926466
H 1.89135200 -2.99929100 1.26088300	H -1.11911670 -3.41281503 -0.93035631
H 0.74066400 -4.01264000 2.17018900	O 0.65062345 -4.01236196 0.04042878
	H 0.91846569 -4.14145305 -0.87530593
TS-CH₃OH-H⁺	TS-HOCH₂OH-H⁻_K

H -0.06455100	1.36584000	-0.36162600	P -2.24306497	0.11936997	0.18111988
Ru -0.03046000	-0.15848900	0.03362700	P 2.33573420	0.32819987	0.35304206
C -0.06851700	-0.52231100	-1.79340400	C -2.39729982	-0.51839593	1.91387273
O -0.09960100	-0.72047000	-2.93187300	C 2.38786292	0.57572225	2.21165682
N -0.00846000	0.07867300	2.19619300	H -2.23777099	-1.60007817	1.87542528
P -2.34475900	-0.01415600	0.35985200	H 2.82688908	-0.33009129	2.64127989
P 2.27984400	0.11696000	0.31466100	H -3.38106070	-0.31986970	2.34632357
C 2.44018900	0.11485600	2.17476700	H 3.05366290	1.40086240	2.47280220
C -2.44527900	-0.13361300	2.21245600	C -1.28147230	0.15301566	2.69889886
H 3.32670400	0.66078100	2.50344100	C 0.97456248	0.79808428	2.73036706
H -3.38277900	0.26123600	2.60681300	H -1.31824427	-0.19879901	3.74617665
H 2.54430000	-0.93061700	2.47743200	H 0.98469561	0.66199077	3.82814006
H -2.40495600	-1.20203300	2.43645900	H -1.49946050	1.23799767	2.74673217
C -1.23556200	0.56970900	2.80995600	H 0.69586764	1.85547553	2.56505199
C 1.17135000	0.69860600	2.77791400	N 0.02251651	-0.10352694	2.10690002
H -1.32986000	1.65743600	2.67191500	H -0.10090376	-1.75041749	-0.33510210
H 1.15280500	1.78773500	2.62373200	C -0.44654801	-3.06154684	-0.78025869
H -1.21875900	0.39277100	3.89722400	Ru 0.06943028	0.08698827	-0.08438619
H 1.19280300	0.54196300	3.86832600	C 0.14668048	0.35412375	-1.93044711
H 0.00778200	-1.23358300	2.01809200	O 0.18969012	0.55437119	-0.306992639
C 3.51244400	-1.13560100	-0.24454400	O -0.27092549	-3.88449666	0.14740949
C -3.47872600	-1.33667800	-0.24132500	H 0.12308779	1.68150876	0.17005998
C 5.32639500	-3.04567300	-1.18188400	K 0.99680076	-2.71156737	1.98179009
C -5.07005700	-3.44556600	-1.14001800	C -3.36864930	-0.91617470	-0.84879433
C 3.34537300	-1.71516700	-1.50285100	C -4.12659516	-1.96693846	-0.33413286
C -3.08602600	-2.66016300	-0.01962500	C -3.44233375	-0.63770024	-2.21648156
C 4.60002900	-1.52638300	0.53909800	C -4.94627028	-2.72025045	-1.16807008
C -4.66152900	-1.08049500	-0.93219500	H -4.08021742	-2.21289601	0.71982794
C 5.49880300	-2.47867100	0.07449000	C -4.26427460	-1.38589672	-3.04560601
C -5.45222100	-2.13303600	-1.37998500	H -2.85260275	0.17073628	-2.63524844
C 4.24981600	-2.65930300	-1.97043600	C -5.01834918	-2.43137145	-2.52315497
C -3.88512500	-3.70537800	-0.45991300	H -5.52580232	-3.53793543	-0.75391104
H 2.49862000	-1.43332500	-2.11742900	H -4.31124959	-1.15661383	-4.10445299
H -2.14449000	-2.85332200	0.48740500	H -5.65561261	-3.02098844	-3.17267357
H 4.75440600	-1.08994400	1.51915100	C 3.57076750	-1.03583301	0.12817005
H -4.96884200	-0.06070800	-1.12966200	C 4.84144336	-0.98248660	0.71273346
H 6.33611100	-2.77622900	0.69626500	C 3.20748844	-2.16673650	-0.60096047
H -6.36931400	-1.92240800	-1.91939000	C 5.72423770	-2.04389338	0.57517936
H 4.10568200	-3.10061900	-2.95030500	H 5.14739931	-0.10308413	1.26983957
H -3.57525500	-4.72923200	-0.28050700	C 4.09516835	-3.23210369	-0.73693394
H 6.02763800	-3.78935800	-1.54385800	H 2.22619494	-2.23019631	-1.06253909
H -5.68882900	-4.26491100	-1.48932400	C 5.35082503	-3.17325746	-0.14922187
C 3.06933700	1.71806500	-0.17842400	H 6.70717427	-1.99060639	1.03091278
C -3.20891600	1.55342900	-0.08209200	H 3.79145301	-4.10377798	-1.30568489
C 4.22601400	4.18827100	-0.80181300	H 6.04271461	-4.00159178	-0.25662387
C -4.50308300	3.91655100	-0.82875300	C 3.22516358	1.78511189	-0.34799341
C 2.31630100	2.89155600	-0.11529200	C 4.20796403	1.64788299	-1.32638209
C -4.36810300	1.96769400	0.57760300	C 2.85352086	3.06688677	0.06157207
C 4.40655200	1.79727600	-0.56890500	C 4.81677021	2.77078488	-1.87540627
C -2.70993500	2.33624100	-1.12230300	H 4.50186209	0.66211050	-1.66707463
C 4.97889600	3.02439500	-0.88145300	C 3.47146718	4.18585303	-0.47740455
C -3.35585100	3.50819700	-1.49623100	H 2.06320482	3.19109777	0.79389880
C 2.89325200	4.11809500	-0.41575700	C 4.45612020	4.04102066	-1.44836046
C -5.00805800	3.14415100	0.21040200	H 5.57637509	2.64828262	-2.63968506
H 1.26715700	2.83452800	0.15092400	H 3.17661896	5.17514169	-0.14474045
H -4.78616600	1.36944200	1.37930900	H 4.93351405	4.91608281	-1.87515113
H 5.00669000	0.89834100	-0.63990500	C -3.17722268	1.71684111	0.21416483
H -1.80192400	2.02781900	-1.62669900	C -4.55524364	1.72673352	0.44358862
H 6.01704700	3.06732100	-1.19247300	C -2.51524937	2.92456359	0.01547037
H -2.95628300	4.10557500	-2.30827200	C -5.25250266	2.92496988	0.48981154
H 2.29391600	5.02033800	-0.36076600	H -5.09155756	0.79274129	0.57468115
H -5.90402500	3.45624500	0.73575300	C -3.21569980	4.12546495	0.05560920
H 4.67367500	5.14512900	-1.04683400	H -1.44658130	2.90919736	-0.16917979
H -5.00322900	4.83488900	-1.11611600	C -4.58262606	4.12855722	0.29514571
O -0.14096100	-2.16006900	1.29256000	H -6.32203377	2.92026079	0.67004848
C 0.77129100	-3.22221500	1.33552800	H -2.68909536	5.05998840	-0.10471654
H 0.65860200	-3.85351900	0.44734100	H -5.12877556	5.06510377	0.32551776
H 1.81892300	-2.88884900	1.35893600	H -1.46905487	-2.79764719	-1.09340138
H 0.59974300	-3.85471000	2.21846800	O 0.38835081	-3.21444800	-1.90392980
			H 0.11718780	-2.56251555	-2.56176041
TS-CH₃OH-H⁺			KRu₂HCOOH		
P -2.26041895	0.13743589	0.31255370	P -2.21938788	0.21618279	0.38452217
P 2.34778516	-0.02223452	0.28459461	P 2.31439632	0.73592023	0.27668433
C -2.40193136	0.12613671	2.17739332	C -2.25780151	-0.30707635	2.16821915
C 2.47328714	-0.31747937	2.12272762	C 2.52237313	0.82212356	2.14008497
H -2.52303745	-0.91481954	2.48789458	H -2.09694553	-1.38964400	2.19620536

H 2.38725217 -1.39688705 2.27413753	H 2.96088178 -0.12397136 2.47400345
H -3.26720453 0.69751910 2.51819956	H -3.21544904 -0.08492364 2.64569687
H 3.43180845 -0.00020736 2.53614063	H 3.22144478 1.61437423 2.41514031
C -1.11819570 0.67582618 2.77504759	C -1.10374322 0.41488182 2.84597655
C 1.31924618 0.40377153 2.79753014	C 1.15123419 1.03005731 2.76485999
H -1.14086244 0.56786151 3.86797180	H -1.07810067 0.11779483 3.91120896
H 1.33023220 0.21277726 3.87899091	H 1.24306218 0.87553895 3.85697623
H -0.99856497 1.73544329 2.53916093	H -1.32932318 1.49987402 2.84394399
H 1.40051722 1.48280769 2.64415715	H 0.86045545 2.08840770 2.62921675
N 0.04145110 -0.03982149 2.21416022	N 0.16239879 0.13476156 2.19447188
O 0.03282481 -0.04018010 -3.00873153	H 0.09915349 -1.22018047 -0.32773338
H -0.04537482 -1.75175927 0.08167939	C -1.05555517 -4.02940292 -0.40668939
H -0.07275113 -1.03543846 2.43108338	Ru 0.04045853 0.46209671 -0.00985581
C -0.67295597 -3.22080243 1.36974925	C -0.03042875 0.83599657 -1.83179650
O -0.64376315 -2.83904492 2.53120331	O -0.07743301 1.08802336 -2.96277728
H 0.14024019 1.62036088 0.10533362	O -0.27429682 -4.44640371 0.41281300
C 0.03519520 -0.03798796 -1.85226362	H -0.05830692 2.07361669 0.41835338
H -1.58945152 -3.18027892 0.76338032	K 1.11741220 -2.42084117 1.66186521
Ru 0.03876486 -0.03242923 -0.00052296	C -3.21147293 -1.07923429 -0.49866142
C 3.44650682 -1.31650867 -0.45161849	C -4.09963462 -1.93853704 0.15141694
C 2.92062453 -2.60264674 -0.58263440	C -3.04602620 -1.21000448 -1.87966810
C 4.74614188 -1.07132533 -0.89377313	C -4.81283532 -2.89868166 -0.55923662
C 3.69086943 -3.63084717 -1.10662682	H -4.24061406 -1.86757558 1.22393197
H 1.88818332 -2.77423384 -0.29722361	C -3.76117152 -2.16416504 -2.59354392
C 5.51198298 -2.09984716 -1.43068986	H -2.34547854 -0.56464493 -2.39696736
H 5.16538824 -0.07497382 -0.83329558	C -4.64778132 -3.01413331 -1.93491949
C 4.99087799 -3.38252881 -1.53091105	H -5.49757757 -3.55775390 -0.03691220
C 3.26846148 -4.62535996 -1.20054255	H -3.62957791 -2.24122525 -3.66753040
H 6.51910775 -1.89281524 -1.77589871	H -5.21439276 -3.75212573 -2.49256531
H 5.59001324 -4.18291422 -1.95098610	C 3.48510964 -0.63284237 -0.18750951
C 3.29057709 1.54534925 0.02030507	C 4.68647395 -0.87263298 0.48710762
C 4.46749116 1.84325165 0.71086209	C 3.12975100 -1.47727560 -1.24044978
C 2.81101261 2.46067061 -0.91538062	C 5.50771103 -1.93313282 0.12067678
C 5.14708134 3.03140119 0.47272344	H 4.99237492 -0.22455999 1.30155715
H 4.86947731 1.14787699 1.43937587	C 3.95672753 -2.53000377 -1.61616302
C 3.49823960 3.64166484 -1.16485018	H 2.18142291 -1.31170974 -1.74110260
H 1.87950816 2.24939081 -1.42683999	C 5.14520037 -2.76261011 -0.93440081
C 4.66507227 3.93162542 -0.46936462	H 6.43535715 -2.10656892 0.65563765
H 6.05537488 3.25181062 1.02291046	H 3.66802936 -3.17335278 -2.44027737
H 3.11370618 4.34161405 -1.89845471	H 5.78704542 -3.58781761 -1.22285343
H 5.19611024 4.85832267 -0.65728757	C 3.19052849 2.23996001 -0.35999011
C -3.18696103 1.66236740 -0.19481947	C 4.48466521 2.21696418 -0.87954284
C -4.58042177 1.68498730 -0.28668902	C 2.50600306 3.45541818 -0.30848574
C -2.47399896 2.82893555 -0.46429538	C 5.08799931 3.38877708 -1.32183184
C -5.24488500 2.85651090 -0.62392946	H 5.02806309 1.28319033 -0.95415641
H -5.15436478 0.78318668 -0.10868111	C 3.11526198 4.62594785 -0.73853274
C -3.14090469 4.00143336 -0.79892946	H 1.48240688 3.46174576 0.05175160
H -1.39017472 2.79725564 -0.41696713	C 4.40834851 4.59689840 -1.24696960
C -4.52681627 4.01893936 -0.87880984	H 6.09194905 3.35292382 -1.73107899
H -6.32713662 2.85830348 -0.69594866	H 2.57035549 5.56260630 -0.69068939
H -2.57209487 4.90099249 -1.00808591	H 4.87987471 5.51012281 -1.59332085
H -5.04703708 4.93207468 -1.14682105	C -3.39405496 1.65156454 0.30915528
C -3.40716861 -1.20525393 -0.22483942	C -4.76927494 1.49754267 0.49813850
C -4.44511186 -1.69018768 0.57247024	C -2.88313904 2.92423596 0.07022447
C -3.22002213 -1.75516053 -1.49407814	C -5.61356600 2.59838607 0.46167422
C -5.27860656 -2.70218806 0.10963138	H -5.19287489 0.51327446 0.66485907
H -4.61013828 -1.28779950 1.56539110	C -3.72977004 4.02651204 0.03011337
C -4.05996437 -2.75701391 -1.96019222	H -1.81265961 3.03023506 -0.07547713
H -2.40272759 -1.40629560 -2.11442151	C -5.09448157 3.86706620 0.22654568
C -5.09029093 -3.23469360 -1.15872624	H -6.67985538 2.46550917 0.61033536
H -6.07616781 -3.07353070 0.74384236	H -3.31875763 5.01227944 -0.15931240
H -3.90191225 -3.17235079 -2.94931763	H -5.75512945 4.72666884 0.19294034
H -5.74082535 -4.02350050 -1.51989552	H -1.06199503 -2.97588549 -0.73610077
H 0.16874032 -3.77824161 0.92624767	O -1.96568189 -4.81696137 -0.97183129
	H -2.56123606 -4.27869714 -1.51930076
HRu-OH-CH₂O	KRu-HCOOH'
P -2.31421145 0.08492597 0.24560886	P -2.29742200 0.40899700 0.35431000
P 2.32097699 0.12346399 0.22485759	P 2.29783900 0.38175000 0.36004900
C -2.42844039 -0.28822397 2.07096819	C -2.45575000 0.39130500 2.21336200
C 2.45658236 -0.25458282 2.04587494	C 2.44707600 0.30891000 2.21675500
H -2.41946740 -1.37686925 2.16502044	H -2.58366600 -0.65041700 2.52584000
H 2.46671046 -1.34301273 2.14424363	H 2.52957400 -0.74529900 2.50129700
H -3.35776889 0.07626190 2.51168913	H -3.33362400 0.94904100 2.54666000
C 3.38287337 0.13195178 2.47499403	H 3.34405100 0.82257000 2.56974800
C -1.21654926 0.29975418 2.77311704	C -1.16560400 0.95735000 2.78304200
C 1.24179793 0.31481662 2.75962313	C 1.17619800 0.91127600 2.79234700

H -1.22094731	0.01171743	3.83122625	H -1.20516200	0.87926100	3.88603200
H 1.25902094	0.02925551	3.81906495	H 1.21121600	0.81975200	3.89440900
H -1.22634865	1.39148677	2.71741343	H -1.12881600	2.04060100	2.55897800
H 1.23599038	1.40638885	2.70384766	H 1.17704600	1.99786700	2.58090700
O -0.01513483	0.23970281	-3.07807215	N -0.00585600	0.26259600	2.25530100
C -0.00987743	0.12967044	-1.92760560	O 0.00494700	0.74532700	-2.96287800
H -0.03698704	1.59420975	-0.00346062	H -0.00175400	-1.40561700	-0.07015200
C 3.48031600	-1.07323729	-0.56402526	H 0.02088200	-2.41148400	-0.96691600
C 3.27681421	-2.43838891	-0.33921198	O 0.03427400	-3.25490100	-1.56761200
C 4.49316143	-0.67178355	-1.43505509	C 0.00294700	0.55386200	-1.82061600
C 4.09409713	-3.37782729	-0.95220379	K -0.07355700	-2.48907300	2.19242600
H 2.44374792	-2.75495542	0.28067330	H 0.00427600	1.95222800	0.28138800
C 5.30566542	-1.61707671	-2.05042785	Ru -0.00010900	0.32560600	0.02976800
H 4.65443027	0.38042091	-1.63621887	C 0.02330100	-4.34924500	-0.86232000
C 5.11489836	-2.96969519	-1.80360275	C 3.38704500	-0.98729900	-0.24037300
H 3.93002624	-4.43390539	-0.76469419	C 3.22310900	-1.42920300	-1.55428500
H 6.08959331	-1.29064615	-2.72500139	C 4.36121000	-1.59511900	0.55361800
H 5.75258994	-3.70506904	-2.28306838	C 4.02015700	-2.44405000	-2.06467900
C -3.44595048	-1.14644002	-0.52467335	H 2.45845100	-0.98060900	-2.17808000
C -2.98993192	-2.46812330	-0.55780177	C 5.15271800	-2.62006500	0.04601500
C -4.67508518	-0.82976961	-1.10016269	H 4.51703200	-1.26882700	1.57584800
C -3.77343776	-3.45916352	-1.12926145	C 4.98545500	-3.04511100	-1.26503800
H -2.00312815	-2.68649525	-0.14928896	H 3.87889900	-2.77275700	-3.08832800
C -5.45186707	-1.82779656	-1.67915598	H 5.90461000	-3.08219100	0.67685100
H -5.02779871	0.19414251	-1.10773769	H 5.60386600	-3.84243800	-1.66238500
C -5.00629387	-3.14233342	-1.69008552	C -3.39023900	-0.97552400	-0.20468600
H -3.41790441	-4.48447356	-1.14953323	C -4.39364800	-1.52980800	0.59266500
H -6.40461930	-1.57067224	-2.12886015	C -3.19675800	-1.48764300	-1.48868900
H -5.61451747	-3.91849373	-2.14342410	C -5.18401000	-2.57113100	0.11763100
C 3.18834048	1.74305599	0.04938859	H -4.57365100	-1.14785500	1.59147800
C 2.58201921	2.77822041	-0.65866090	C -3.99294700	-2.51862600	-1.96755400
C 4.45258881	1.95383544	0.60702406	H -2.40891100	-1.08115500	-2.11241900
C 3.22508986	4.00146565	-0.80703357	C -4.98680700	-3.06614500	-1.16451200
H 1.59382998	2.61831972	-1.07448928	H -5.95869900	-2.99084600	0.75053200
C 5.09088515	3.17715381	0.46547606	H -3.82879800	-2.90168900	-2.96865000
H 4.95199163	1.15516395	1.14468942	H -5.60437400	-3.87619400	-1.53663400
C 4.47721693	4.20467962	-0.24370373	C 3.29819700	1.87326500	-0.10525700
H 2.74207291	4.79865478	-1.36087011	C 4.69467500	1.84994000	-0.11492500
H 6.06938707	3.33018724	0.90644438	C 2.64137300	3.05842200	-0.42745500
H 4.97615025	5.16043430	-0.35495984	C 5.41660300	2.99379400	-0.42683400
C -3.19417163	1.69409014	0.04308916	H 5.22674100	0.93203100	0.10745700
C -2.68575985	2.63462107	-0.85116834	C 3.36514600	4.20336500	-0.73973100
C -4.37209241	1.98912059	0.73401389	H 1.55683400	3.06568800	-0.43010300
C -3.33942188	3.84483326	-1.05002115	C 4.75294500	4.17474800	-0.73944400
H -1.76108586	2.41993012	-1.37165045	H 6.50080900	2.96036900	-0.43376700
C -5.01970605	3.20204002	0.54359601	H 2.83960400	5.11821500	-0.99139600
H -4.79770359	1.26836971	1.42444512	H 5.31769100	5.06669100	-0.98826100
C -4.50370933	4.13285968	-0.35080772	C -3.28589400	1.89158100	-0.16196100
H -2.93033100	4.56551835	-1.75000764	C -4.68090200	1.86695900	-0.22317900
H -5.92875147	3.42111114	1.09308717	C -2.61840700	3.07495800	-0.46993700
H -5.01019190	5.08027830	-0.50219846	C -5.39146700	3.00775900	-0.57116600
N 0.01247750	-0.17558171	2.11903672	H -5.22051700	0.95075400	-0.01315500
H 0.25844532	-2.66442576	-0.54845420	C -3.33084400	4.21675600	-0.81698000
O 0.10271665	-2.22981140	0.29620995	H -1.53439900	3.08279500	-0.43581900
C -0.14900173	-3.83613212	2.11850707	C -4.71780000	4.18691800	-0.86783600
H -1.00255241	-4.22238955	1.53197957	H -6.47461100	2.97283200	-0.61856800
O -0.30363222	-3.18727243	3.12954791	H -2.79685000	5.12992100	-1.05667000
H 0.01573510	-1.19798522	2.15520394	H -5.27354000	5.07629800	-1.14450300
Ru 0.00054856	-0.00584113	-0.08106894	O -0.00300600	-4.43593400	0.35255200
H 0.85099521	-4.16981247	1.78300056	H 0.04068200	-5.24233500	-1.50437400
TS-CH₂O-OH⁻			TS-H₂/HCOOH_k		
P -2.31521900	0.09294700	0.25248000	P -2.38891300	0.33091100	0.27674000
P 2.32347800	0.06777100	0.26329400	P 2.22719800	0.33314200	0.28814600
C -2.44441800	-0.23232400	2.08260300	C -2.54747500	0.32043500	2.14084900
C 2.44240600	-0.25990800	2.09278200	C 2.34757700	-0.18245300	2.06530000
H -2.43786900	-1.31759000	2.21323300	H -2.83336900	-0.69608200	2.42910800
H 2.43808600	-1.34597300	2.21874000	H 2.33037800	-1.27632000	2.08356300
H -3.37139000	0.15718900	2.50880100	H -3.34446000	0.98874700	2.47282500
H 3.36738500	0.12344300	2.52026700	H 3.27695000	0.15591600	2.52924300
C -1.22777200	0.36592500	2.76571200	C -1.20153400	0.69592500	2.74238300
C 1.22557500	0.34773900	2.77468600	C 1.12490400	0.38804600	2.76580700
H -1.25165000	0.13943700	3.83901400	H -1.24204300	0.50015900	3.83042200
H 1.24299600	0.11587200	3.84746500	H 1.14587100	0.07785000	3.82692800
H -1.20704300	1.45269800	2.65069100	H -1.06220900	1.78943000	2.64775000
H 1.22442100	1.43299000	2.66205600	H 1.21637300	1.49144500	2.78103600
O 0.01081000	0.17342100	-3.05263100	N -0.11090000	-0.03877900	2.12641800

C	0.00883500	0.06070900	-1.90244200	O	-0.09824000	0.89047600	-3.00556100
H	-0.00188800	1.51937500	0.03139400	H	-0.29598900	-1.60084700	-0.25440900
C	3.51142800	-1.12766900	-0.48311900	H	0.35897900	-2.09551400	-0.49442900
C	3.22858400	-2.49010600	-0.34275400	O	1.16415400	-3.30997900	-0.98822600
C	4.62833400	-0.73560500	-1.22284800	C	-0.09153500	0.58833600	-1.89188700
C	4.06759300	-3.43903900	-0.90610300	K	-0.50002800	-2.80504600	2.10872800
H	2.32067300	-2.78948400	0.17115200	H	-0.13697800	1.77705000	0.25083900
C	5.46319400	-1.69072900	-1.79087400	Ru	-0.08847600	0.21529800	-0.05300900
H	4.85063700	0.31668400	-1.36065600	C	1.39739400	-4.30528100	-0.25216000
C	5.18899300	-3.04334500	-1.62806200	C	3.43558900	-0.71363200	-0.62322400
H	3.84218100	-4.49440000	-0.78815700	C	3.43135500	-0.65942800	-2.01738500
H	6.32784800	-1.37464600	-2.36533600	C	4.35531200	-1.54054200	0.01922900
H	5.84439200	-3.78933200	-2.06945400	C	4.33652100	-1.40865000	-2.75280300
C	-3.50196800	-1.09861900	-0.50335800	H	2.70960100	-0.03625300	-2.53307700
C	-3.12955100	-2.44533300	-0.49704500	C	5.25758100	-2.29661200	-0.71971000
C	-4.70182000	-0.72181900	-1.10547100	H	4.37253700	-1.61160900	-1.10037200
C	-3.96749600	-3.40042000	-1.05528500	C	5.25167400	-2.23038500	-2.10575100
H	-2.16570500	-2.72361400	-0.07818300	H	4.31780400	-1.36094200	-3.83581400
C	-5.52901200	-1.68263600	-1.67519800	H	5.96280300	-2.94218400	-0.20774100
H	-4.98949300	0.32378900	-1.14367900	H	5.95305300	-2.82374700	-2.68180900
C	-5.17032200	-3.02384300	-1.64180100	C	-3.48804700	-1.05858100	-0.24600500
H	-3.67623300	-4.44502700	-1.04034600	C	-4.71393300	-1.30812400	0.37892700
H	-6.45979800	-1.37521500	-2.14427500	C	-3.07433400	-1.89708100	-1.28055100
H	-5.82042800	-3.76824200	-2.08511200	C	-5.50415700	-2.37747600	-0.02076600
C	3.15899100	1.70121000	0.04840600	H	-5.06086900	-0.66022700	-1.17689500
C	2.58147700	2.66635600	-0.77279400	C	-3.86934100	-2.96428300	-1.68433300
C	4.36853900	1.99206600	0.68494500	H	-2.11836700	-1.72056000	-1.76003900
C	3.19881800	3.89751300	-0.96090200	C	-5.08243600	-3.20738400	-1.05439800
H	1.63131900	2.45088700	-1.25156500	H	-6.45258400	-2.56109600	0.47235100
C	4.98312800	3.22566400	0.50457100	H	-3.53267500	-3.60841100	-2.48877700
H	4.84832100	1.25302700	1.31351800	H	-5.70004800	-4.04230900	-1.36647500
C	4.39903300	4.18072500	-0.32050600	C	3.07333100	1.97995300	0.24604300
H	2.73825700	4.63674800	-1.60574100	C	4.43725000	2.07582900	0.53312200
H	5.91820300	3.43701200	1.00722000	C	2.36897900	3.13659000	-0.07522300
H	4.87684900	5.14058100	-0.46249200	C	5.07619000	3.30682600	0.51847900
C	-3.12431300	1.73311200	0.01675300	H	5.01051700	1.18198400	0.75440800
C	-2.57215700	2.64099900	-0.88665800	C	3.01144500	4.36987900	-0.09783900
C	-4.28754500	2.08799800	0.70130000	H	1.31344000	3.06107000	-0.30824300
C	-3.17311600	3.87376400	-1.10482400	C	4.36325700	4.45846900	0.20211400
H	-1.65902600	2.37847400	-1.40738100	H	6.13524100	3.36695000	0.74454000
C	-4.88247000	3.32428500	0.49180700	H	2.45114900	5.26214400	-0.35513700
H	-4.74698200	1.39677100	1.40057600	H	4.86426300	5.42016800	0.18365800
C	-4.32756800	4.22145400	-0.41417900	C	-3.31542500	1.83410400	-0.26356100
H	-2.73676100	4.56654100	-1.81598100	C	-4.46438900	1.77114900	-1.04979400
H	-5.78248900	3.58782500	1.03751000	C	-2.82482900	3.08535000	0.11690000
H	-4.79181100	5.18661100	-0.57896200	C	-5.11662700	2.93638700	-1.43807800
N	-0.00175700	-0.17924300	2.15812500	H	-4.85333200	0.81256100	-1.37033700
H	0.10349900	-2.75296300	-0.67244700	C	-3.48670300	4.24536400	-0.25714100
O	0.04295700	-2.33301500	0.19316400	H	-1.90860800	3.14903400	0.69328700
C	-0.14377900	-3.68265200	1.79748100	C	-4.63499400	4.17448500	-1.03800000
H	-0.97741200	-4.19058900	1.28283900	H	-6.00443400	2.87140200	-2.05751100
O	-0.33208100	-2.99202600	2.79183100	H	-3.09618300	5.20926900	0.05029600
H	-0.01734800	-1.19345400	2.32013100	H	-5.14561700	5.08211800	-1.34002600
Ru	0.00332600	-0.07719000	-0.05651500	O	1.04132600	-4.48270900	0.93155000
H	0.85707600	-4.07503200	1.54848000	H	1.99081700	-5.11335400	-0.73073400
HRu_OCH₂OH_{OH}				KRu-OOCH			
P	-2.33006302	-0.03594500	0.26369942	P	-2.35000258	0.09867544	0.48390388
P	2.29525055	0.15224624	0.41260929	P	2.24085303	0.00666353	0.23622085
C	-2.48646963	-0.51497967	2.05170075	C	-2.40209995	0.17068960	2.34238922
C	2.38645626	0.00379359	2.26534163	C	2.49022844	-0.19600722	2.06390364
H	-2.41143573	-1.60530600	2.06668395	H	-2.59799127	-0.85746148	2.66289434
H	2.52734491	-1.05190708	2.49947107	H	2.50958710	-1.27107707	2.26698638
H	-3.45523331	-0.25321091	2.48196341	H	-3.23133095	0.77796263	2.71309069
H	3.22698559	0.57479000	2.66272893	H	3.43478327	0.23626335	2.40236967
C	-1.33204552	0.10106678	2.82470306	C	-1.04850181	0.64913078	2.84698980
C	1.06474452	0.47326837	2.84916776	C	1.28980072	0.45032745	2.74007445
H	-1.35230317	-0.24936774	3.86570324	H	-1.03268861	0.55852645	3.95075194
H	1.05775292	0.28090984	3.93111826	H	1.38312621	0.31069891	3.83435872
H	-1.43257235	1.19195138	2.84467083	H	-0.95648584	1.73347409	2.64405983
H	0.93256311	1.55003281	2.70174628	H	1.34756674	1.54476061	2.58204865
O	0.06041674	0.42531311	-2.97337910	N	0.03902747	-0.10462085	2.24780924
C	0.04026612	0.20237032	-1.84077954	C	0.75761493	-3.44695466	0.06555299
H	-0.09870277	1.49508654	0.18875590	Ru	-0.07845709	-0.17914803	0.05637659
C	3.46548270	-1.12193145	-0.22863998	C	-0.19181841	-0.12331872	-1.80670814
C	3.47169620	-2.40601355	0.32749753	O	-0.26278114	-0.02114344	-2.95713054
C	4.26287057	-0.86044223	-1.34502235	O	1.05219022	-4.31296130	0.90515911

C 4.28875461	-3.39345276	-0.21165418	H -0.10870061	1.39640045	0.09496535
H 2.81841430	-2.64455029	1.16527800	C 3.40706422	-1.17725425	-0.56457204
C 5.07216532	-1.85378737	-1.87996462	C 4.31524984	-1.96237186	0.14335777
H 4.25974335	0.12481586	-1.79665741	C 3.36028778	-1.28916671	-1.95654400
C 5.09192316	-3.12150181	-1.31178204	C 5.16244246	-2.83905713	-0.52567425
H 4.29075326	-4.38241309	0.23353865	H 4.36903138	-1.90306551	1.22384159
H 5.68920438	-1.63426554	-2.74437268	C 4.21067635	-2.15795782	-2.62319480
H 5.72662658	-3.89550528	-1.72889005	H 2.64987464	-0.69629303	-2.52238259
C -3.48073319	-1.17506166	-0.61261671	C 5.11388685	-2.93746977	-1.90857599
C -2.94601478	-2.29719628	-1.24545400	H 5.85834918	-3.44909014	0.03965593
C -4.85963816	-0.96020182	-0.63884829	H 4.16157538	-2.23353249	-3.70382649
C -3.78747448	-3.20001281	-1.88497215	H 5.77254140	-3.62361858	-2.42923432
H -1.87291031	-2.45898155	-1.22970004	C -3.64248666	-1.15591793	0.07894504
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H -3.36550814	-4.07008025	-2.37576558	H -5.33556001	0.07669834	0.58908686
H -6.76488037	-1.69002646	-1.29896676	C -4.17513230	-3.39435303	-0.64707624
H -5.81287652	-3.68969190	-2.40809905	H -2.17115416	-2.60047853	-0.51035665
C 3.15113852	1.74203953	0.04220394	C -5.52765964	-3.13722717	-0.46695385
C 2.48534560	2.75949637	-0.63594061	H -6.99786954	-1.68131045	0.12017511
C 4.47051276	1.94972801	0.45508982	H -3.84877890	-4.36376406	-1.00800826
C 3.12557488	3.96622405	-0.89769856	H -6.26169286	-3.90582672	-0.68369339
H 1.45903137	2.60379727	-0.94572817	C -3.13002443	1.65841871	-0.11416412
C 5.10672101	3.15475681	0.19684637	C -3.46712114	1.75121016	-1.46655711
H 5.00937040	1.16250362	0.97182645	C -3.33035205	2.76692633	0.70576042
C 4.43413475	4.16608079	-0.48177476	C -4.00933914	2.91969457	-1.98025137
H 2.59642605	4.75047000	-1.42755101	H -3.30585080	0.90370289	-2.12392234
H 6.12999115	3.30499617	0.52304545	C -3.86984476	3.94001362	0.18888428
H 4.93252344	5.10753359	-0.68504337	H -3.05798577	2.73135439	1.75378515
C -3.16270405	1.59968723	0.09161141	C -4.21334788	4.01883189	-1.15323027
C -3.02155400	2.27099811	-1.12525422	H -4.26798467	2.97386160	-3.03196542
C -3.91546846	2.19317879	1.10281440	H -4.01942697	4.79404137	0.84055080
C -3.63234818	3.49887324	-1.32904068	H -4.63437465	4.93344592	-1.55574483
H -2.42583493	1.83134717	-1.91737608	C 3.06748431	1.61967916	-0.14198089
C -4.51664450	3.43184651	0.90276915	C 2.32741755	2.71326161	-0.58254249
H -4.03995128	1.70147594	2.06010878	C 4.44908512	1.75594228	0.01571989
C -4.37988168	4.08518196	-0.31332442	C 2.95412912	3.92554590	-0.85089179
H -3.51724764	4.00413764	-2.28156006	H 1.25703385	2.60584082	-0.71285137
H -5.09439436	3.88305663	1.70199809	C 5.07297385	2.96667716	-0.24651921
H -4.85072873	5.04925373	-0.46997419	H 5.04641970	0.90714339	0.33134254
N -0.04772453	-0.23733888	2.20238804	C 4.32510571	4.05594018	-0.68131101
H 1.03720469	-2.55986242	-0.53788856	H 2.36520034	4.76793222	-1.19690853
O 0.14684459	-2.41133015	-0.19895358	H 6.14623240	3.05874942	-0.11980038
C 0.04165947	-3.24464037	1.09328478	H 4.81335577	5.00118228	-0.89208551
H -1.06196746	-3.26770637	1.20006801	O -0.09747963	-2.52171251	0.24868410
O 0.71307666	-2.72636741	2.08778438	H 1.26292928	-3.47153226	-0.91962540
H 0.16834715	-1.29850639	2.28609291	K -0.20406814	-2.85624707	2.82952421
Ru -0.00144377	-0.07238563	-0.00202732			
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HRu_OCH₂OH_o			KRu-HCOO		
H -0.09521600	1.49791600	-0.27326500	P -2.31194375	0.28285014	0.30491401
Ru -0.03113600	-0.05993700	0.07455800	P 2.31275048	0.28080780	0.30515824
C -0.04531400	-0.37676100	-1.74815400	C -2.46613293	0.18771993	2.16428188
O -0.05528200	-0.53707800	-2.89397400	C 2.46677540	0.18651899	2.16461111
N -0.02930700	0.29404000	2.25375900	H -2.62554716	-0.86869310	2.40393040
P -2.36017100	0.08575600	0.37686100	H 2.62590209	-0.86980846	2.40484462
P 2.27893100	0.19632800	0.35917000	H -3.33313465	0.74357922	2.52745291
C 2.41087800	0.24976400	2.21863400	H 3.33395380	0.74226221	2.52753414
C -2.45290500	0.02637700	2.23504900	C -1.17296319	0.69757792	2.77890429
H 3.32449900	0.74804900	2.54799700	C 1.17375082	0.69714691	2.77892016
H -3.40674400	0.38709100	2.62191800	H -1.20809469	0.51756574	3.87061212
H 2.43233400	-0.78764300	2.56332700	H 1.20864027	0.51738715	3.87068019
H -2.36086500	-1.03217500	2.49193300	H -1.14355166	1.79862798	2.67276104
C -1.28431600	0.80565200	2.81635500	H 1.14490594	1.79818564	2.67250033
C 1.17725500	0.94002400	2.78044600	N 0.00028454	0.07292856	2.18692670
H -1.36526400	1.86877700	2.57201800	Ru 0.00038476	0.15618297	0.00532044
H 1.15780900	1.99547400	2.49508600	C 0.00061240	0.39798244	-1.85745516
H -1.27915600	0.71642900	3.91153300	O 0.00079080	0.63795301	-2.98384141
H 1.19321100	0.89393700	3.87822100	H 0.00112551	1.72496105	0.15778606
H 0.02403100	-0.73349500	2.38665500	K 0.00094366	-2.66979916	2.55613394
C 3.50551700	-1.07713400	-0.16066900	C -3.44792394	-1.03837504	-0.28984708
C -3.52847500	-1.22608300	-0.16934300	C -4.64418133	-1.33418930	0.37145605
C 5.31297800	-2.99340900	-1.09459800	C -3.09719588	-1.77344802	-1.42083110
C -5.18195100	-3.31758600	-0.98229200	C -5.47282640	-2.34585512	-0.09360525
C 3.50535600	-1.45812800	-1.50430200	H -4.93878390	-0.76887396	1.24918073

C -3.13102800	-2.55138700	0.02558000	C -3.92960139	-2.78532370	-1.88515614
C 4.42194400	-1.66854400	0.70838200	H -2.15858439	-1.58218378	-1.92718897
C -4.74808400	-0.95595000	-0.78962100	C -5.11563822	-3.07281468	-1.22451586
C 5.31851700	-2.62369900	0.24312000	H -6.39811074	-2.56735503	0.42734219
C -5.57071100	-2.00105200	-1.19299300	H -3.63231040	-3.35888176	-2.75526725
C 4.40541100	-2.40573000	-1.96818500	H -5.76049373	-3.86688493	-1.58475249
C -3.96054900	-3.58891200	-0.37658500	C 3.44748485	-1.04187560	-0.28879434
H 2.79215100	-1.01654600	-2.19164000	C 4.64338334	-1.33857230	0.37276657
H -2.15921600	-2.76333000	0.46233900	C 3.09610845	-1.77717316	-1.41943569
H 4.44284400	-1.39751900	1.75728700	C 5.47102960	-2.35133651	-0.09168992
H -5.05790200	0.06630200	-0.96881000	H 4.93850040	-0.77307930	1.25020577
H 6.02081100	-3.08077400	0.93154700	C 3.92751654	-2.79014663	-1.88315782
H -6.51616900	-1.78229900	-1.67745300	H 2.15775759	-1.58517992	-1.92600772
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H -3.63659200	-4.61302100	-0.22920200	H 6.39604916	-2.57350286	0.42944460
H 6.00971400	-3.74162600	-1.45540500	H 3.62971793	-3.36383965	-2.75300651
H -5.82463300	-4.13104700	-1.30122700	H 5.75726740	-3.87343670	-1.58202087
C 3.13002900	1.75707500	-0.16400400	C 3.19485971	1.84198867	-0.15131821
C -3.20256800	1.66025800	-0.08675800	C 4.43378892	1.84261787	-0.79124436
C 4.41151400	4.13482000	-0.88232200	C 2.59459576	3.06589088	0.15211134
C -4.46496300	4.02705000	-0.87799900	C 5.06444389	3.04081674	-1.10675022
C 2.39953400	2.82644300	-0.67530200	H 4.90913229	0.90642552	-1.05584192
C -4.32993200	2.12654900	0.59290200	C 3.23243690	4.26053813	-0.14910385
C 4.51456000	1.88754600	-0.02599400	H 1.61092186	3.07886033	0.60700290
C -2.71968200	2.39368500	-1.16984000	C 4.47024978	4.25186419	-0.78129454
C 5.14980000	3.06927200	-0.37876400	H 6.02300256	3.02304136	-1.61377342
C -3.35063100	3.56586400	-1.56683300	H 2.75283904	5.20199872	0.09561749
C 3.03757000	4.00976500	-1.03108600	H 4.96312611	5.18561908	-1.02844157
C -4.95306600	3.30556500	0.20447800	C -3.19245677	1.84515103	-0.15083124
H 1.32744200	2.71878900	-0.79411100	C -4.43141169	1.84731572	-0.79070645
H -4.73902300	1.56746400	1.42677800	C -2.59095050	3.06831852	0.15310407
H 5.10549100	1.05680300	0.34384600	C -5.06087005	3.04628671	-1.10566825
H -1.83459400	2.04710200	-1.68950800	H -4.90771453	0.91171807	-1.05568238
H 6.22526600	3.15577700	-0.26874200	C -3.22759760	4.26374024	-0.14756401
H -2.96497600	4.12291900	-2.41351600	H -1.60724412	3.08010287	0.60795416
H 2.45602500	4.83317400	-1.43107300	C -4.46544311	4.25659284	-0.77971049
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H 4.90917200	5.05652200	-1.16317700	H -2.74704135	5.20460955	0.09755237
H -4.95258100	4.94638700	-1.18301100	H -4.95738731	5.19095241	-1.02642984
O -0.06546600	-2.03040300	1.14277000	H -0.00078329	-1.83462809	-0.27681578
C 0.57236200	-3.17421700	0.77243800	C -0.00131852	-2.98957754	-0.66085699
H 1.63618200	-3.00091800	0.52625100	O -0.00177745	-3.79315087	0.28660164
H 0.52422000	-3.92333100	1.57825300	O -0.00126463	-3.09682178	-1.87174002
O -0.03250000	-3.84276000	-0.33971300			
H -0.02895000	-3.21192300	-1.06850500			
HRu_OCH₂OH_H			TS-HCOOH-H_K		
P -2.35398851	0.13048677	0.33360859	P -2.30291027	-0.26831768	-0.22231059
P 2.28451438	0.10105342	0.27661947	P 2.29372859	-0.27963326	-0.25652395
C -2.46620883	0.13467093	2.19455979	C -2.46935409	0.21282894	-2.01746508
C 2.40781302	-0.27542825	2.09014222	C 2.43571264	0.20176927	-2.05367399
H -2.57017438	-0.90333961	2.51326924	H -2.57716736	1.30198715	-2.06045070
H 2.29499488	-1.35874242	2.19345316	H 2.54758398	1.29047641	-2.09768107
H -3.33973063	0.69320713	2.53367493	H -3.36007687	-0.22739050	-2.47101764
H 3.36725223	0.03317676	2.51023147	H 3.31768060	-0.24207354	-2.52061081
C -1.18025183	0.70803608	2.76613550	C -1.19433310	-0.21913491	-2.72200165
C 1.24870563	0.42102356	2.78580687	C 1.14850590	-0.22425060	-2.73941418
H -1.17326869	0.57391118	3.85640007	H -1.23913658	0.12454700	-3.77269082
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H -1.10032559	1.77896106	2.56108760	H -1.17747162	-1.32471662	-2.76823559
H 1.34889987	1.50864189	2.71557407	H 1.12599251	-1.32973618	-2.78561939
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O -0.09256265	-0.02004938	-3.03317535	H 0.00690763	1.36648555	0.73728064
H 0.01433019	-1.83806682	0.27029040	C 0.02026478	2.75573393	1.98827255
H -0.16901850	-1.03190404	2.33481461	Ru -0.00214122	-0.28309833	0.09432017
C -0.03920193	-2.84025105	1.03231893	C 0.00910290	-0.96139658	1.83206525
O -0.49709113	-2.55522799	2.19299663	O 0.01577209	-1.43408087	2.88731171
H -0.07833446	1.61847974	-0.05456127	O 0.01703135	3.67763647	1.24076470
C -0.07176848	-0.01524931	-1.87901131	O 0.02656735	2.19753033	3.01319708
H -0.66027433	-3.49394698	0.38895809	H -0.01072096	-1.79384103	-0.54461564
Ru -0.03881811	0.02487262	-0.01644953	K -0.00590664	2.91275534	-1.31276110
C 3.41009040	-1.08508830	-0.56964369	C -3.38648512	0.93712686	0.66886505
C 4.18646103	-2.02267760	0.11007225	C -4.38650801	1.68016757	0.03815971
C 3.47312977	-1.03593663	-1.96459512	C -3.18774320	1.10890680	2.03990209
C 5.01633717	-2.88933808	-0.59308351	C -5.16839781	2.57490677	0.76127550
H 4.13931691	-2.09771172	1.18901771	H -4.57051042	1.56175470	-1.02395612
C 4.30561825	-1.89771144	-2.66321605	C -3.97488584	1.99396448	2.76343617

H 2.86715321 -0.32044202 -2.50968394	H -2.40050738 0.55667785 2.53987987
C 5.07981012 -2.82782666 -1.97837891	C -4.96520589 2.73230499 2.12576506
H 5.61159326 -3.61650465 -0.05195073	H -5.94085288 3.14501462 0.25606887
H 4.34368279 -1.84760977 -3.74566297	H -3.80480831 2.11459069 3.82749149
H 5.72681629 -3.50533218 -2.52434493	H -5.57513015 3.42872327 2.69056126
C 3.21338513 1.69013416 0.08961259	C 3.39660919 0.91968829 0.61906077
C 4.60014530 1.71987681 0.25868896	C 4.39045962 1.65848647 -0.02620553
C 2.54135688 2.87566770 -0.19458009	C 3.21971331 1.09107745 1.99313531
C 5.29581039 2.91563688 0.15720500	C 5.18768132 2.54869514 0.68567075
H 5.14359111 0.80235851 0.45735176	H 4.55758053 1.54025683 -1.09112657
C 3.23969281 4.07386081 -0.29811642	C 4.02213602 1.97159056 2.70533617
H 1.46685046 2.84798472 -0.33677782	H 2.43755432 0.54218775 2.50462363
C 4.61588614 4.09666014 -0.12136687	C 5.00617129 2.70573278 2.05325283
H 6.37222269 2.92547219 0.28904279	H 5.95507390 3.11554915 0.16921327
H 2.70431164 4.98993051 -0.52252439	H 3.86894490 2.09200234 3.77197736
H 5.16087301 5.03047650 -0.20512214	H 5.62805353 3.39862393 2.60927864
C -3.29052340 1.63549423 -0.17857150	C 3.28228888 -1.84521367 -0.13947052
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C -2.69949701 2.58517271 -1.00727553	C 2.61502378 -3.06811268 -0.13124570
C -5.30166540 2.97575702 -0.11633485	C 5.38889092 -3.02833136 -0.04339010
H -5.08716277 1.09933616 0.88848473	H 5.21750295 -0.89705014 -0.06601455
C -3.40376823 3.72191394 -1.38979179	C 3.32781097 -4.26047826 -0.08816973
H -1.68030101 2.43143145 -1.34104215	H 1.53076902 -3.06794480 -0.15488058
C -4.70250187 3.92048918 -0.94330184	C 4.71524283 -4.24423392 -0.04505998
H -6.31769076 3.12379303 0.23268573	H 6.47248902 -3.00635656 0.00105496
H -2.93279334 4.45284335 -2.03772916	H 2.79389355 -5.20456463 -0.07932078
H -5.25061319 4.80817950 -1.23926505	H 5.27140069 -5.17453288 -0.00511756
C -3.46168990 -1.24534451 -0.19688929	C -3.29745983 -1.82883329 -0.08946894
C -3.40773370 -2.47801318 0.45953360	C -4.69198134 -1.81336256 -0.01578674
C -4.28498013 -1.10643710 -1.31546403	C -2.63628655 -3.05506957 -0.09128716
C -4.19073876 -3.53718503 0.01847708	C -5.40821637 -3.00135491 0.03963328
H -2.73931301 -2.62404859 1.30330634	H -5.22652405 -0.87096590 0.01378806
C -5.05865976 -2.17205496 -1.75635549	C -3.35428787 -4.24383296 -0.03685593
H -4.32955926 -0.16160786 -1.84438790	H -1.55254057 -3.06035348 -0.13170840
C -5.01908111 -3.38819230 -1.08677261	C -4.74078575 -4.22062098 0.02779887
H -4.14520108 -4.48604652 0.54157433	H -6.49086862 -2.97393206 0.10091173
H -5.69543232 -2.04834466 -2.62544985	H -2.82503646 -5.19058379 -0.03605626
H -5.62659445 -4.21870004 -1.42898041	H -5.30091337 -5.14811042 0.07661368
O 1.30073549 -3.32499546 1.05216114	
H 1.56296041 -3.53263544 0.14743918	
TS-HOCH₂OH-H⁻	KRu-H₂CO₂
P -2.37145890 0.32094863 0.16620593	P -2.28909404 0.39584078 0.38754649
P 2.22998762 0.01176228 0.44599064	P 2.28915662 0.39546746 0.38774534
C -2.63121801 0.30214814 2.01437187	C -2.45074811 0.36635123 2.24829965
C 2.21695871 -0.29361904 2.28161015	C 2.45056081 0.36525955 2.24848747
H -2.79905118 -0.73321621 2.31479140	H -2.56243020 -0.67864484 2.55763366
H 2.06052407 -1.36677483 2.42347339	H 2.56160748 -0.67991462 2.55744742
H -3.50761409 0.88905848 2.29302892	H -3.33820554 0.90817104 2.58273070
H 3.15728337 -0.00248768 2.75407398	H 3.33825407 0.90649153 2.58324789
C -1.37558935 0.82650493 2.69085717	C -1.17094912 0.95108035 2.82247340
C 1.04521447 0.47226766 2.87506478	C 1.17098481 0.95047253 2.82265974
H -1.46424967 0.70979935 3.77951603	H -1.21183008 0.87022731 3.92550367
H 0.96871246 0.26431749 3.95046342	H 1.21174482 0.86944189 3.92568090
H -1.22680756 1.88692242 2.47463098	H -1.15027638 2.03462516 2.59824672
H 1.18243252 1.54990865 2.75207890	H 1.15082126 2.03406318 2.59859694
N -0.20222352 0.08668903 2.19275109	N -0.00011479 0.27710804 2.29410518
O 0.09281823 0.06691720 -3.01132386	H 0.00010830 -1.33488015 -0.14666219
H -0.14514889 -1.65345985 0.18910130	C 0.00052004 -3.91789430 -1.25541501
H -0.37743864 -0.92185473 2.37772698	Ru 0.00003673 0.37036023 0.05798387
C -0.32325883 -2.91051493 1.07844704	C 0.00012814 0.59168144 -1.78969423
O -0.85018000 -2.59863863 2.15711753	O 0.00019838 0.75811051 -2.93663050
H 0.00338660 1.73241708 0.04134314	O 0.00020994 -4.24651149 -0.13708625
C 0.03701093 0.07394651 -1.85665038	O 0.00080080 -3.65414076 -2.37774928
H -0.91146833 -3.37285865 0.27134801	H 0.00006015 2.01483149 0.33943973
Ru -0.05670103 0.09813425 -0.00303392	K -0.00115943 -2.43065366 2.07465513
C 3.30835099 -1.30593848 -0.26113603	C -3.34012963 -1.02568154 -0.16845519
C 4.06079187 -2.18521806 0.51725467	C -4.35180587 -1.58613171 0.61386078
C 3.36689389 -1.41681125 -1.65266216	C -3.09801666 -1.56481358 -1.43343786
C 4.85869311 -3.15266500 -0.08394798	C -5.10186222 -2.66022624 0.14455087
H 4.02193432 -2.13427328 1.59841627	H -4.56925204 -1.18384559 1.59728566
C 4.16914154 -2.37775794 -2.25107393	C -3.85610110 -2.62614655 -1.90899710
H 2.77870860 -0.75024915 -2.27337232	H -2.29916646 -1.15426499 -2.04043948
C 4.91698495 -3.24960340 -1.46757055	C -4.85775827 -3.18060520 -1.11926862
H 5.43338598 -3.83311731 0.53470413	H -5.88363631 -3.08360728 0.76636587
H 4.20381790 -2.45005141 -3.33242068	H -3.65893874 -3.02546663 -2.89798871
H 5.53944233 -4.00457588 -1.93478340	H -5.44609686 -4.01338494 -1.48881612

C 3.31084952	1.50456227	0.25952766	C 3.34014594	-1.02589891	-0.16869043
C 4.68714346	1.42567750	0.48700969	C 4.35147967	-1.58689551	0.61367143
C 2.75191416	2.73070619	-0.08978607	C 3.09837816	-1.56433350	-1.43403387
C 5.48363944	2.55664848	0.38065156	C 5.10156269	-2.66082908	0.14404122
H 5.14493878	0.47421503	0.73513870	H 4.56862073	-1.18518123	1.59739696
C 3.55144877	3.86336527	-0.19827854	C 3.85648563	-2.62551230	-1.90989900
H 1.68423266	2.78133243	-0.27557515	H 2.29979306	-1.15337083	-2.04110197
C 4.91648106	3.77946935	0.03766830	C 4.85781553	-3.18050865	-1.12013418
H 6.55100711	2.48251039	0.55821392	H 5.88306825	-3.08464379	0.76589828
H 3.10398926	4.81213921	-0.47388510	H 3.65958616	-3.02429703	-2.89915832
H 5.54053745	4.66207039	-0.05041442	H 5.44617020	-4.01316892	-1.48992551
C -3.20640782	1.87835892	-0.37231536	C 3.32867974	1.84588969	-0.12418129
C -4.55230900	2.10645462	-0.07181709	C 4.72025885	1.77782362	-0.21702471
C -2.49692762	2.84503413	-1.07871602	C 2.69238127	3.05446491	-0.39980409
C -5.17066608	3.28475687	-0.46322878	C 5.45935075	2.90107507	-0.56388054
H -5.12662599	1.35504900	0.46005081	H 5.23525389	0.84221811	-0.03263996
C -3.11967974	4.02305148	-1.47797220	C 3.43344368	4.17847879	-0.74453062
H -1.45000088	2.66923536	-1.29743064	H 1.60923739	3.09241017	-0.34243255
C -4.45402802	4.24599062	-1.16912143	C 4.81749432	4.10558855	-0.82694641
H -6.21454174	3.45232094	-0.22150123	H 6.53955656	2.83254255	-0.63662355
H -2.55699491	4.76745476	-2.03051423	H 2.92389213	5.11187532	-0.95842205
H -4.93859820	5.16576102	-1.47795502	H 5.39532996	4.98119712	-1.10252219
C -3.50916983	-0.98114929	-0.48075197	C -3.32843447	1.84613396	-0.12509548
C -3.61894749	-2.21387902	0.16733023	C -4.71998050	1.77807559	-0.21840962
C -4.18550584	-0.78984711	-1.68683895	C -2.69200931	3.05462914	-0.40079047
C -4.41548346	-3.21844272	-0.36761782	C -5.45892480	2.90126115	-0.56579799
H -3.06930629	-2.40568119	1.08301900	H -5.23506302	0.84252902	-0.03397111
C -4.97283629	-1.80051463	-2.22266228	C -3.43292623	4.17857629	-0.74604007
H -4.10327063	0.15486519	-2.21155596	H -1.60888407	3.09256199	-0.34307161
C -5.09606161	-3.01560759	-1.56154333	C -4.81695068	4.10569707	-0.82892431
H -4.49829860	-4.16659009	0.15242391	H -6.53910620	2.83273323	-0.63890567
H -5.49252794	-1.63457602	-3.15994917	H -2.92327777	5.11190857	-0.95998003
H -5.71485701	-3.80287835	-1.97766773	H -5.39467000	4.98125222	-1.10491278
O 0.97823104	-3.37839844	1.12945014			
H 1.29931665	-3.50565786	0.22832664			
HRu_HCOOH			KRu-OH		
P -2.32564846	0.16869912	0.26515287	Ru 0.01390500	-0.07141300	0.01243400
P 2.26880251	0.26016013	0.26510615	C 0.02754300	-0.30237600	-1.87932200
C -2.46885745	-0.13476540	2.10227808	O 0.03710100	-0.51670600	-3.00602700
C 2.43010106	0.10388272	2.12700402	N -0.00401300	-0.20937900	2.04900600
H -2.44846576	-1.21159682	2.28012880	P 2.33633200	-0.17825200	0.32033400
H 2.54212781	-0.96089137	2.34815885	P -2.31248600	-0.11912300	0.30427900
H -3.40919145	0.25744035	2.49329672	C -2.40089900	0.28012800	2.10897800
H 3.31268266	0.62750613	2.49916626	C 2.43811100	-0.00882600	2.16442100
C -1.27741916	0.51514421	2.78383583	H -3.35819000	-0.00360000	2.55036900
C 1.16997603	0.63821783	2.78505765	H 3.34815200	-0.44767400	2.57858700
H -1.29760663	0.30697204	3.86203829	H -2.27123000	1.36192500	2.20668100
H 1.20193193	0.44839710	3.86678532	H 2.48765100	1.06946500	2.34299600
H -1.29431555	1.59812491	2.64256952	C 1.17901800	-0.57130100	2.80567000
H 1.08044721	1.71518908	2.62946349	C -1.23280900	-0.41288300	2.79273400
N -0.02441623	0.01455308	2.18766297	H 1.23957500	-1.66808700	2.88632800
O -0.05885870	0.60348205	-3.01580184	H -1.43148300	-1.49131500	2.89923400
H -0.01739605	-1.43789164	-0.19381175	H 1.09008200	-0.18843700	3.83234900
H 0.01372214	-0.98967542	2.36407463	H -1.11828900	-0.01504200	3.81103000
C 0.17966607	-3.39045317	1.36997278	C -3.37975300	1.10700700	-0.55528800
O -0.48952543	-3.15629157	2.34103566	C 3.48280700	1.10716200	-0.31390100
H -0.06796251	1.89112865	0.30214619	C -4.90628300	2.94523700	-2.00593600
C -0.04586100	0.46400569	-1.86766240	C 5.14078700	3.14987200	-1.21972300
H -0.23598445	-3.69575830	0.40117658	C -3.59658700	0.92801400	-1.92464100
Ru -0.02770353	0.24039391	-0.03185616	C 2.92653500	2.29622700	-0.78780600
C 3.31311200	-1.14015321	-0.34562182	C -3.92702400	2.22417100	0.07436500
C 4.45300603	-1.58786852	0.32656531	C 4.86946000	0.94383200	-0.29525200
C 2.92254937	-1.79493807	-1.51496884	C -4.68826500	3.13613500	-0.64919500
C 5.18824764	-2.66162177	-0.16169697	C 5.69432400	1.96464300	-0.74573000
H 4.77118877	-1.10711330	1.24492932	C -4.35784900	1.83731300	-2.64320000
C 3.66443710	-2.86203967	-2.00952709	C 3.76205000	3.31334300	-1.23788500
H 2.02029799	-1.47499686	-2.02340848	H -3.17359700	0.06762300	-2.43258400
C 4.79786879	-3.29848015	-1.33330696	H 1.84109400	2.40803200	-0.78815200
H 6.06580764	-3.00217729	0.37679744	H -3.76855600	2.39792800	1.13166100
H 3.35105953	-3.35578680	-2.92285941	H 5.30603300	0.01618300	0.05861500
H 5.37202912	-4.13537757	-1.71507628	H -5.10711900	4.00008900	-0.14541300
C 3.29029149	1.75003690	-0.15899860	H 6.77084500	1.83409500	-0.73175600
C 4.65457399	1.68556154	-0.44765361	H -4.51946100	1.68300900	-3.70417600
C 2.65713446	2.99294053	-0.17250832	H 3.33037700	4.23635700	-1.60981800
C 5.37268257	2.84286601	-0.72163318	H -5.49866600	3.65859300	-2.56781200
H 5.16442055	0.73056669	-0.47562399	H 5.78754500	3.94459200	-1.57528500

C 3.37885339	4.14962657	-0.43773951	C -3.27484100	-1.68232500	0.13541100
H 1.58700155	3.03076748	0.00725583	C 3.18106100	-1.75308000	-0.11826200
C 4.73848989	4.07867751	-0.71211760	C -4.71941100	-4.06508600	-0.03257400
H 6.43069765	2.77547668	-0.95094126	C 4.36658900	-4.16093600	-0.90332400
H 2.87147035	5.10830502	-0.44485482	C -2.61761200	-2.89038200	-0.08611600
H 5.30015276	4.98072788	-0.92908167	C 3.54538100	-2.70557300	0.83096900
C -3.37828412	1.66990623	0.01677905	C -4.66653700	-1.67711300	0.26676300
C -4.74074005	1.65760313	0.32877178	C 3.41163600	-2.02464000	-1.46913800
C -2.80398860	2.84051349	-0.46924434	C -5.38295300	-2.86196000	0.18490500
C -5.50974413	2.80042313	0.16485884	C 4.00416500	-3.21647600	-1.85763600
H -5.20838792	0.74791294	0.69111855	C -3.33799700	-4.07674500	-0.16829000
C -3.57771919	3.98384283	-0.64121532	C 4.13453100	-3.90315500	0.44007100
H -1.74203815	2.84326039	-0.69119762	H -1.53886900	-2.89079300	-0.19701000
C -4.92839540	3.96672806	-0.32317931	H 3.37217800	-2.52670000	1.88543300
H -6.56541846	2.78094792	0.41302541	H -5.19458800	-0.74234100	0.42159800
H -3.12016684	4.88952512	-1.02420033	H 3.13227000	-1.29711400	-2.22365800
H -5.53096529	4.85880411	-0.45543149	H -6.46257600	-2.84650600	0.28597300
C -3.35444631	-1.15119624	-0.51685287	H 4.18021700	-3.41037500	-2.90984000
C -3.36735330	-2.45299832	-0.01373339	H -2.81581300	-5.01064600	-0.34463100
C -4.04296537	-0.88286751	-1.70081402	H 4.41346200	-4.63396700	1.19118500
C -4.07854365	-3.45345991	-0.66353909	H -5.28117900	-4.99015400	-0.10038200
H -2.81552214	-2.70200167	0.88539698	H 4.82750600	-5.09392200	-1.20761000
C -4.74343405	-1.88731146	-2.35592744	H 0.12133500	-1.68032700	-0.01452800
H -4.03645717	0.11839394	-2.11600635	O -0.13035600	2.13300700	-0.09241300
C -4.76921428	-3.17481523	-1.83633776	H -0.76129800	2.33665400	-0.78813200
H -4.08901735	-4.45657691	-0.25094869	K 0.14769100	3.81784800	1.91160900
H -5.27120498	-1.65986540	-3.27562071			
H -5.32092374	-3.95798521	-2.34437200			
O 1.51727898	-3.33917836	1.41645030			
H 1.87969687	-3.35594999	0.51841282			
HRu_HCOOH'			¹TS-H₂/H₂O_K		
P 2.25423599	-0.22750637	0.25932441	P -2.38313800	-0.07223800	0.24733100
P -2.35581741	-0.10364602	0.24393340	P 2.26231300	0.53484700	0.27160800
C 2.40598468	-0.05449563	2.11736172	C -2.23155200	-0.73568700	1.96734000
C -2.47876645	0.36177668	2.04726144	C 2.32000400	0.74715000	2.13081300
H 2.54702502	1.00720040	2.33471345	H -1.75978300	-1.73161400	1.87898400
H -2.42015841	1.45125818	2.10838067	H 2.56978000	-0.22640000	2.55782500
H 3.26902110	-0.60158100	2.50104062	H -3.19832500	-0.81846900	2.46864700
H -3.42992154	0.05364108	2.48462252	H 3.09443700	1.45642300	2.42867300
C 1.12242737	-0.53890954	2.76870649	C -1.28622400	0.18034600	2.72460700
C -1.30918220	-0.27280144	2.77929398	C 0.94732200	1.17071600	2.64088900
H 1.15334350	-0.33744864	3.84821395	H -0.99143900	-0.28496100	3.67534400
H -1.32193222	0.01568985	3.83881267	H 0.87923800	0.99234800	3.72171800
H 0.99631607	-1.61426281	2.62481258	H -1.77601000	1.13442700	2.98313100
H -1.37401230	-1.36267657	2.72475263	H 0.79946100	2.24799700	2.48139400
N -0.03740645	0.13153619	2.15527940	N -0.10203500	0.45896700	1.94041400
O -0.06887960	-0.54973086	-3.03096515	O -0.16968500	0.86382300	-3.10836700
H -0.03586991	1.57736456	-0.23853946	H 0.01718400	-1.84361800	-0.62583000
H 0.07804327	1.14057209	2.29976799	H -0.28136200	-2.31332600	-0.07776600
H 0.36540330	2.77612425	0.23948777	O -0.56028600	-3.42310300	1.48706300
O 0.57467808	3.74567145	0.51480154	C -0.11953500	0.64008600	-1.98205500
C -0.06111669	-0.38306503	-1.88785523	H -1.22469500	-4.03135700	1.81957100
C 0.62472639	3.88264785	1.81286233	K 1.84518700	-3.48228600	0.89600300
H 0.85091873	4.92217766	2.09370950	Ru -0.06172700	0.37544400	-0.09431600
O 0.45169924	3.01664747	2.64762542	H -0.17521200	1.96994100	-0.05465400
Ru -0.05001602	-0.12558039	-0.05275606	C 3.17434000	2.00876200	-0.39366600
H -0.11065954	-1.75106100	0.26796238	C 4.54825500	1.95734200	-0.62985500
C -3.44162078	1.12418080	-0.61033812	C 2.49088400	3.19996700	-0.62863800
C -3.09040013	2.47402009	-0.54236549	C 5.22649600	3.08180600	-1.08326500
C -4.55014110	0.75579556	-1.37108365	H 5.08627300	1.02985300	-0.46938300
C -3.85260136	3.43619846	-1.18736954	C 3.17051400	4.32578800	-1.07514500
H -2.19668502	2.76974375	-0.00534986	H 1.41666800	3.23123600	-0.47402100
C -5.30432782	1.72019967	-2.03063746	C 4.54005400	4.26963000	-1.30355100
H -4.82797755	-0.28701625	-1.45936505	H 6.29374000	3.02759900	-1.26951200
C -4.96433264	3.06180805	-1.93384267	H 2.62598800	5.24601600	-1.25820100
H -3.56690017	4.48014677	-1.12050131	H 5.06975500	5.14666700	-1.65930100
H -6.16026293	1.41633432	-2.62330143	C -3.55287800	1.34894300	0.39825900
H -5.55441267	3.81282312	-2.44730261	C -4.81929000	1.17445600	0.96307000
C 3.36757206	1.09144855	-0.39065260	C -3.17822400	2.61545400	-0.04268700
C 4.44531187	1.60382118	0.33399972	C -5.68768500	2.24898700	1.09020400
C 3.11387417	1.59427951	-1.66666718	H -5.13465000	0.19057600	1.29387300
C 5.25378143	2.59546097	-0.20869460	C -4.05119800	3.69149800	0.07884400
H 4.66293014	1.23611658	1.33057018	H -2.19114700	2.75113800	-0.47083000
C 3.92902774	2.57595055	-2.21308761	C -5.30461200	3.51089400	0.64691900
H 2.26160950	1.22738704	-2.22646304	H -6.66731200	2.10161600	1.53176600
C 4.99949541	3.08023581	-1.48504176	H -3.74856400	4.67220000	-0.27186000

H 6.08369236	2.98858911	0.36843825	H -5.98479600	4.35005100	0.74416400
H 3.71768411	2.95710448	-3.20590066	C -3.35509600	-1.31502100	-0.69152900
H 5.63012382	3.85409569	-1.90853135	C -4.28789500	-0.91044900	-1.65125000
C -3.32783309	-1.67171456	0.14274566	C -3.07922000	-2.67817200	-0.53884200
C -4.59431658	-1.79049776	0.72149713	C -4.95347700	-1.85053500	-2.42553500
C -2.78834517	-2.76533741	-0.52995434	H -4.50326200	0.14276500	-1.79074800
C -5.30117681	-2.98191420	0.63457936	C -3.75544000	-3.61082100	-1.31491000
H -5.04294470	-0.94707828	1.23559056	H -2.32200200	-3.01342000	0.17034200
C -3.50117075	-3.95490910	-0.62713256	C -4.69449400	-3.20539800	-2.25591500
H -1.79453711	-2.67979088	-0.95359764	H -5.67834800	-1.52163300	-3.16239700
C -4.75555065	-4.06671036	-0.04308331	H -3.53962300	-4.66586000	-1.18283800
H -6.28066214	-3.06254885	1.09321092	H -5.21721200	-3.93988100	-2.85892500
H -3.06993488	-4.79760463	-1.15618179	C 3.39168100	-0.85531400	-0.04859100
H -5.30859665	-4.99698081	-0.11312724	C 4.26827000	-1.41716300	0.92052700
C 3.20102176	-1.77663662	-0.12128546	C 3.29028100	-1.52997800	-1.29307900
C 4.58765373	-1.77873925	-0.28671544	C 4.95123500	-2.59761400	0.66728200
C 2.50888702	-2.98267358	-0.21953445	H 4.45031700	-0.90497500	1.85796500
C 5.26680247	-2.96612081	-0.52611909	C 3.98681700	-2.69497900	-1.54127500
H 5.14407632	-0.85016752	-0.24404391	H 2.64330000	-1.12383900	-2.06437700
C 3.19063229	-4.17035425	-0.45476974	C 4.81319800	-3.26628400	-0.55360800
H 1.42832527	-2.97079792	-0.12135677	H 5.62993700	-2.98660500	1.42077600
C 4.57062289	-4.16593285	-0.60784325	H 3.89740500	-3.17083800	-2.51235400
H 6.34330719	-2.95116081	-0.65787866	H 5.36888700	-4.17425900	-0.75403400
H 2.63749848	-5.10031178	-0.53043393			
H 5.10207366	-5.09172399	-0.79945118			
TS-H₂/HCOOH			¹KRu-OCOOCH₃		
P -2.30516490	0.15670108	-0.03787107	P 1.19520300	-2.22172200	0.49380800
P 2.32885997	0.16762080	0.18300294	P -2.50147800	0.52922800	0.53406700
C -2.35756299	0.61475784	-1.84538717	C 0.89670000	-2.79153100	2.24660400
C 2.51535950	0.93574120	-1.50224081	C -2.81851900	0.20498800	2.33845900
H -2.43077185	1.70347139	-1.90463123	H 1.37154500	-2.05690100	2.90075400
H 2.44668226	2.01840266	-1.37334266	H -2.13578700	0.82742400	2.91955500
H -3.22047205	0.17255930	-2.34619887	H 1.34432900	-3.76902400	2.43465900
H 3.48436883	0.70932171	-1.95011363	H -3.84464000	0.44737600	2.62056200
C -1.05577143	0.17753748	-2.49583309	C -0.60231100	-2.80553600	2.50874100
C 1.37452235	0.43470499	-2.37228313	C -2.48751400	-1.25862800	2.59855700
H -1.02783741	0.53095140	-3.53480528	H -0.79504400	-2.90509200	3.58529200
H 1.42567812	0.89947617	-3.36517965	H -2.46240300	-1.45384100	3.67888800
H -0.96135102	-0.91106342	-2.50229307	H -1.06563200	-3.67772900	2.02118800
H 1.44435109	-0.64879823	-2.50445661	H -3.27423200	-1.90570200	2.17834700
N 0.07880927	0.73991929	-1.74037369	N -1.21775300	-1.60068000	1.99644000
O -0.09953431	-0.77577904	3.25163872	C -0.54580800	-0.63062600	-1.74952600
H -0.14803165	1.87121594	0.98045871	O -0.49072900	-0.50736000	-2.89189500
H -0.05112921	1.77239675	-1.77384785	C 3.56661300	4.01579500	-0.78296100
O 0.15976888	2.56840029	0.44512791	O 2.86768800	4.46924400	0.15450000
O 0.50785721	3.80141392	0.01029672	O 3.34472700	2.99851200	-1.47364100
C -0.06431656	-0.39234660	2.16524415	H -1.66335000	-2.18490800	-0.37659000
C 0.03106333	4.18169848	-1.10762017	Ru -0.73355400	-0.92829100	0.12674900
H 0.06711551	5.27599835	-1.27001882	C -2.26505500	2.35327500	0.37040000
O -0.44290013	3.46879126	-2.00112522	C -1.98818800	3.20389200	1.44443700
Ru -0.00293981	0.18712305	0.39780188	C -2.23596300	2.88641600	-0.92586100
H 0.03965490	-1.34372473	-0.11293962	C -1.68603800	4.54474300	1.22881100
C 3.43868351	1.14073317	1.28843785	H -2.00962200	2.83282200	2.46203500
C 3.25528853	2.52246027	1.38699981	C -1.93630300	4.22448200	-1.13783500
C 4.39859058	0.52436183	2.09158175	H -2.45497800	2.24867700	-1.77621100
C 4.04420487	3.27144404	2.24877236	C -1.64986300	5.05861000	-0.06110300
H 2.48466431	3.02350701	0.81127769	H -1.47095600	5.18778100	2.07487400
C 5.17692616	1.27815081	2.96177444	H -1.91624300	4.61597700	-2.14877700
H 4.54234130	-0.54803146	2.04449756	H -1.39868700	6.09927400	-0.22728700
C 5.00757598	2.65360463	3.03731926	C -4.15985600	0.29668900	-0.25181700
H 3.89260640	4.34329743	2.31082565	C -5.19815500	1.20482400	-0.03077600
H 5.91714281	0.78439056	3.58179340	C -4.38913400	-0.82060200	-1.04958900
H 5.61669886	3.24146271	3.71508147	C -6.44741800	0.99100400	-0.59471000
C -3.42985386	1.35846858	0.78588686	H -5.02878100	2.08951900	0.57424800
C -4.37877548	2.11040045	0.09297602	C -5.64101100	-1.03142200	-1.61732700
C -3.32197118	1.51398795	2.16851152	H -3.57703700	-1.52133200	-1.21653100
C -5.20576897	2.99808431	0.77118510	C -6.67037300	-0.12855100	-1.39014300
H -4.47766509	2.01758504	-0.98218071	H -7.24766800	1.70150700	-0.41892700
C -4.15463847	2.39332923	2.84548116	H -5.80847500	-1.90210200	-2.24175500
H -2.57442959	0.95302217	2.71744321	H -7.64587100	-0.29197400	-1.83476100
C -5.09748070	3.13895174	2.14800605	C 2.86347900	-1.44361500	0.55470600
H -5.93357219	3.58231471	0.21897739	C 3.80178700	-1.73013300	1.54868800
H -4.05738390	2.50519579	3.91951900	C 3.18266100	-0.49288700	-0.41716800
H -5.74134113	3.83343671	2.67604305	C 5.02347000	-1.06679400	1.57094100
C 3.20829853	-1.44778231	0.01955310	H 3.58942100	-2.46965800	2.31246900
C 4.49021172	-1.51612406	-0.53302901	C 4.39906900	0.17650300	-0.39413300

C 2.60113956	-2.62058253	0.46139213	H 2.46925500	-0.26790500	-1.20361700
C 5.14300653	-2.73481114	-0.65205911	C 5.31908600	-0.10963600	0.60861300
H 4.99292693	-0.61294957	-0.86181473	H 5.74145100	-1.29346400	2.35188000
C 3.25945722	-3.84032256	0.35182047	H 4.58990400	0.95450600	-1.12551600
H 1.60191015	-2.57116888	0.87673960	H 6.26362900	0.42149300	0.64125800
C 4.52797753	-3.90042599	-0.20819901	C 1.47902300	-3.78394100	-0.45522100
H 6.13534398	-2.77429851	-1.08763561	C 0.38439200	-4.42598800	-1.03347100
H 2.77568800	-4.74519845	0.70260144	C 2.74747000	-4.35091400	-0.58731800
H 5.03910165	-4.85252125	-0.29904902	C 0.55154200	-5.62588900	-1.71292000
C -3.26224073	-1.42432269	0.05411861	H -0.59572400	-3.96527300	-0.95981300
C -4.65880525	-1.42724864	0.07365868	C 2.91251200	-5.54767800	-1.27241900
C -2.58410917	-2.64163335	0.06689203	H 3.61312600	-3.85177200	-0.16797000
C -5.35948262	-2.62539406	0.09087289	C 1.81521100	-6.18970000	-1.83325100
H -5.20523020	-0.49138277	0.08962767	H -0.30722100	-6.11399900	-2.16080900
C -3.28729876	-3.84026871	0.08149196	H 3.90407800	-5.97478500	-1.37498600
H -1.49999099	-2.63760427	0.07386011	H 1.94723800	-7.12190800	-2.37136500
C -4.67543601	-3.83534812	0.09295830	O 4.72606100	4.68824900	-1.11264100
H -6.44375798	-2.61302541	0.11045344	C 5.00435800	5.85300200	-0.35693000
H -2.74608961	-4.78002977	0.09376489	H 5.94406100	6.24759100	-0.74668500
H -5.22426677	-4.77048160	0.11107146	H 4.21650700	6.60305700	-0.46701900
			H 5.11156800	5.62811200	0.70768300
			K 1.16073000	2.44153400	-0.06382700
HRu_OCHO_H ₂			TS-CH _k		
P 2.34319173	-0.26066071	0.16567720	P -2.29220100	0.57896200	0.27873700
P -2.31523728	0.00944506	0.33275070	P 2.25780200	0.25476100	0.38238000
C 2.54141180	-0.11082902	2.00917935	C -2.43177000	0.84902200	2.12330800
C -2.32160473	0.49902760	2.11847736	C 2.33273500	-0.33299400	2.13220200
H 2.70941742	0.94292024	2.23752309	H -2.88439300	-0.06286400	2.52576500
H -2.17327269	1.58398310	2.15654162	H 2.16553000	-1.41404000	2.10144600
H 3.40096516	-0.68636957	2.35571979	H -3.12052600	1.66464400	2.35559800
H -3.26558592	0.24264795	2.60250435	H 3.29452300	-0.12256200	2.60683900
C 1.25692606	-0.56660108	2.67709034	C -1.04708300	1.06742800	2.70782900
C -1.14391035	-0.18140337	2.79250626	C 1.18393800	0.36707700	2.83977100
H 1.31610321	-0.36599128	3.75445100	H -1.12159200	0.99648700	3.80955100
H -1.08315577	0.14019504	3.83969924	H 1.16513300	0.04523000	3.89740700
H 1.09821136	-1.63989673	2.54054729	H -0.72925400	2.10686500	2.49850300
H -1.25954743	-1.27005669	2.78423407	H 1.40776400	1.45167600	2.86963500
N 0.11140968	0.15711502	2.09773551	N -0.09272100	0.10524600	2.19117800
O -0.16580746	-0.51610138	-3.06616354	H 0.19643500	-1.70159300	-0.12111500
H 0.48160143	1.76497142	-0.27910558	C 0.72121900	-3.16181300	-0.14187400
H 0.31900419	1.18593642	2.24482241	Ru -0.03233200	0.13085800	-0.01994500
H -0.31186567	1.82229607	-0.12692265	C 0.00107500	0.24682600	-1.88399400
O -1.05855531	3.46936359	1.96686791	O 0.02750800	0.36451200	-3.03428400
C -0.09566952	-0.30320810	-1.93855124	O 1.16303600	-3.38033800	0.99660300
C 0.12398333	3.60944012	2.32222870	H -0.08448100	1.74173800	0.12099500
H 0.47305433	4.64380095	2.54298283	K -0.99984600	-2.51585600	2.19038200
O 0.99377862	2.70175004	2.46113092	C -3.72983100	-0.57282300	0.02784500
Ru 0.00811976	-0.02525437	-0.08910195	C -5.05125900	-0.17171700	0.24160200
H -0.04893447	-1.60151243	0.13166229	C -3.47406900	-1.90252600	-0.29252700
C -3.39451117	1.21900548	-0.53489970	C -6.08881900	-1.08840400	0.14571200
C -3.26679647	2.58182680	-0.25238691	H -5.27156700	0.86434700	0.47493700
C -4.27075599	0.80344555	-1.53846380	C -4.51334500	-2.82432100	-0.38655000
C -4.03189603	3.50536843	-0.95302605	H -2.44949700	-2.20303800	-0.48387700
H -2.57193688	2.93625471	0.50490534	C -5.82213600	-2.41831000	-0.16591800
C -5.02476209	1.73554981	-2.23952388	H -7.11079800	-0.76478600	0.31138000
H -4.37089919	-0.24944120	-1.77492118	H -4.30011300	-3.85611100	-0.64496700
C -4.91083802	3.08792864	-1.94491579	H -6.63511100	-3.13175600	-0.24399500
H -3.93196042	4.55941293	-0.71935073	C 3.53777500	-0.71348600	-0.53219700
H -5.70262199	1.40112714	-3.01715064	C 4.27058600	-1.74782800	0.05275300
H -5.50218439	3.81509921	-2.49043362	C 3.77017000	-0.39733900	-1.87411200
C 3.45886355	1.02684358	-0.53265705	C 5.22190200	-2.44479100	-0.68847300
C 3.39939366	2.32432696	-0.01525766	H 4.09667600	-2.02628200	1.08477900
C 4.28187669	0.76318860	-1.62714842	C 4.72099200	-1.08949500	-2.60790100
C 4.17793464	3.32925394	-0.57284396	H 3.19915600	0.39347800	-2.34819700
H 2.74067571	2.56274250	0.81689906	C 5.45111100	-2.11579800	-2.01676300
C 5.05170526	1.77662955	-2.18486596	H 5.77978400	-3.24872200	-0.22115200
H 4.32748973	-0.23429352	-2.04809832	H 4.88700000	-0.83325500	-3.64832000
C 5.00585297	3.05951642	-1.65627883	H 6.19015600	-2.66074300	-2.59327700
H 4.12995303	4.33014716	-0.15865821	C 3.10435200	1.90392500	0.42515600
H 5.68813257	1.55947777	-3.03560393	C 4.43590600	1.99590100	0.83876900
H 5.60877958	3.84912648	-2.09075553	C 2.43648200	3.06210400	0.04042500
C -3.27745920	-1.56041345	0.26950125	C 5.07788300	3.22456100	0.88368700
C -4.57317962	-1.60600283	0.79245977	H 4.98178400	1.10112900	1.11906400
C -2.73354511	-2.71214022	-0.29198025	C 3.08273600	4.29341600	0.07661800
C -5.30246527	-2.78529004	0.76161658	H 1.40339600	2.98715100	-0.28052300
H -5.02176413	-0.71372751	1.21582442	C 4.40126300	4.37809100	0.50053700

C -3.46746516	-3.89290141	-0.32753942	H 6.11045100	3.28218300	1.21076100
H -1.72699809	-2.68021059	-0.69094983	H 2.55056300	5.18753500	-0.22957100
C -4.75005171	-3.93203013	0.20043827	H 4.90450100	5.33844500	0.52994900
H -6.30548653	-2.80918781	1.17295906	C -2.94023300	2.11567500	-0.51143200
H -3.03273200	-4.78298822	-0.76859744	C -3.48572300	2.05455200	-1.79411700
H -5.32154865	-4.85323422	0.17504901	C -2.81412200	3.35834400	0.10770100
C 3.16429677	-1.85021254	-0.26647971	C -3.91126000	3.20962800	-2.43628400
C 4.48833961	-2.08690285	0.11466784	H -3.58010500	1.09897600	-2.29826100
C 2.47508709	-2.83482589	-0.96893623	C -3.24439500	4.51335300	-0.53323100
C 5.10466540	-3.28961374	-0.19704841	H -2.36292000	3.43446100	1.09049600
H 5.04671472	-1.32498392	0.64805837	C -3.79594900	4.44239100	-1.80604800
C 3.09562095	-4.03834207	-1.28553985	H -4.33118400	3.14512600	-3.43405700
H 1.44629274	-2.65784541	-1.25698175	H -3.14300900	5.47226100	-0.03659800
C 4.40834799	-4.26806006	-0.89913706	H -4.12854600	5.34451400	-2.30738900
H 6.13133925	-3.46315610	0.10562526	O -0.47967400	-3.78354300	-0.47681000
H 2.54871603	-4.79672206	-1.83451524	O 1.53640500	-3.12750400	-1.23796600
H 4.89150567	-5.20739376	-1.14410815	C -0.88093400	-3.69486800	-1.84067200
			H -1.87455800	-4.13841500	-1.89766700
			H -0.91667100	-2.65134600	-2.16687900
			H -0.19533900	-4.24660600	-2.48422400
			H 2.39813900	-2.81290100	-0.93301800
HRu_HCOO			¹TS-CO_{2,K}		
P -2.32644964	0.13893268	0.33713922	P -2.27537400	0.34905100	0.34530200
P 2.32574984	0.13827868	0.33689613	P 2.39433800	0.28401900	0.29301400
C -2.44077078	0.10106682	2.19683106	C -2.39934400	-0.03417500	2.14740500
C 2.44047944	0.09826042	2.19627015	C 2.51880800	0.08660900	2.13002700
H -2.41651166	-0.94899447	2.49924718	H -2.46269900	-1.12321900	2.19359200
H 2.41432127	-0.95196300	2.49792192	H 2.60256800	-0.98406700	2.35786200
H -3.36878372	0.55062980	2.55432304	H -3.29544200	0.37526300	2.61758700
H 3.36922661	0.54596387	2.55419267	H 3.40988500	0.57729900	2.52590900
C -1.22612190	0.81184660	2.77015114	C -1.13592500	0.45500800	2.83708200
C 1.22681444	0.81042963	2.77005433	C 1.25322500	0.62582800	2.76903400
H -1.22615001	0.72149659	3.86447592	H -1.03925700	-0.02796100	3.82143200
H 1.22695713	0.71985759	3.86435386	H 1.20325200	0.28804900	3.81493900
H -1.24222232	1.87714703	2.52375143	H -1.19622500	1.53675500	3.03408300
H 1.24410799	1.87574739	2.52380248	H 1.27042000	1.72596300	2.79269300
N -0.00002754	0.22019854	2.21143936	N 0.06186400	0.18484400	2.05931300
H -0.00031994	-1.78425941	0.33428558	O 0.08495300	0.56749000	-2.98674200
H -0.00045779	-0.80784761	2.42393708	C 0.06302200	0.30702200	-1.87049500
C -0.00071211	-2.78950031	1.07203319	C -1.70863700	-3.43417300	0.03022000
Ru -0.00025534	0.08066170	0.02340944	C 0.73571700	-2.76127400	-1.26698300
C -0.00007794	0.00930810	-1.83637368	O 0.02168700	-2.23792100	-0.17731900
O -0.00018909	0.00057134	-2.98964266	O -1.96030300	-3.20875200	1.16370300
O -0.00000112	-2.49651838	2.27708956	H 1.71107800	-2.27925400	-1.38469800
O -0.00161839	-3.80037214	0.41369515	H 0.91742100	-3.83876200	-1.13735400
H 0.00038364	1.66966040	-0.07059534	C -3.65090900	-0.55823900	-0.46821500
C 3.38781213	-1.24815723	-0.23791461	C -4.94917000	-0.51122600	0.04550500
C 4.27561437	-1.92322235	0.59929504	C -3.40812800	-1.25151300	-1.65049900
C 3.29266047	-1.63219211	-1.57646826	C -5.98315800	-1.15974200	-0.61130600
C 5.05539176	-2.96191730	0.10510491	H -5.15944500	0.03927200	0.95594500
H 4.36190885	-1.65577671	1.64564803	C -4.44883500	-1.89377100	-2.31256000
C 4.07737696	-2.66400907	-2.06898211	H -2.40081600	-1.30677500	-2.04522000
H 2.59427990	-1.13103840	-2.23660005	C -5.73417900	-1.84992600	-1.79393700
C 4.95965705	-3.32332300	-1.22887510	H -6.98726300	-1.12394400	-0.20345800
H 5.73417406	-3.48559297	0.76894541	H -4.24595200	-2.43950700	-3.22663300
H 3.98784893	-2.95622697	-3.10906353	H -6.54466100	-2.35537400	-2.30707400
H 5.56366295	-4.14727317	-1.61155970	C -2.84307400	2.09310300	0.14490500
C -3.38783871	-1.24927387	-0.23443717	C -3.24003700	2.89297800	1.21432100
C -4.28300149	-1.91532714	0.60228781	C -2.86916500	2.63137800	-1.14403700
C -3.28485281	-1.64430937	-1.56913908	C -3.65039400	4.20518500	1.00163200
C -5.06221418	-2.95592774	0.11135012	H -3.23463900	2.50570400	2.22599400
H -4.37554538	-1.63904306	1.64583120	C -3.28517600	3.93633500	-1.35623500
C -4.06906779	-2.67804325	-2.05855330	H -2.56524800	2.02587800	-1.99111100
H -2.58057622	-1.15049048	-2.22846909	C -3.67545900	4.72967600	-0.28212300
C -4.95861295	-3.33728084	-1.21900429	H -3.95409600	4.81499600	1.84543400
H -5.74675225	-3.47251734	0.77483643	H -3.30348900	4.33678300	-2.36375200
H -3.97331941	-2.97893829	-3.09559518	H -3.99796600	5.75140200	-0.44773500
H -5.56217119	-4.15375482	-1.59912354	C 3.67241000	-0.84000600	-0.40079300
C -3.31124222	1.62888918	-0.14000350	C 3.97970500	-0.71038600	-1.76099900
C -4.70485931	1.62389603	-0.04297549	C 4.26964400	-1.87244000	0.32848600
C -2.66721804	2.78319244	-0.57816046	C 4.87738900	-1.57130600	-2.36906400
C -5.43534254	2.75873660	-0.36432500	H 3.51935600	0.07896200	-2.34619400
H -5.22562038	0.72534338	0.26894616	C 5.16404200	-2.74153400	-0.28972100
C -3.40054313	3.91925655	-0.90149195	H 4.06173500	-2.00797300	1.38281900
H -1.58721221	2.77943300	-0.67016401	C 5.47342500	-2.59391800	-1.63294600
C -4.78409161	3.91009798	-0.79346303	H 5.11071800	-1.44929100	-3.42084600

H -6.51696549 2.74173927 -0.28794285	H 5.62012500 -3.53528100 0.29137100
H -2.88709781 4.81031057 -1.24564609	H 6.17430400 -3.27050900 -2.10860300
H -5.35666642 4.79458676 -1.04989964	C 3.13846200 1.93898500 -0.04109300
C 3.31023390 1.62870714 -0.13904956	C 2.37273900 3.03158100 -0.44500300
C 2.66782507 2.77760283 -0.59322939	C 4.51507200 2.11451800 0.14893000
C 4.70274350 1.62829814 -0.02680421	C 2.96467900 4.27171600 -0.65149000
C 3.40164937 3.91303667 -0.91788105	H 1.30779200 2.90879800 -0.59869100
H 1.58884500 2.77028267 -0.69618722	C 5.10299000 3.35358100 -0.05388400
C 5.43363439 2.76257802 -0.34894131	H 5.13232600 1.27372300 0.44572000
H 5.22248479 0.73353880 0.29765569	C 4.32957600 4.43789400 -0.45492300
C 4.78390187 3.90862419 -0.79449825	H 2.35414700 5.10890400 -0.97133400
H 2.88961830 4.79989797 -1.27472837	H 6.17024100 3.47247700 0.09771600
H 6.51438272 2.74936391 -0.26042121	H 4.79057400 5.40597400 -0.61605100
H 5.35684011 4.79267282 -1.05164240	H 0.01181700 1.62078100 0.03900600
	Ru 0.04421000 0.03062800 0.01681900
	H 0.19051300 -2.65096500 -2.21580800
	K 0.59075600 -3.21140500 2.35429100
	O -1.80309700 -3.93852200 -1.02045300
HRu_OOCH	
P -2.32124628 0.18317324 0.31905247	
P 2.32090482 0.18192340 0.32049315	
C -2.44723968 0.09353645 2.17915272	
C 2.44555571 0.09052532 2.18050546	
H -2.45339584 -0.96663289 2.44464662	
H 2.44980187 -0.96983596 2.44527113	
H -3.36641498 0.55428340 2.54574047	
H 3.36516007 0.54959419 2.54813277	
C -1.22177036 0.75780921 2.78337316	
C 1.22059570 0.75621163 2.78423161	
H -1.23309865 0.63200635 3.87475221	
H 1.23114121 0.63012745 3.87558232	
H -1.21979141 1.83143716 2.57289097	
H 1.22007021 1.82989409 2.57399016	
N -0.00077254 0.17242528 2.21427687	
H -0.00143118 -0.86139256 2.37913432	
C -0.00103144 -2.86479625 0.97074559	
Ru -0.00008035 0.15571799 0.00125051	
C 0.00042051 0.33888251 -1.84492817	
O 0.00074131 0.50680965 -2.98728442	
O -0.00164931 -2.55541183 2.17854715	
H 0.00029937 1.74752185 0.10424564	
C 3.34568761 -1.22590703 -0.27171468	
C 4.35694337 -1.80193304 0.49858872	
C 3.09339223 -1.73272584 -1.54629909	
C 5.10926686 -2.85724727 -0.00213270	
H 4.56230434 -1.43860403 1.49908896	
C 3.85122817 -2.78126792 -2.04836008	
H 2.28807872 -1.31775482 -2.14004678	
C 4.86039780 -3.34559420 -1.27811256	
H 5.88842163 -3.29969608 0.60877584	
H 3.64189270 -3.16748683 -3.03957493	
H 5.44605553 -4.17073475 -1.66797743	
C -3.34590595 -1.22516406 -0.27208734	
C -4.36046430 -1.79728054 0.49684113	
C -3.09000741 -1.73666177 -1.54406372	
C -5.11251844 -2.85328688 -0.00277595	
H -4.56866816 -1.43022507 1.49540198	
C -3.84758516 -2.78592240 -2.04507249	
H -2.28202432 -1.32489015 -2.13638882	
C -4.86005290 -3.34627751 -1.27628181	
H -5.89427604 -3.29264807 0.60703448	
H -3.63543173 -3.17583109 -3.03424031	
H -5.44550767 -4.17196925 -1.66528710	
C -3.32897752 1.66541562 -0.13576961	
C -4.72432156 1.61842936 -0.17167213	
C -2.68612057 2.86822419 -0.42276383	
C -5.45897291 2.75680067 -0.47313759	
H -5.24314422 0.68618493 0.01917976	
C -3.42326122 4.00762971 -0.72279696	
H -1.60254034 2.89694382 -0.41948692	
C -4.81015549 3.95529462 -0.74704659	
H -6.54187701 2.70509755 -0.50242451	
H -2.90937339 4.93572715 -0.94802408	
H -5.38543345 4.84258719 -0.98745784	
C 3.32964476 1.66411802 -0.13213178	
C 2.68758517 2.86588235 -0.42503467	

C 4.72519611	1.61780574	-0.16071646
C 3.42565601	4.00499728	-0.72400186
H 1.60399330	2.89405090	-0.42692274
C 5.46077354	2.75587709	-0.46092862
H 5.24352600	0.68624690	0.03488724
C 4.81266882	3.95336674	-0.74099006
H 2.91243688	4.93230484	-0.95395202
H 6.54384631	2.70477152	-0.48443993
H 5.38868906	4.84043187	-0.98046399
O -0.00030421	-2.09866624	-0.03203241
H -0.00109726	-3.94474491	0.72025136
TS-HCOOH-H⁻		
P 2.31134071	-0.14212912	0.19741971
P -2.31106497	-0.15359551	0.19147914
C 2.44811654	-0.02911260	2.06037822
C -2.45314206	-0.04041751	2.05397505
H 2.47828915	1.03327411	2.31683285
H -2.48859447	1.02191593	2.30996513
H 3.36342235	-0.49745341	2.42681297
H -3.36728602	-0.51265749	2.41830598
C 1.22363733	-0.67391721	2.68471977
C -1.22735499	-0.67954046	2.68159529
H 1.23809655	-0.53493016	3.77439403
H -1.24529516	-0.54051266	3.77121066
H 1.20595056	-1.74703245	2.48133196
H -1.20418649	-1.75258408	2.47836202
N -0.00245896	-0.09434756	2.10884218
H -0.00351718	1.57213558	-0.07104227
H -0.00504651	0.91230948	2.29163303
C -0.01007931	3.14571483	0.69889330
Ru 0.00053538	-0.15373042	-0.10455375
C 0.00323821	-0.27114121	-1.95263026
O 0.00496438	-0.35965066	-3.10506184
O -0.01077533	2.87657816	1.85530886
O -0.01112620	3.84757247	-0.23962044
H 0.00438169	-1.80082953	0.05175198
C -3.34704778	1.24748349	-0.40682097
C -4.38531560	1.79796610	0.34695386
C -3.07611116	1.77552405	-1.66889400
C -5.13992283	2.85135267	-0.15480539
H -4.61211527	1.41492454	1.33559216
C -3.83732818	2.82054719	-2.17350808
H -2.25197409	1.38053338	-2.25060182
C -4.86979879	3.36153810	-1.41781314
H -5.93838159	3.27449916	0.44485923
H -3.61100218	3.22334494	-3.15423479
H -5.45682139	4.18528569	-1.80842156
C 3.34160190	1.26466795	-0.39730323
C 4.37634179	1.81864178	0.35878604
C 3.06985311	1.79363538	-1.65880054
C 5.12671552	2.87636949	-0.14016094
H 4.60363903	1.43489292	1.34704103
C 3.82689380	2.84304256	-2.16062173
H 2.24824732	1.39587861	-2.24219421
C 4.85586259	3.38748748	-1.40264689
H 5.92242939	3.30216861	0.46127216
H 3.59996442	3.24650150	-3.14093619
H 5.43957495	4.21461700	-1.79106488
C 3.34625259	-1.61869084	-0.23297412
C 4.73948925	-1.55142024	-0.30404382
C 2.71621788	-2.83862950	-0.47096754
C 5.48513911	-2.68748944	-0.58794066
H 5.24907538	-0.60685290	-0.15471651
C 3.46438941	-3.97530354	-0.75355885
H 1.63227906	-2.87765722	-0.44213793
C 4.84952439	-3.90342872	-0.81081541
H 6.56614914	-2.61990929	-0.64457609
H 2.95990679	-4.91711131	-0.94035545
H 5.43332498	-4.78868592	-1.03815360
C -3.33744034	-1.63554770	-0.24078484
C -2.70061302	-2.85168763	-0.48001838
C -4.73101828	-1.57587305	-0.31209555
C -3.44243969	-3.99212378	-0.76423921
H -1.61649604	-2.88480446	-0.45065225
C -5.47032507	-2.71568828	-0.59749685
H -5.24583179	-0.63428582	-0.16180420

C	-4.82792889	-3.92782368	-0.82173385
H	-2.93272673	-4.93091204	-0.95203043
H	-6.55168289	-2.65403695	-0.65425811
H	-5.40677901	-4.81601675	-1.05027798
HRu_CO₂			
P	-2.30092542	0.22891149	0.29740744
P	2.30073182	0.22898193	0.29754292
C	-2.45227090	0.15319980	2.16501851
C	2.45194146	0.15291313	2.16513367
H	-2.50505120	-0.90326679	2.44250127
H	2.50450552	-0.90360505	2.44245423
H	-3.36322725	0.64215090	2.51519296
H	3.36294566	0.64166312	2.51546851
C	-1.22496197	0.79284755	2.78801595
C	1.22467985	0.79266497	2.78811685
H	-1.24844983	0.67598600	3.88056107
H	1.24809588	0.67573116	3.88065453
H	-1.19092295	1.86023992	2.55935461
H	1.19077888	1.86007806	2.55952198
N	-0.00016275	0.19401635	2.23009715
H	-0.00001689	-1.41310311	-0.02605095
H	-0.00024840	-0.80192425	2.44097811
C	0.00098326	-3.72878700	1.37161956
Ru	-0.00009109	0.27084984	0.00367420
C	-0.00005675	0.39746033	-1.83947819
O	-0.00005120	0.48042193	-2.99386120
O	0.00112432	-3.11208349	2.35835837
O	0.00088035	-4.39370789	0.42684078
H	-0.00015936	1.94321166	0.23422643
C	3.31161023	-1.21169042	-0.25690677
C	4.38767799	-1.71102371	0.47973893
C	2.97887516	-1.82639831	-1.46349099
C	5.11841371	-2.79858938	0.01611120
H	4.66427494	-1.25769810	1.42531185
C	3.71751750	-2.90406764	-1.93311695
H	2.12220017	-1.47121067	-2.02364879
C	4.78733348	-3.39397140	-1.19424910
H	5.94754207	-3.17960241	0.60248473
H	3.44578304	-3.37136702	-2.87305331
H	5.35740451	-4.24205662	-1.55718574
C	-3.31165278	-1.21197874	-0.25674863
C	-4.38804658	-1.71087685	0.47972146
C	-2.97844013	-1.82734677	-1.46286121
C	-5.11863800	-2.79865426	0.01637249
H	-4.66501596	-1.25702502	1.42493442
C	-3.71694064	-2.90523207	-1.93222259
H	-2.12149651	-1.47250321	-2.02282470
C	-4.78708298	-3.39469383	-1.19353717
H	-5.94802293	-3.17932241	0.60260704
H	-3.44483526	-3.37304546	-2.87179584
H	-5.35704173	-4.24294842	-1.55625719
C	-3.36374251	1.67710723	-0.17030987
C	-4.74680198	1.57740533	-0.33510220
C	-2.75099224	2.91708472	-0.34485658
C	-5.50146663	2.70096709	-0.64620899
H	-5.24158051	0.61862207	-0.23791785
C	-3.50849873	4.04083717	-0.65177369
H	-1.67098201	2.97735219	-0.25027670
C	-4.88497409	3.93671777	-0.80147230
H	-6.57420709	2.60748394	-0.77678235
H	-3.01710370	4.99830350	-0.78739238
H	-5.47546177	4.81207208	-1.04931658
C	3.36351998	1.67732194	-0.16979165
C	2.75064227	2.91712643	-0.34506760
C	4.74671856	1.57785225	-0.33357736
C	3.50814028	4.04094954	-0.65176761
H	1.67056361	2.97720926	-0.25115740
C	5.50137897	2.70148168	-0.64443019
H	5.24161728	0.61918688	-0.23580835
C	4.88473852	3.93706649	-0.80046717
H	3.01664970	4.99828270	-0.78797870
H	6.57423306	2.60818904	-0.77420287
H	5.47522469	4.81247487	-1.04812449
¹Ru amido			
H	-0.08741900	1.85876300	-0.09226700

Ru	-0.01727900	0.21889500	0.05432300
C	-0.02835100	0.25557400	-1.85917800
O	-0.03696300	0.34216400	-3.00699800
N	-0.01615200	0.56998800	2.06243900
P	-2.30925300	-0.06000800	0.41330600
P	2.29033100	0.04180400	0.39829700
C	2.38274100	0.18122000	2.25552500
C	-2.36901100	-0.02858800	2.27606400
H	3.32793500	0.61601900	2.58663900
H	-3.34101100	0.30542200	2.64335600
H	2.30010000	-0.83204500	2.65541000
H	-2.20376000	-1.05078400	2.62197300
C	-1.24363100	0.87219900	2.76423600
C	1.19202600	1.00447200	2.72791900
H	-1.50915400	1.92871500	2.59724200
H	1.36125500	2.07181800	2.51427700
H	-1.10384900	0.74895700	3.84702500
H	1.08318900	0.91334400	3.81727000
C	3.23356300	-1.49518600	0.00725200
C	-3.17168000	-1.63364000	-0.03349700
C	4.57863400	-3.84643900	-0.70001600
C	-4.27504300	-4.09651300	-0.78049300
C	3.04630700	-2.07281400	-1.25080000
C	-2.64517000	-2.83128000	0.45961400
C	4.10479500	-2.11423800	0.90581700
C	-4.24020500	-1.69070200	-0.92802700
C	4.76698100	-3.28582100	0.55588800
C	-4.78457300	-2.91540100	-1.30017500
C	3.71938800	-3.23239100	-1.60510800
C	-3.20106300	-4.04981300	0.10326500
H	2.35714800	-1.61545800	-1.95247000
H	-1.77489100	-2.80885000	1.10834400
H	4.27655000	-1.68785200	1.88747700
H	-4.65211200	-0.77806400	-1.34121500
H	5.43555400	-3.75766200	1.26795200
H	-5.61264800	-2.94147400	-2.00026700
H	3.56317100	-3.66522700	-2.58706500
H	-2.78476900	-4.96802300	0.50315200
H	5.09624400	-4.75939400	-0.97260900
H	-4.70241800	-5.05009700	-1.06986600
C	3.43838500	1.36972600	-0.20136900
C	-3.52370300	1.24737800	-0.07123300
C	5.10731800	3.45422100	-1.02315600
C	-5.30636300	3.26995900	-0.80289200
C	2.90230700	2.60747500	-0.55223900
C	-4.82947600	1.25681900	0.42683800
C	4.81967000	1.18190900	-0.27811900
C	-3.12271400	2.26299800	-0.93510800
C	5.64834400	2.21909900	-0.68523400
C	-4.01155800	3.26706000	-1.30307600
C	3.73340600	3.64515500	-0.95674900
C	-5.71429300	2.26329900	0.06607300
H	1.82496500	2.74005000	-0.51381000
H	-5.16486600	0.46851400	1.09280800
H	5.25234900	0.21863800	-0.03302100
H	-2.09990400	2.27214200	-1.29491100
H	6.71954000	2.05941500	-0.74568400
H	-3.68669900	4.05119300	-1.97813100
H	3.30298100	4.60256800	-1.23014400
H	-6.72425500	2.26139700	0.46151000
H	5.75559900	4.26215500	-1.34461600
H	-5.99812800	4.05586700	-1.08585400
¹HRu-H			
H	0.61587900	1.81910500	-0.01141300
Ru	-0.07465700	0.32529100	-0.15301300
C	-0.11418600	0.62470300	-1.99002600
O	-0.15103700	0.81260900	-3.12825300
N	-0.02540100	-0.00612700	2.10145800
P	2.58233100	0.16891200	0.23499500
P	-2.58458000	0.09156000	0.33406000
C	-2.49268200	-0.04827300	2.19457400
C	2.43296700	0.20215500	2.09876700
H	-3.35278000	-0.58627500	2.59957300
H	3.34373600	-0.18174600	2.56213500
H	-2.50621300	0.96571300	2.60662400
H	2.33620700	1.24847400	2.40184000

C	1.23501000	-0.59613100	2.57858300
C	-1.20141200	-0.74257300	2.59609300
H	1.28064000	-1.62065200	2.20032200
H	-1.15834300	-1.74963100	2.17311500
H	1.23702500	-0.64673300	3.67709600
H	-1.15797400	-0.84147600	3.69005200
C	-3.92227700	1.31635800	0.04187200
C	3.82241100	1.49427500	-0.05476600
C	-5.84352100	3.25661600	-0.58562600
C	5.53179500	3.63023000	-0.69150100
C	-4.14232800	1.70289300	-1.28572000
C	3.52684900	2.80100100	0.35697000
C	-4.67291100	1.92762100	1.04920400
C	4.97524900	1.28682600	-0.82031800
C	-5.62398900	2.89188500	0.73587500
C	5.82037600	2.34340200	-1.13041900
C	-5.10064200	2.65460000	-1.59627700
C	4.37728100	3.85282000	0.05043400
H	-3.55205900	1.25746800	-2.07979000
H	2.61045900	3.00345400	0.90102100
H	-4.53397900	1.65037000	2.08743600
H	5.21863800	0.29164400	-1.17261200
H	-6.19939400	3.35451400	1.53058000
H	6.71237300	2.15736800	-1.71915700
H	-5.25889200	2.93806100	-2.63090900
H	4.13069200	4.85481700	0.38506400
H	-6.58565600	4.00890000	-0.82786800
H	6.19406900	4.45355300	-0.93420600
C	-3.38213300	-1.50714100	-0.13827900
C	3.55889300	-1.38675100	-0.02125000
C	-4.49364400	-3.97605900	-0.82387800
C	4.95189800	-3.76038300	-0.52269400
C	-2.56856300	-2.54834400	-0.58616300
C	4.70887000	-1.70452800	0.70644800
C	-4.76155000	-1.71021800	-0.05148200
C	3.12089500	-2.27310200	-1.00454300
C	-5.31236100	-2.93773000	-0.39239200
C	3.81388600	-3.45257100	-1.25535600
C	-3.12255800	-3.77856400	-0.92023100
C	5.40000300	-2.88284000	0.45912300
H	-1.49966300	-2.37814900	-0.68440500
H	5.08413300	-1.01993800	1.45976200
H	-5.40906300	-0.90319500	0.27321400
H	2.22280100	-2.03670000	-1.56434900
H	-6.38513300	-3.08330300	-0.32492200
H	3.46138900	-4.13087500	-2.02465800
H	-2.48005500	-4.57976100	-1.26901300
H	6.29305500	-3.11476700	1.02960600
H	-4.92655400	-4.93353100	-1.09219900
H	5.49254300	-4.68045400	-0.71626700
H	-0.07692800	0.94491700	2.45984400
H	0.42400200	-1.22013100	-0.45507300
¹H Ru-OCOOCH₃			
P	-2.59621900	0.23023100	0.26827100
P	2.62383300	0.18938900	0.28243900
C	-2.41877800	0.22500500	2.12669100
C	2.46475600	0.09862900	2.13788000
H	-2.34076400	-0.81964400	2.43468000
H	2.32310700	-0.94951900	2.40917000
H	-3.31125600	0.64208400	2.59661700
H	3.37877600	0.45304500	2.61814900
C	-1.18197500	0.97684200	2.59201200
C	1.26449600	0.90695100	2.60844000
H	-1.11673200	0.90144800	3.68685000
H	1.18705100	0.82769000	3.70173300
H	-1.24476900	2.03788800	2.33697700
H	1.38525300	1.96765300	2.36697100
N	0.03012300	0.41379600	1.98160200
C	0.09210400	0.74521200	-2.09831500
O	0.10212800	0.90281200	-3.23775000
C	-0.03107700	-2.56198800	0.52608100
O	-0.03558000	-2.33390900	1.74737600
O	-0.02291100	-1.72537700	-0.42570500
H	0.00118900	-0.62228700	2.08345400
H	-0.52302400	2.02060500	-0.16874800
Ru	0.06293900	0.51307500	-0.23963000

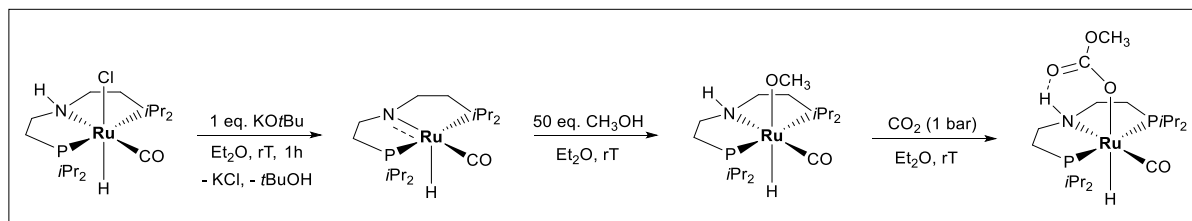
C	3.79865000	-1.15936300	-0.13223700
C	4.78833300	-0.97405100	-1.10208800
C	3.61266600	-2.43796000	0.40415400
C	5.59413100	-2.03263700	-1.49794400
H	4.93695800	0.00360900	-1.54571900
C	4.42410100	-3.49146300	0.00749300
H	2.82643500	-2.62658600	1.12660000
C	5.41965700	-3.29382800	-0.94175200
H	6.36201700	-1.86899100	-2.24619600
H	4.26931700	-4.47371200	0.43993300
H	6.05017500	-4.11950700	-1.25174600
C	3.59798800	1.73692400	0.05095300
C	3.05207200	2.77724100	-0.69910100
C	4.85928900	1.90678800	0.62938300
C	3.75174700	3.96730500	-0.86857400
H	2.07212200	2.65443500	-1.14743200
C	5.55745900	3.09289600	0.45785300
H	5.30552100	1.10250200	1.20462400
C	5.00335500	4.12641700	-0.29125700
H	3.31542400	4.76851000	-1.45451600
H	6.53694700	3.21192500	0.90795600
H	5.55034000	5.05322300	-0.42461700
C	-3.77589200	-1.15575700	-0.02175700
C	-4.82982400	-1.02494600	-0.93115900
C	-3.53739800	-2.41043000	0.55034900
C	-5.64130300	-2.10978700	-1.23425100
H	-5.02591400	-0.06747400	-1.39931000
C	-4.35488100	-3.49042500	0.24798400
H	-2.70536300	-2.56064600	1.22958400
C	-5.41168300	-3.34568600	-0.64275300
H	-6.45890100	-1.98552700	-1.93616400
H	-4.15648400	-4.45190900	0.70858900
H	-6.04715100	-4.19173100	-0.87929800
C	-3.63257200	1.72486900	-0.05227500
C	-4.80093200	1.98395700	0.66889400
C	-3.25722900	2.60675700	-1.06442000
C	-5.56966600	3.10489100	0.38954300
H	-5.12704100	1.29732200	1.44266300
C	-4.02931600	3.72812300	-1.34765300
H	-2.35049200	2.41731700	-1.62583200
C	-5.18343200	3.98083000	-0.61947000
H	-6.47456000	3.29317400	0.95699300
H	-3.72473200	4.40441800	-2.13866500
H	-5.78479400	4.85639800	-0.83813600
O	-0.03035800	-3.87623300	0.17702700
C	-0.03904100	-4.17828900	-1.21566400
H	0.84822000	-3.78158000	-1.71199200
H	-0.04594800	-5.26603800	-1.27851900
H	-0.92640100	-3.77074700	-1.70264600
TS-CH			
P	-2.56085500	0.15892600	0.19683400
P	2.63299100	0.16865600	0.31105800
C	-2.36092700	0.01623400	2.04303000
C	2.53531000	0.10350900	2.17013800
H	-2.22082700	-1.04715100	2.25396500
H	2.46945300	-0.94863800	2.45342800
H	-3.26791300	0.34414800	2.55540100
H	3.43181400	0.52990400	2.62352800
C	-1.16122000	0.78420700	2.57410200
C	1.28928000	0.83846600	2.64083900
H	-1.13642200	0.68502400	3.66856700
H	1.20787800	0.75648100	3.73334400
H	-1.23657200	1.84866600	2.33873900
H	1.34149400	1.90253200	2.39281900
N	0.09097700	0.26693700	2.00217000
O	0.20854400	0.34624100	-3.21807500
H	-0.19609700	-1.40615700	-0.08945800
H	0.12686800	-0.75700200	2.15420500
C	-0.05861100	-2.73945000	0.69888800
O	0.47475200	-2.50125500	1.78598600
H	-0.62429700	1.72264100	-0.22727100
C	0.20296300	0.33633800	-2.06385200
Ru	0.17713200	0.31019800	-0.20001400
C	3.89806500	-1.08869100	-0.12625600
C	3.78676200	-2.38206700	0.39447600
C	4.89510900	-0.81828500	-1.06740600

C	4.68688400	-3.36644500	0.01227700
H	2.97927800	-2.63411000	1.07272900
C	5.78678100	-1.81115200	-1.45063800
H	4.98297900	0.17218300	-1.49811400
C	5.69154900	-3.08584100	-0.90651100
H	4.59162700	-4.36311500	0.42870000
H	6.55947400	-1.58472600	-2.17732300
H	6.39045600	-3.85952900	-1.20442300
C	3.47623800	1.78338500	0.01486200
C	4.71845900	2.07200900	0.58735100
C	2.85422100	2.74957500	-0.77344400
C	5.32215900	3.30263300	0.37462200
H	5.22543200	1.32666600	1.19090400
C	3.46004700	3.98322300	-0.98635600
H	1.88604000	2.53378300	-1.21292500
C	4.69268700	4.26134700	-0.41315900
H	6.28705200	3.51423000	0.82225200
H	2.96473300	4.72593400	-1.60178900
H	5.16580800	5.22292800	-0.57907500
C	-3.43735200	1.78095000	-0.01224700
C	-4.57320700	2.09497600	0.73702500
C	-3.00450300	2.68201800	-0.98367500
C	-5.24651900	3.29175600	0.53495300
H	-4.95015000	1.39409900	1.47405900
C	-3.68399000	3.87692800	-1.19413800
H	-2.12456600	2.44917100	-1.57137000
C	-4.80166600	4.18687500	-0.43162700
H	-6.12548000	3.52226400	1.12716400
H	-3.33622300	4.56560700	-1.95629800
H	-5.32985000	5.12027400	-0.59258800
C	-3.98282800	-0.98398900	-0.14093300
C	-4.39962900	-2.00747800	0.71467300
C	-4.60049200	-0.87499800	-1.39442200
C	-5.41590100	-2.87860900	0.33547700
H	-3.93524700	-2.14126400	1.68289000
C	-5.61634100	-1.74016000	-1.76703000
H	-4.28856000	-0.09408500	-2.08066700
C	-6.03010800	-2.74911400	-0.90210500
H	-5.72709600	-3.66198500	1.01822000
H	-6.08628100	-1.62895000	-2.73824200
H	-6.82237500	-3.42925500	-1.19392300
O	0.68668600	-3.42865900	-0.23189300
C	0.13476000	-3.62248300	-1.51871900
H	0.93524700	-4.01538600	-2.14293100
H	-0.68643400	-4.34863100	-1.50428500
H	-0.20853100	-2.67064100	-1.94167900
O	-1.40965500	-3.05782400	0.72070200
H	-1.78586400	-3.01894200	-0.16644800
TS-CO₂			
P	-2.65114500	0.20649500	0.21904500
P	2.64574500	0.18594700	0.18561700
C	-2.48754000	0.08122900	2.06989500
C	2.46367900	-0.12463400	2.01376500
H	-2.50144900	-0.97769800	2.33551700
H	2.38536700	-1.20449800	2.16113700
H	-3.33634300	0.55756900	2.56456300
H	3.35011000	0.21360200	2.55431000
C	-1.18849600	0.71360600	2.53944600
C	1.22685700	0.57178900	2.55457700
H	-1.14558700	0.67235100	3.63698800
H	1.19802200	0.46411500	3.64797700
H	-1.14413300	1.76663100	2.24870900
H	1.26713500	1.64252300	2.33503600
N	-0.01178900	0.03717300	1.96814000
O	-0.01218900	0.40464200	-3.29298500
C	-0.01616700	0.18590600	-2.16189900
C	-0.08423000	-3.48954800	1.27459200
C	0.32568000	-2.83712300	-1.47187700
O	0.12886600	-2.17211400	-0.24299100
O	-0.44872500	-2.78895500	2.16091100
H	1.21082100	-2.45301900	-1.99095900
H	-0.07980600	-0.95518400	2.20405300
H	0.47185900	-3.90761600	-1.30218900
C	-4.01099900	-0.96721100	-0.16643600
C	-3.94387500	-2.28336400	0.30556500
C	-5.03471900	-0.62787100	-1.05647000

C	-4.89675800	-3.21858300	-0.07097200
H	-3.13881200	-2.58907200	0.96411000
C	-5.98265600	-1.56895600	-1.43460400
H	-5.09795700	0.37947700	-1.45080500
C	-5.92217900	-2.86604500	-0.94064100
H	-4.83146000	-4.23096700	0.31230800
H	-6.77353700	-1.28424900	-2.12010200
H	-6.66362700	-3.59935300	-1.23689600
C	-3.42048700	1.86686000	-0.00867500
C	-2.82443500	2.76941600	-0.88786000
C	-4.58440500	2.24553900	0.66621000
C	-3.37957700	4.02859500	-1.08894900
H	-1.91520400	2.48457800	-1.40370200
C	-5.13659700	3.50259000	0.46669400
H	-5.07429800	1.54994300	1.33931100
C	-4.53356300	4.39702000	-0.41188300
H	-2.90653300	4.72107700	-1.77633900
H	-6.04122000	3.78438300	0.99444800
H	-4.96634400	5.37907500	-0.56791500
C	4.01069700	-0.95070400	-0.28618000
C	5.12377700	-0.51675100	-1.01189600
C	3.86365400	-2.32131300	-0.04064500
C	6.08006000	-1.42502300	-1.44687300
H	5.25009000	0.53625000	-1.23343000
C	4.82514800	-3.22351900	-0.47097700
H	2.98259400	-2.69348200	0.47007800
C	5.93977000	-2.77963500	-1.17342000
H	6.94051200	-1.06867600	-2.00290600
H	4.69500300	-4.28021900	-0.26516800
H	6.68824000	-3.48644700	-1.51333500
C	3.41302900	1.86232300	0.14524700
C	2.84383700	2.82951100	-0.68230100
C	4.53667100	2.19767200	0.90563300
C	3.38697800	4.10783100	-0.75053100
H	1.96359100	2.57836800	-1.26252200
C	5.07691700	3.47411500	0.83909800
H	5.00559200	1.45507400	1.54232900
C	4.50170700	4.43182400	0.01011500
H	2.93504400	4.85049800	-1.39859900
H	5.95060800	3.72181400	1.43207400
H	4.92501600	5.42891600	-0.04167400
H	-0.02189000	1.58857600	-0.25183000
Ru	-0.02343300	-0.05186700	-0.30497000
H	-0.54196100	-2.71138600	-2.13060400
O	0.22260300	-4.51744000	0.80147800

Synthesis, characterization and solid-state structure of the complex [H-Ru-OCOOCH₃].

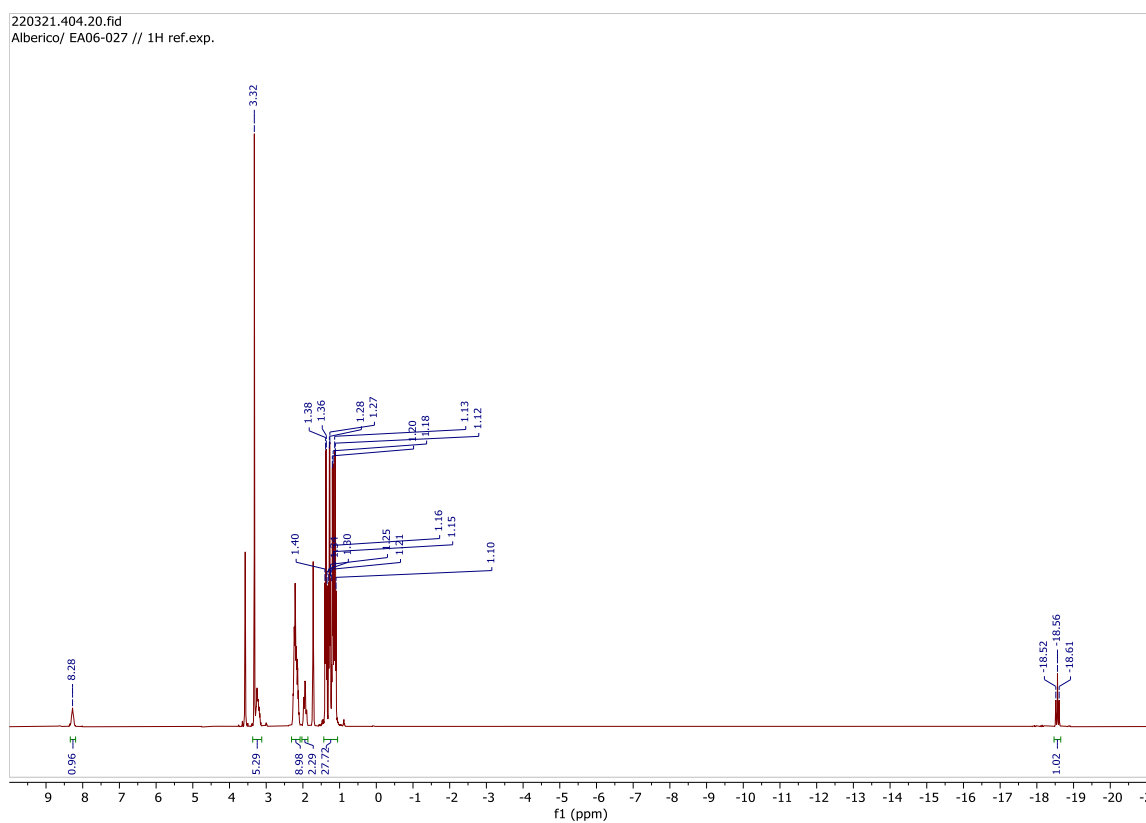
Synthesis of [H-Ru-OCOOCH₃]



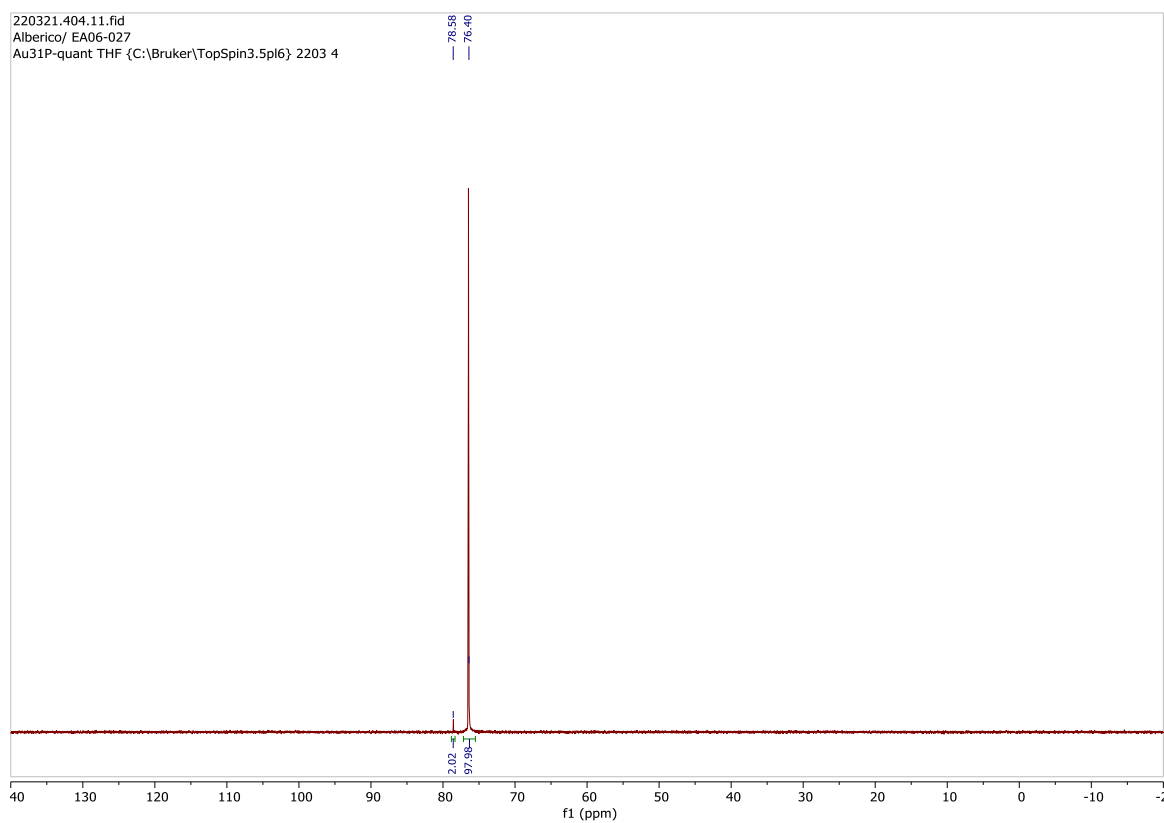
Supplementary Fig. 13 Synthesis of complex [H-Ru-OCOOCH₃].

To a suspension of [RuHCl(CO)(HN(CH₂CH₂P(CH(CH₃)₂)₂)₂)] (100 mg, 0.21 mmol, 1 eq.) in diethyl ether (10 mL) *t*BuOK (28.6 mg, 0.25 mmol, 1.2 eqs.) was added. The resulting orange suspension was stirred at room temperature for 1 hour and then filtered through a short pad of Celite S (pH ≈ 7) to remove KCl. To the resulting clear orange solution, CH₃OH (429 μL, 340 mg, 10.6 mmol, 50 eqs.) was added, upon which the orange color faded. The solution was then frozen with liquid nitrogen, the head space evacuated and argon replaced by CO₂. The solution was then let warm up to room temperature and stirred for 1 h. Solvents were removed in vacuo and the sample dried to leave a white solid complex [RuH(OC(O)OCH₃)(CO)(HN(CH₂CH₂P(CH(CH₃)₂)₂)₂)] ([H-Ru-OCOOCH₃]). Yield was quantitative. Crystals suitable for X-ray analysis were obtained by suspending the solid in *n*-heptane, heating until the solid dissolved, and then allowing the resulting solution to cool down to room temperature.

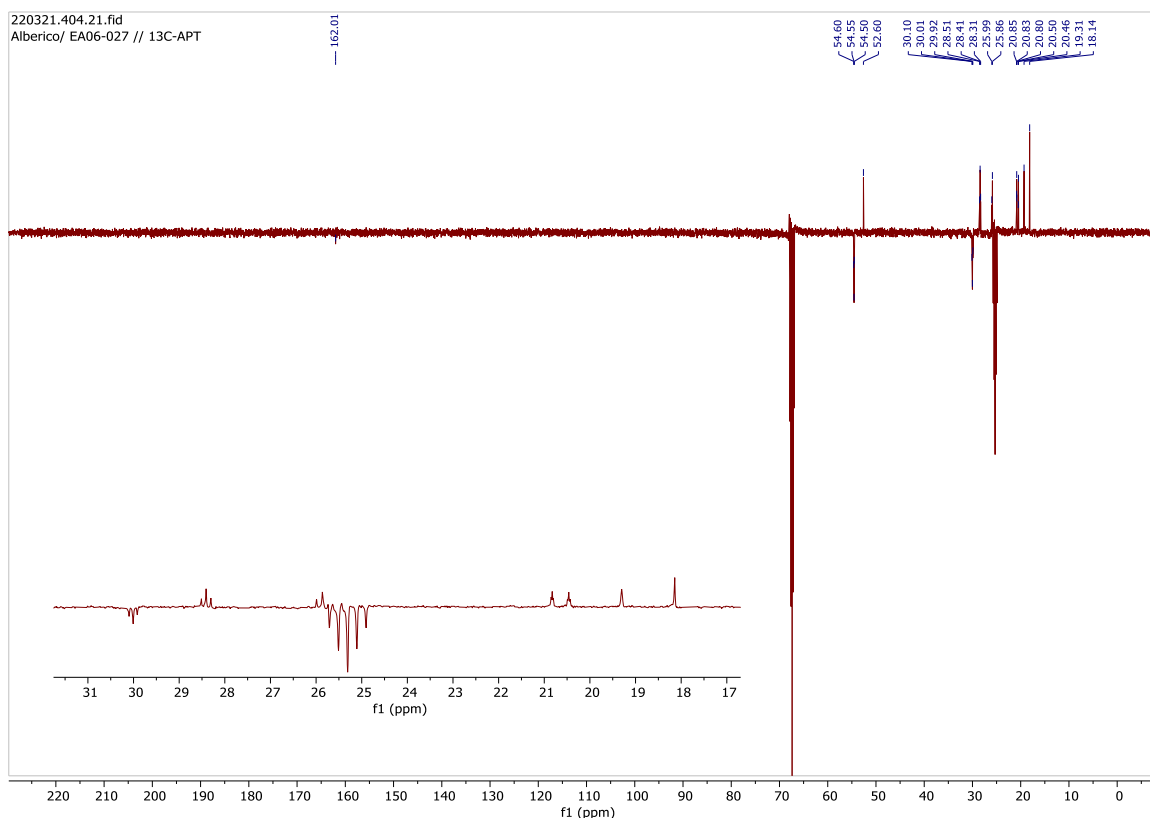
NMR of the complex [H-Ru-OCOOCH₃]



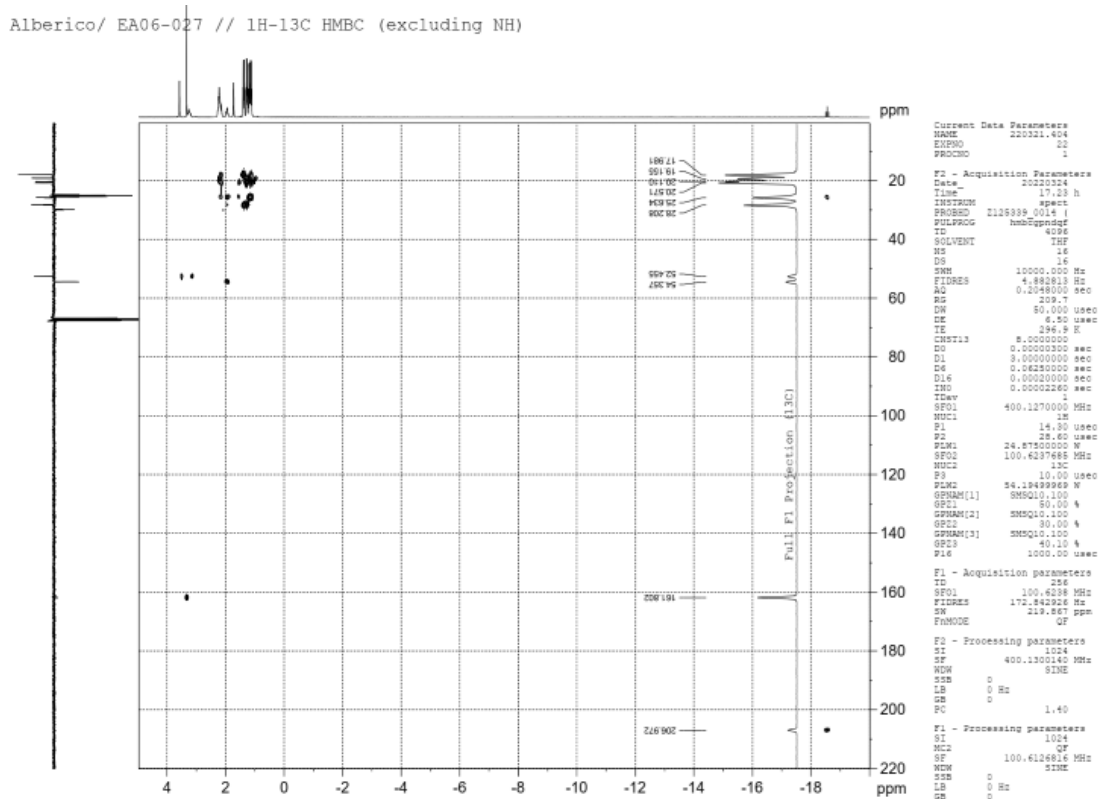
Supplementary Fig. 14 ¹H NMR of the complex [H-Ru-OCOOCH₃].



Supplementary Fig. 15 ³¹P{¹H} NMR of the complex [H-Ru-OCOOCH₃].



Supplementary Fig. 16 ^{13}C APT NMR of the complex $[\text{H-Ru-OCOOCH}_3]$.



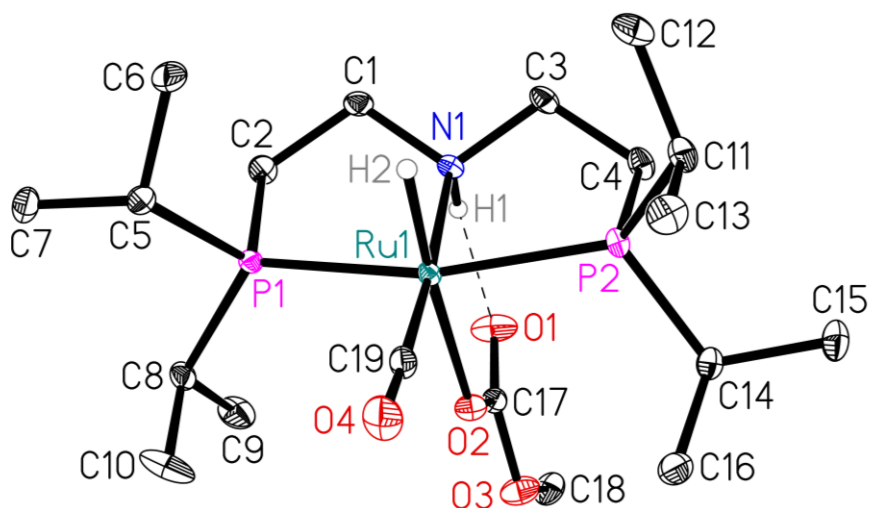
Supplementary Fig. 17 ^1H - ^{13}C HMBC NMR of the complex $[\text{H-Ru-OCOOCH}_3]$. The spectrum allows to detect the signal of the coordinated CO carbon (207.0 ppm) by means of its two-bond interaction with the ruthenium hydride and the signal of the carbonyl carbon of the RuOC(O)OCH_3 moiety (161.8 ppm) through its three-bond interaction with the CH_3O hydrogens.

X-ray crystal structure analysis of [H-Ru-OCOOCH₃]

Data were collected on a Bruker Kappa APEX II Duo diffractometer. The structure was solved by direct methods (SHELXS-97)¹⁵ and refined by full-matrix least-squares procedures on F^2 (SHELXL-2018)¹⁶. XP (Bruker AXS) was used for graphical representations.

Crystal data of [H-Ru-OCOOCH₃]: C₁₉H₄₁NO₄P₂Ru, $M = 510.54$, triclinic, space group $P\bar{1}$, $a = 8.3457(5)$, $b = 11.6744(7)$, $c = 12.9415(7)$ Å, $\alpha = 83.8813(12)$, $\beta = 80.1704(11)$, $\gamma = 70.8719(11)^\circ$, $V = 1172.06(12)$ Å³, $T = 150(2)$ K, $Z = 2$, 67818 reflections measured, 6368 independent reflections ($R_{\text{int}} = 0.0223$), final R values ($I > 2\sigma(I)$): $R_1 = 0.0180$, $wR_2 = 0.0443$, final R values (all data): $R_1 = 0.0187$, $wR_2 = 0.0448$, 261 parameters.

CCDC 2162048 contains the supplementary crystallographic data for this paper. These data are provided free of charge by the joint Cambridge Crystallographic Data Centre and Fachinformationszentrum Karlsruhe Access Structures service www.ccdc.cam.ac.uk/structures.

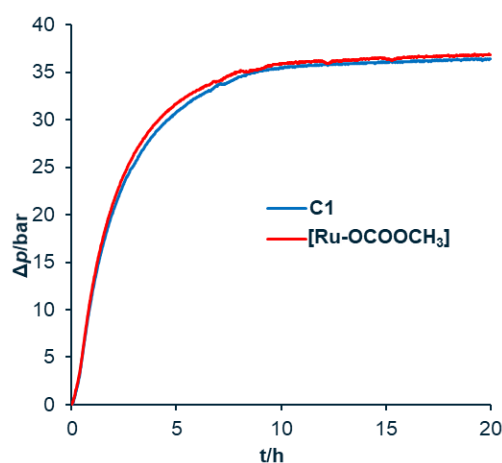


Supplementary Fig. 18 ORTEP representation of [H-Ru-OCOOCH₃]. Displacement ellipsoids correspond to 30% probability. C-bound hydrogen atoms are omitted for clarity. The intramolecular hydrogen bond is shown as dashed line (N1-H1...O1: N1-H1 = 0.86(2), H1...O1 = 1.97(2), N1...O1 = 2.7923(14) Å, N1-H1...O1 = 159(2)°).

H1 and H2 could be found from the difference Fourier map and were refined freely. All other H atoms were placed in idealized positions with $d(\text{C-H}) = 1.00$ Å (CH), 0.99 Å (CH₂), 0.98 Å (CH₃) and refined using a riding model with $U_{\text{iso}}(\text{H})$ fixed at 1.2 $U_{\text{eq}}(\text{C})$ for CH, CH₂ and 1.5 $U_{\text{eq}}(\text{C})$ for CH₃.

Comparative MF dehydrogenation using [H-Ru-OCOOCH₃] and catalyst precursor C1

Supplementary Table 16. Comparison test for dehydrogenation of MeOH, FA, and MF using C1 and [H-Ru-OCOOMe] catalysts.



Entry	Cat.	Δp_{20h} (bar)	V_{20h} (mL)	$H_2:CO_2$ (%)	CO (ppm)	TON	TOF _{max} (h ⁻¹)
1	C1	36.4	3,747	55:45	undetectable	21,046	8,672
2	[H-Ru-OCOOMe]	36.8	3,751	55:45	undetectable	21,069	8,931

General conditions: Under argon atmosphere 4 μ mol catalyst and 10 mmol K₃PO₄ (2.12 g) were added to a 100 mL autoclave. Then 10.0 mL triglyme, 168 mmol H₂O (3.0 mL) and 84 mmol MF (5.2 mL) were injected by a syringe under ice-bath. After that, the autoclave was flushed with N₂ (5 bar) and the pressure was released three times. The reaction was performed at 90 °C for 20 h. After that the autoclave was cooled down using ice-bath and the pressure was carefully released through a room temperature (25 °C) condenser (the water temperature was controlled by a thermostat) to a manual burette to get the gas volume. The gas was analyzed by GC. Additional CO₂ was collected via burette by adding HCl aqueous solution to the reaction liquid phase.

NMR study for the mechanistic insight of MF dehydrogenation

The mechanistic insight experiments were performed using Ru-PNP^{iPr} instead Ru-PNP^{Ph} as catalyst precursor for the following reasons: a) the Ru-PNP^{iPr} catalyst precursor performs almost as well (see Table 1, Entry 1); b) Ru-PNP^{Ph} derived amido species quickly degrades under basic conditions when no substrate is present,¹⁷ which might complicate the synthesis and detection of possible stable intermediates; and c) the NMR data of the ruthenium formate and methylcarbonate species are available from previous mechanistic investigations into the Ru-PNP^{iPr}-promoted MeOH aqueous reforming;¹ however, to the best of our knowledge, NMR data for the analogous Ru-PNP^{Ph} methylcarbonate derived species have not been reported.

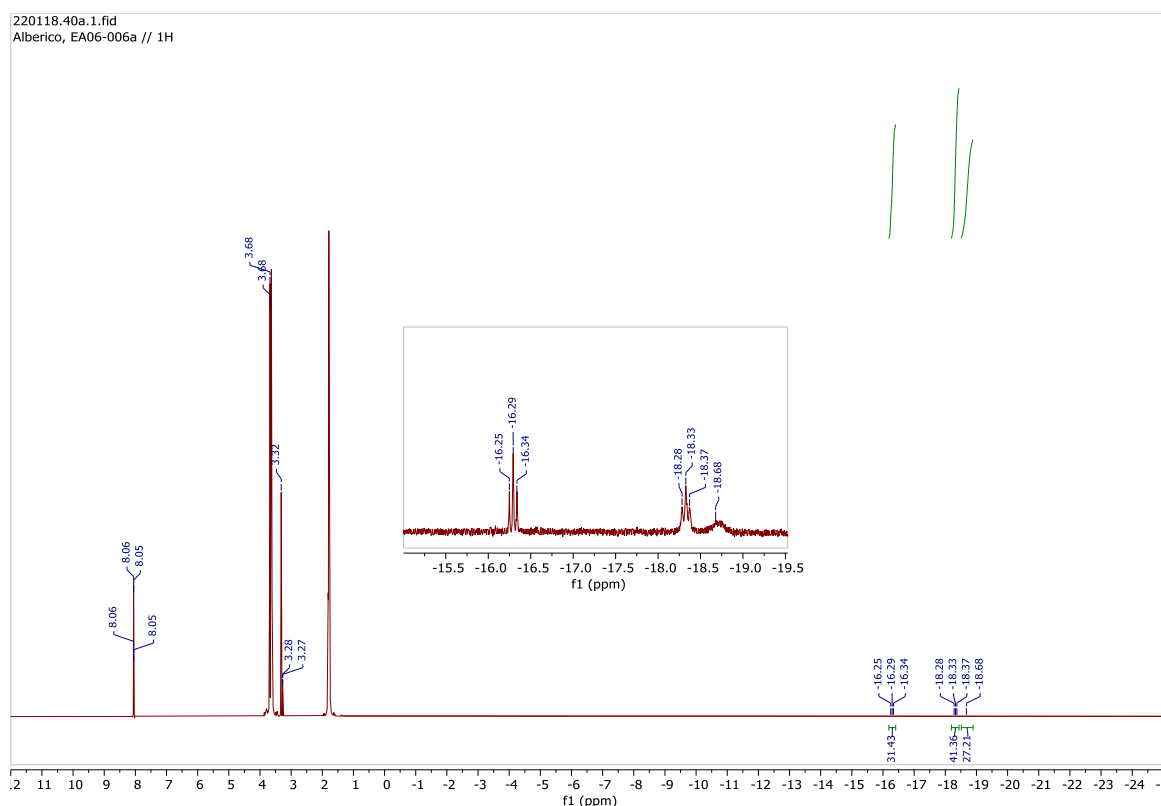
Supplementary Table 17. Selected NMR data for the species detected in the experiments of later on.

Complex	NH δ (ppm)	RuH δ (ppm)	P δ (ppm)
[H-Ru-PNP ^{iPr} -Cl]	3.78	- 15.99	75.22
[H-Ru-PNP ^{iPr} -OH]	-	- 16.44	76.31
[H-Ru-PNP ^{iPr} -OCH ₃]	-	- 17.71	74.21
[H-Ru-PNP ^{iPr} -OC(O)H]	8.35	- 18.21	76,24
[H-Ru-PNP ^{iPr} -OC(O)OH]	8.25	- 18.55	76.00
[H-Ru-PNP ^{iPr} -OC(O)OCH ₃]	8.04	- 18.65	76.35
Uncertain Ru species	9.64	- 18.11	77.80

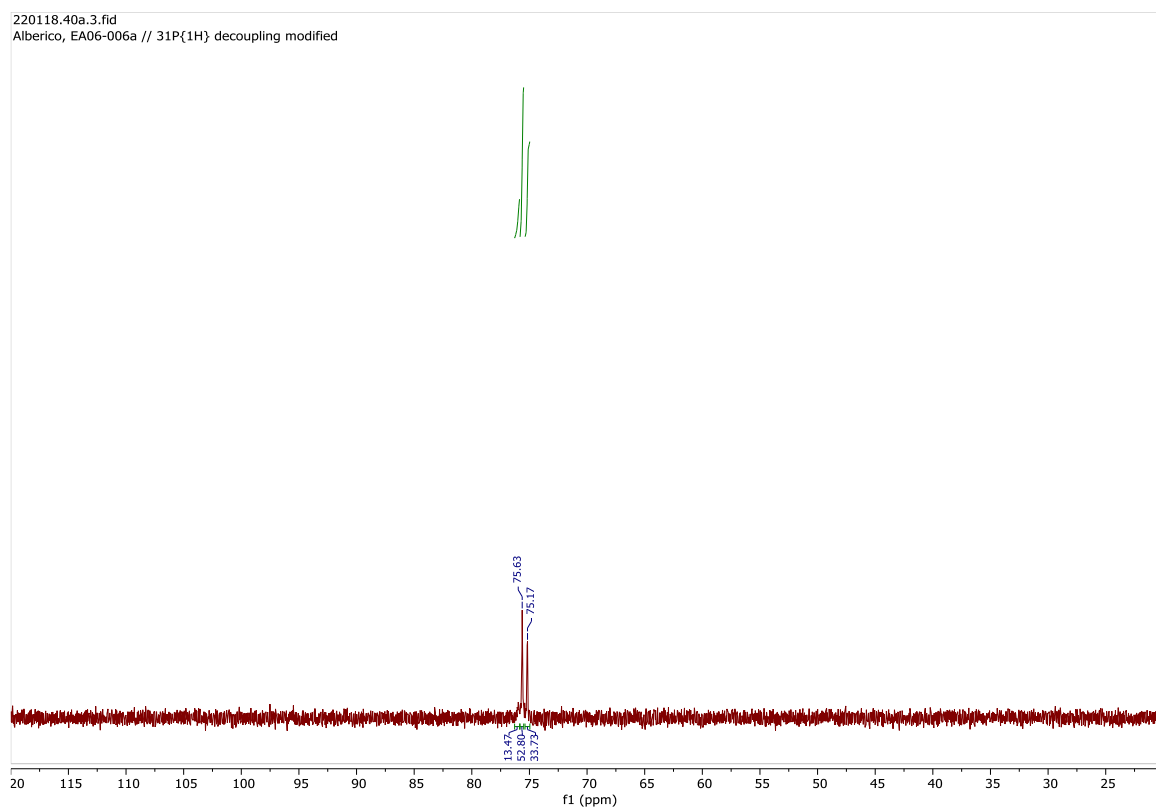
NMR data were recorded in THF-*d*₈. Although the chemical shift of hydrogen on nitrogen NH of the ligand may vary depending on sample concentration, data are reported here to highlight the low field shift due to hydrogen bonding, when present, with the X ligand on Ru (X = OC(O)H, OC(O)OH, and OC(O)OCH₃). Such effect is observed also for the unknown species. The complete set of NMR data for the known species can be found in reference.¹ Slight differences between the chemical shifts reported here, those in the two series of experiments (Supplementary Figs. 34 and 42, *vide infra*), and reference 1 are due to the different composition of the medium in which they were measured (variable amounts of H₂O, CH₃OH and HCOOCH₃).

Autoclave experiment – Detection of catalytic reaction resting states

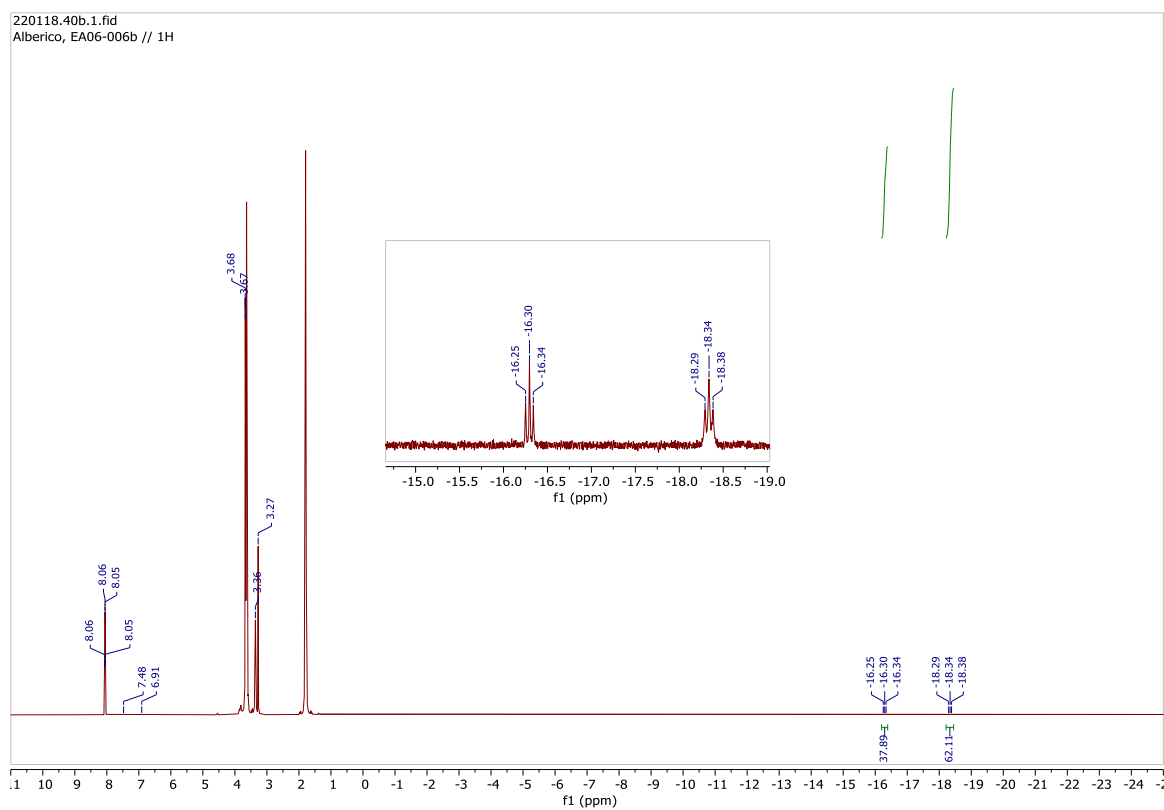
The catalyst precursor Ru-PNPⁱPr **C1** (80 mg, 0.170 mmol) and KOH (841 mg, 15 mmol) were introduced in a stainless-steel autoclave. After purging with argon, THF (15 mL), water (3 mL, 168 mmol) and methyl formate (5.2 mL, 84 mmol) were added, and the autoclave sealed. The resulting solution was stirred at room temperature for 15 minutes. A sample was then withdrawn through an autoclave inlet under a stream of argon, and 0.1 mL of tetrahydrofuran- d_8 added to it for lock purposes and subjected to ^1H and ^{31}P $\{^1\text{H}\}$ NMR analysis (Supplementary Figs. 19-20). The autoclave was sealed again, heated to 90 °C and kept at this temperature for 30 minutes. After this time, it was cooled down, pressure carefully released, and a second sample withdrawn for ^1H and ^{31}P $\{^1\text{H}\}$ NMR analysis (Supplementary Figs. 21-22). The autoclave was sealed again, heated to 90 °C and kept at this temperature until no further pressure was developed. It was cooled down, pressure carefully released, and a third sample withdrawn for ^1H and ^{31}P $\{^1\text{H}\}$ NMR analysis (Supplementary Figs. 23-24).



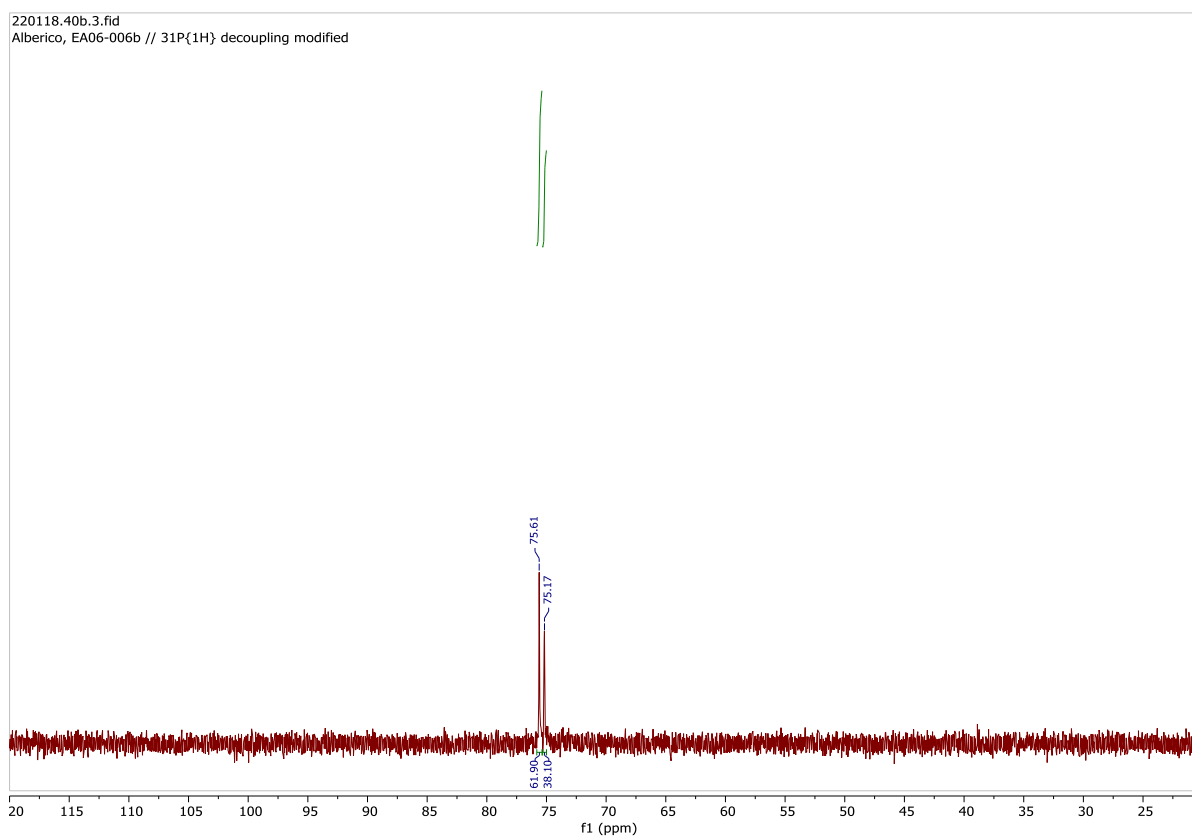
Supplementary Fig. 19 ^1H NMR (400 MHz, THF- d_8 , 298K)



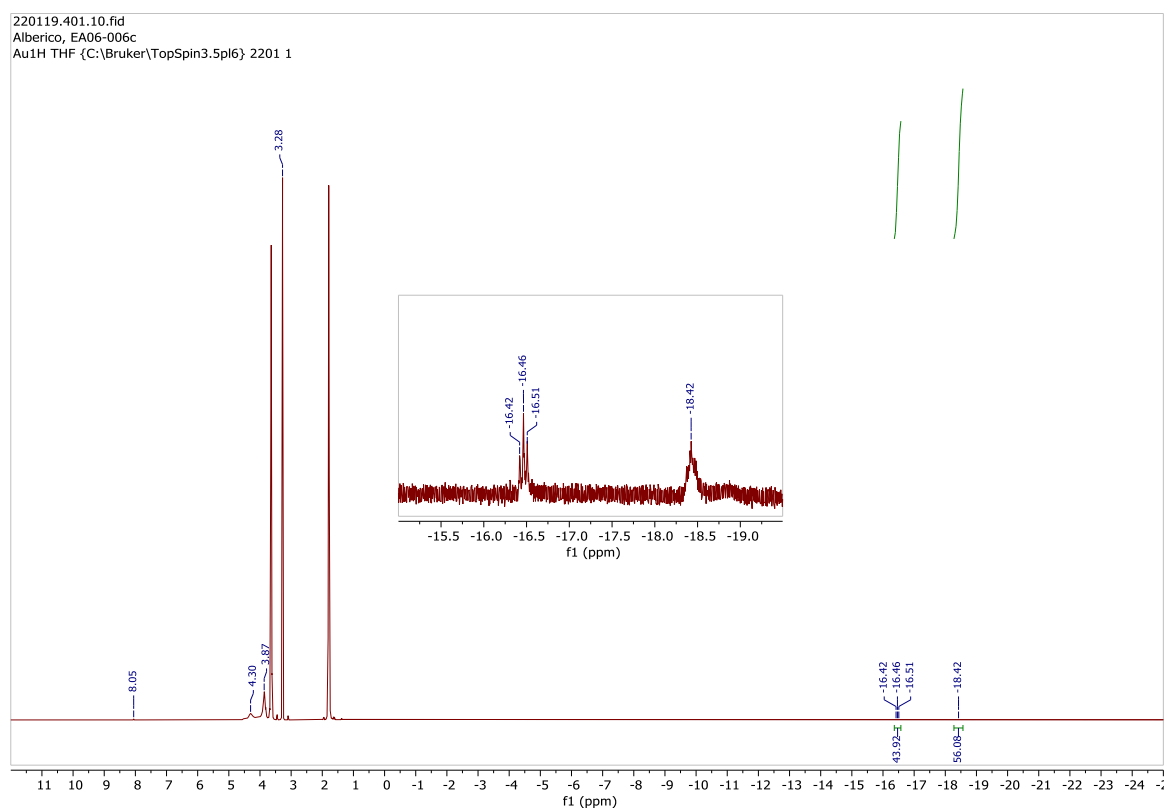
Supplementary Fig. 20 $^{31}\text{P}\{^1\text{H}\}$ NMR (131 MHz, THF- d_8 , 298K)



Supplementary Fig. 21 ^1H NMR (400 MHz, THF- d_8 , 298K)

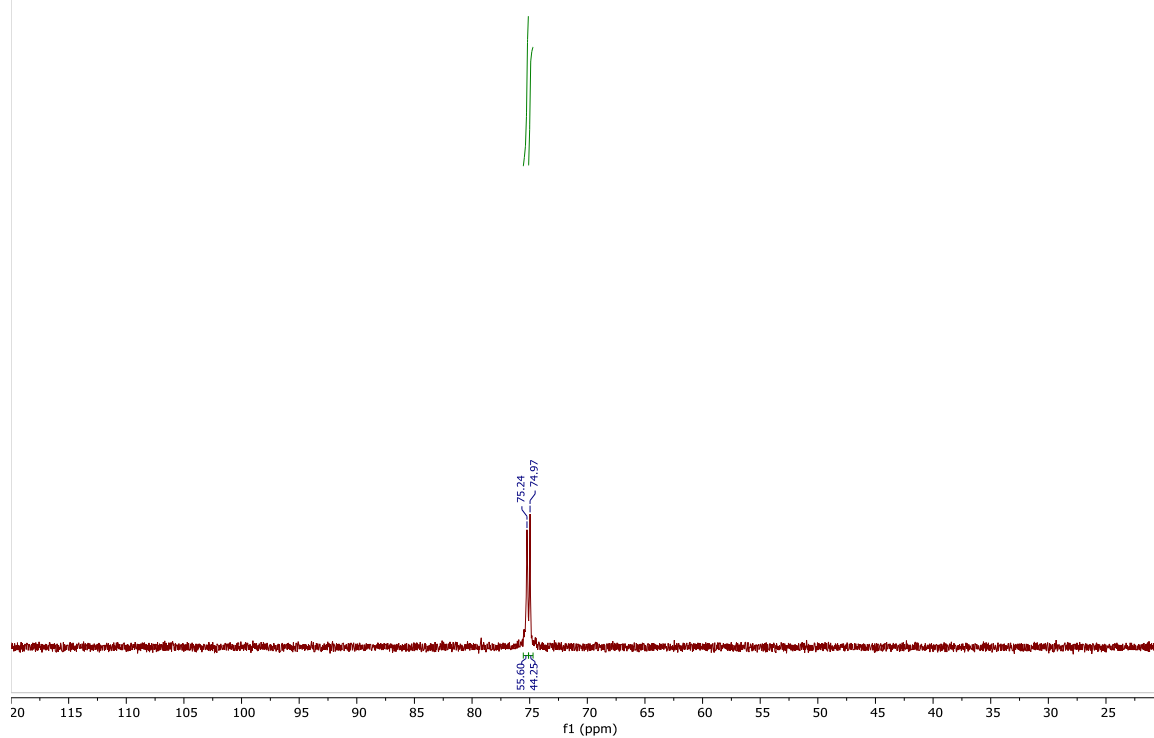


Supplementary Fig. 22 $^{31}\text{P}\{^1\text{H}\}$ NMR (131 MHz, THF-d_8 , 298K)



Supplementary Fig. 23 ^1H NMR (400 MHz, THF-d_8 , 298K)

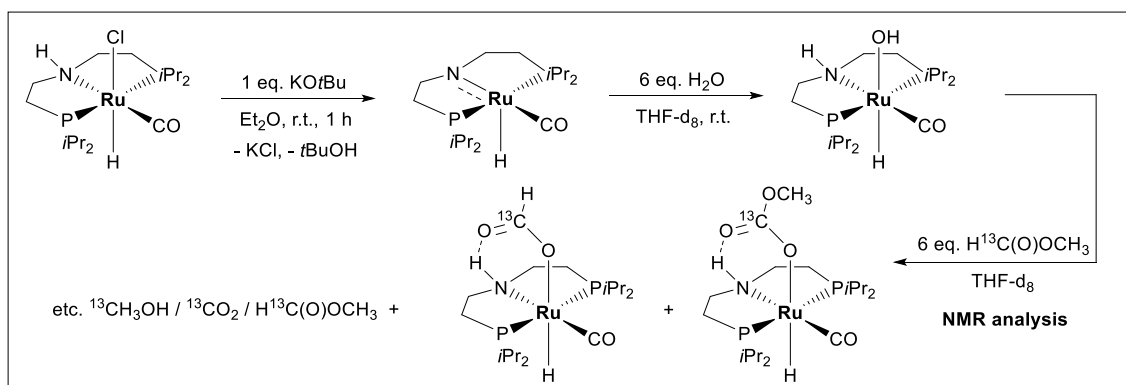
220119.401.11.fid
Alberico, EA06-006c
Au31P-quant THF {C:\Bruker\TopSpin3.5pl6} 2201 1



Supplementary Fig. 24 $^{31}\text{P}\{^1\text{H}\}$ NMR (131 MHz, THF- d_8 , 298K)

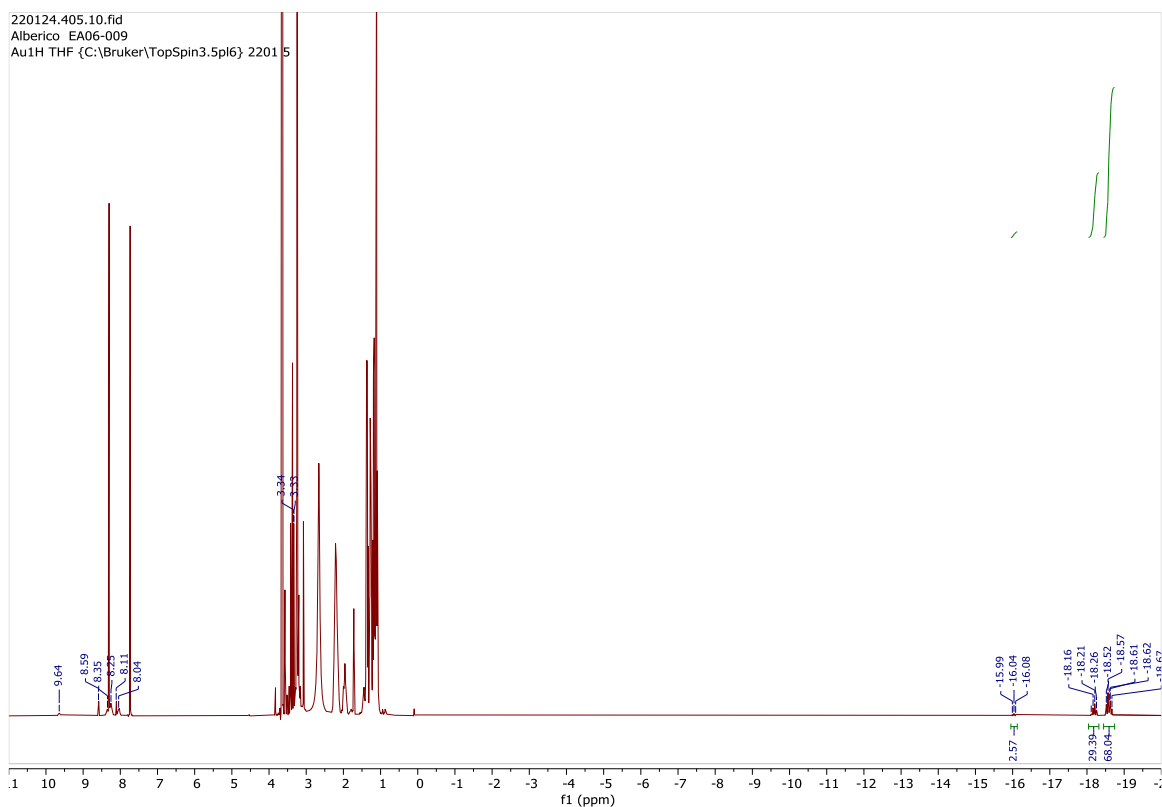
Stoichiometric Experiments – Identification of resting states

Reaction of [H-Ru-OH] with $\text{H}^{13}\text{C}(\text{O})\text{OCH}_3$

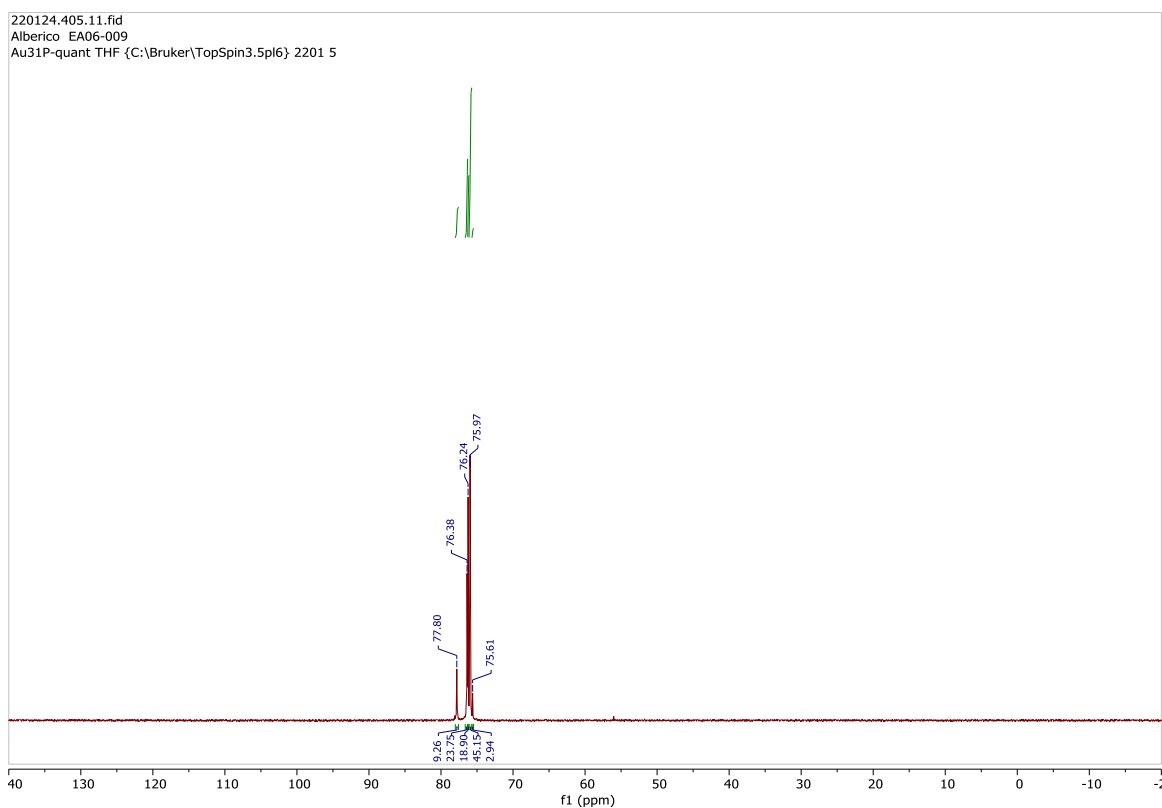


Supplementary Fig. 25 Reaction of [H-Ru-OH] with $\text{H}^{13}\text{C}(\text{O})\text{OCH}_3$

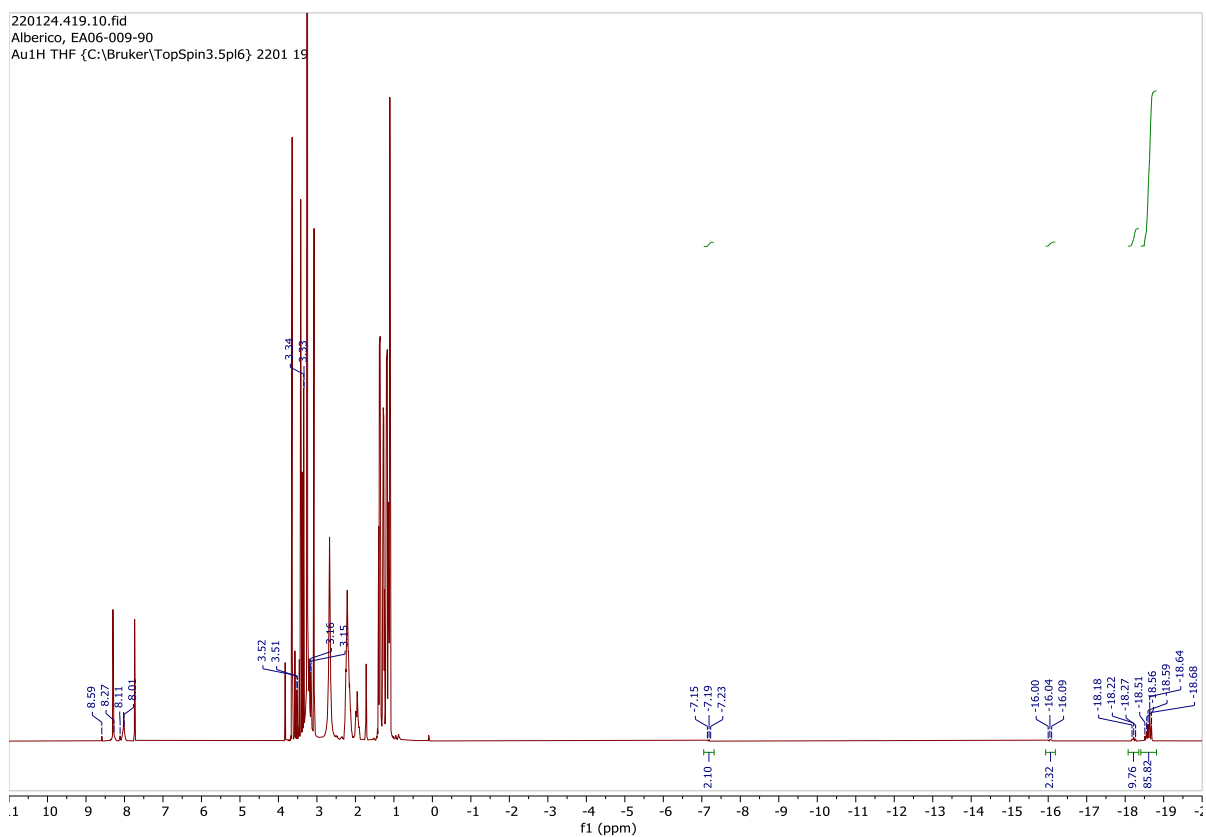
To a suspension of the catalyst precursor Ru-PNPiPr **C1** (150 mg, 0.32 mmol, 1 eq.) in diethyl ether (20 mL), $t\text{BuOK}$ (35.7 mg, 0.32 mmol, 1 eq.) was added. The resulting orange suspension was stirred at room temperature for 1 hour and then filtered through a short path of Celite S ($\text{pH} \approx 7$) to remove KCl. Solvent was removed in vacuo and the orange residue dissolved in tetrahydrofuran- d_8 to give a clear orange solution. To the latter, H_2O (36 μL , 2 mmol, 6.3 eq.) was first added, upon which the orange color faded, followed by $\text{H}^{13}\text{C}(\text{O})\text{OCH}_3$ (118 μL , 1.9 mmol, 6.0 eq.). The resulting clear solution was stirred at room temperature for 15 minutes, after which a sample was withdrawn for NMR analysis (Supplementary Figs. 26-27). The rest of the solution was transferred into a 25 mL pressure tube and immersed in a preheated oil bath at 90°C and kept at this temperature for 90°C for 2 hours. After this time, the pressure tube was cooled down and a second sample was withdrawn and subjected to NMR analysis (Supplementary Figs. 28-30). The pressure tube was sealed again and heated at 90°C for further 7 hours. A third sample was withdrawn and subjected to NMR analysis (Supplementary Figs. 31-33).



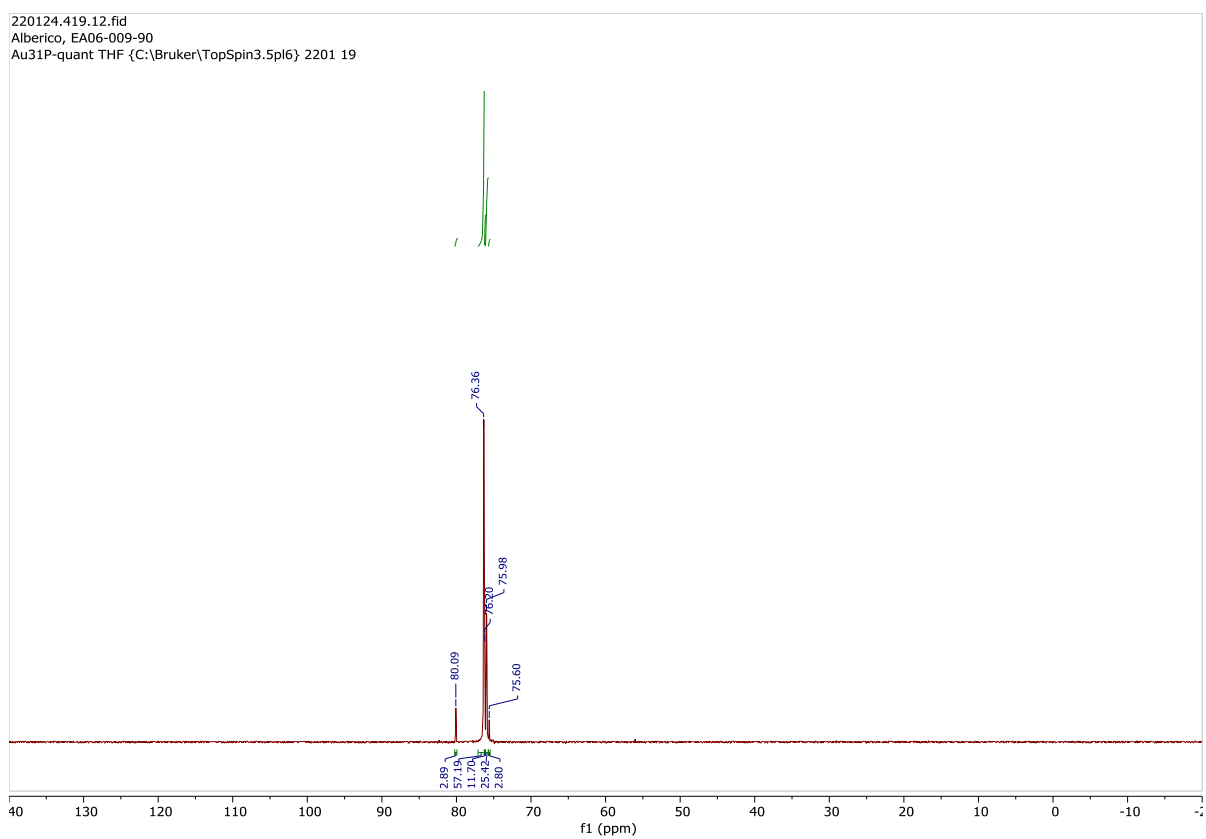
Supplementary Fig. 26 ^1H NMR (400 MHz, THF- d_8 , 298K)

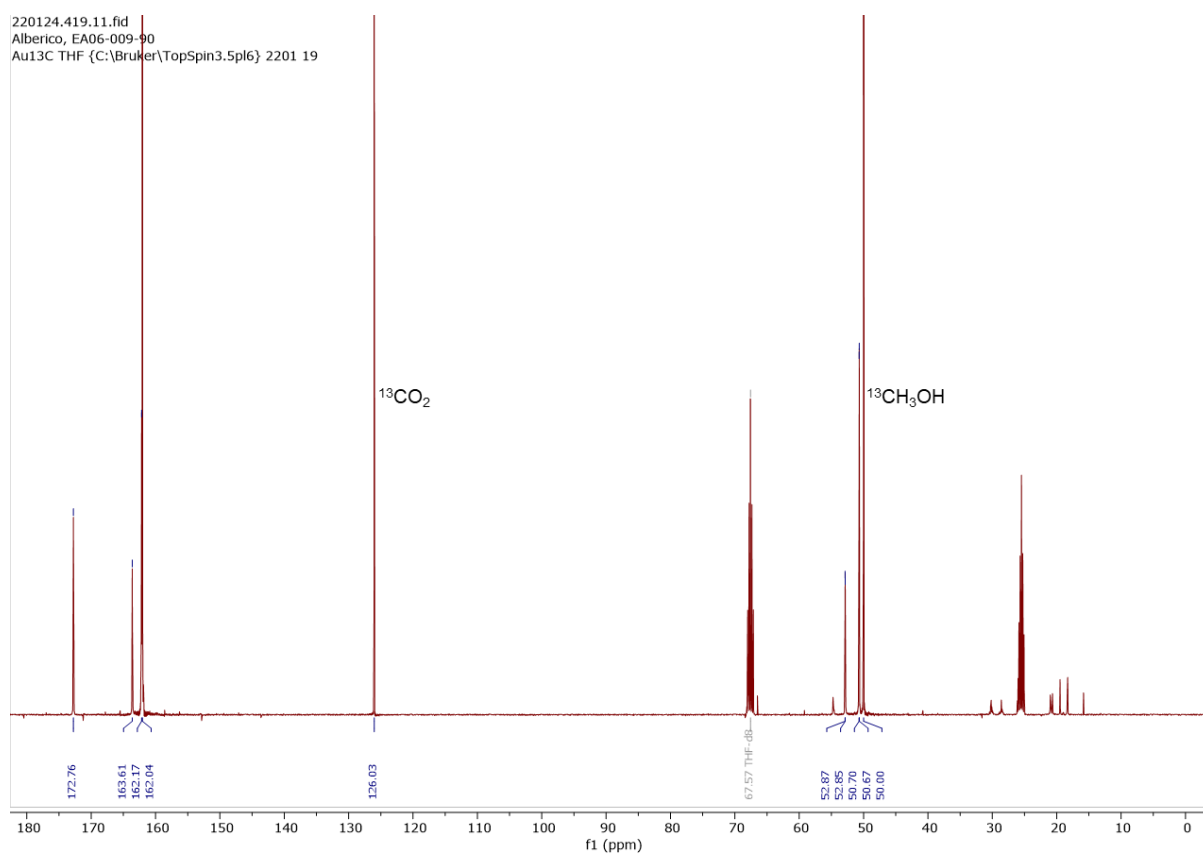


Supplementary Fig. 27 $^{31}\text{P}\{^1\text{H}\}$ NMR (131 MHz, THF- d_8 , 298K)

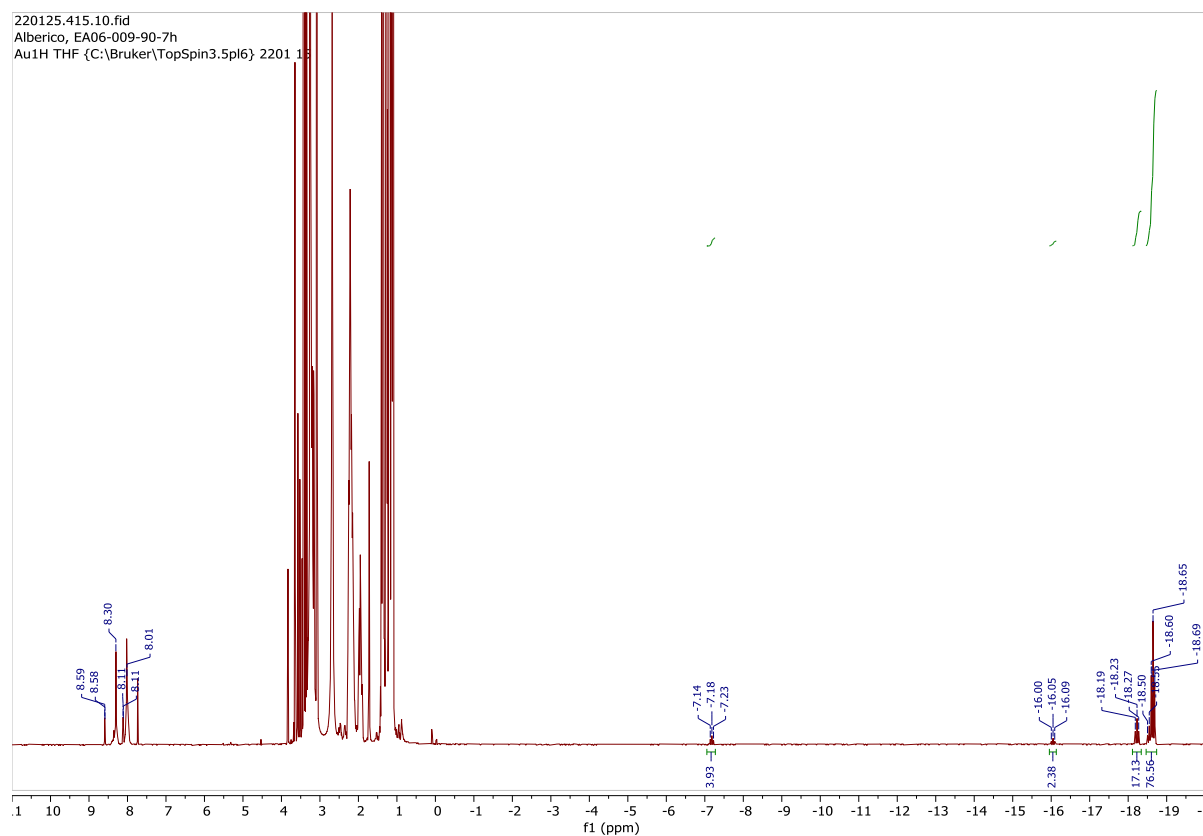


Supplementary Fig. 28 ^1H NMR (400 MHz, THF- d_8 , 298K)



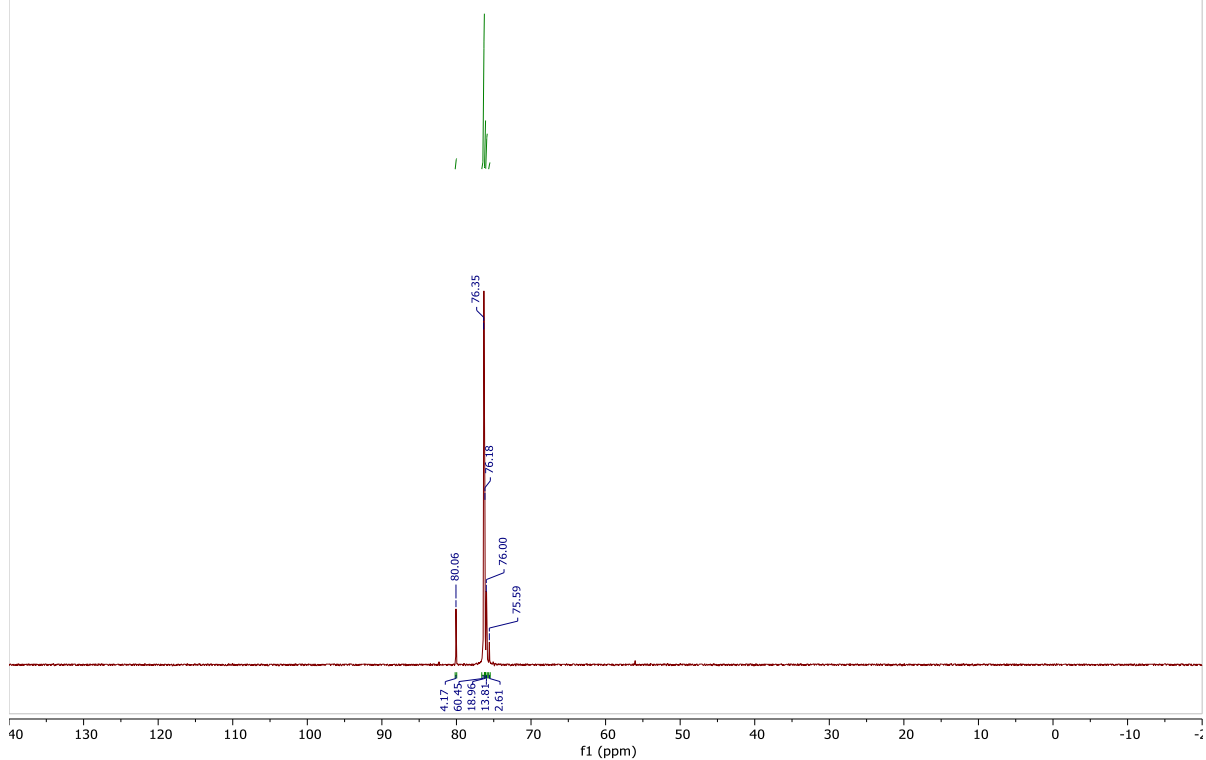


Supplementary Fig. 30 ^{13}C NMR (100 MHz, THF- d_8 , 298K)



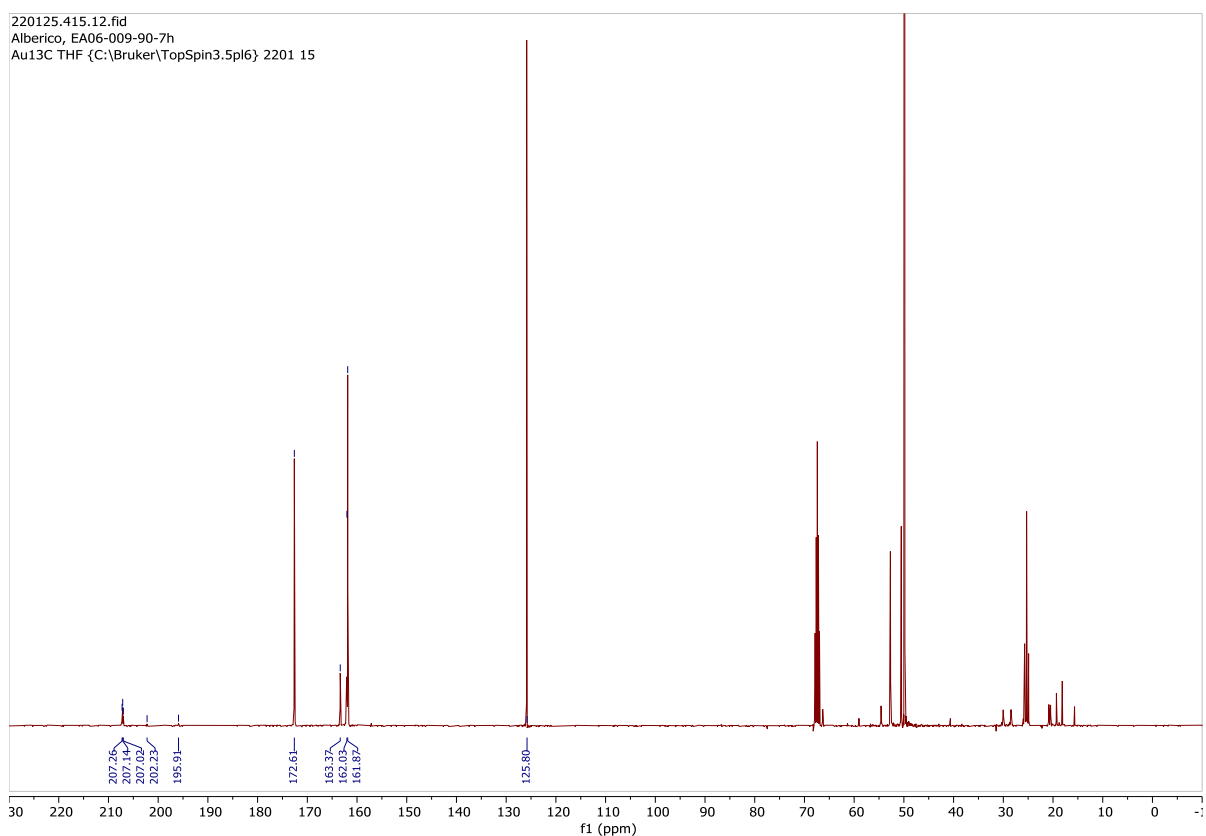
Supplementary Fig. 31 ^1H NMR (400 MHz, THF- d_8 , 298K)

220125.415.11.fid
 Alberico, EA06-009-90-7h
 Au31P-quant THF {C:\Bruker\TopSpin3.5pl6} 2201 15

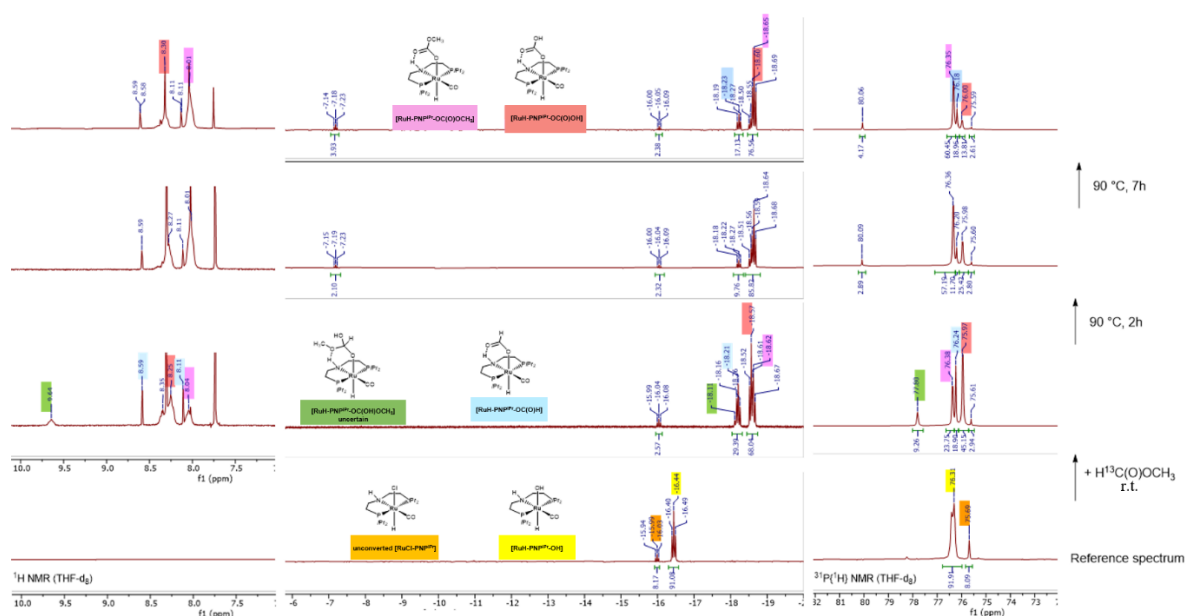


Supplementary Fig. 32 $^{31}\text{P}\{^1\text{H}\}$ NMR (131 MHz, THF-d₈, 298K)

220125.415.12.fid
 Alberico, EA06-009-90-7h
 Au13C THF {C:\Bruker\TopSpin3.5pl6} 2201 15



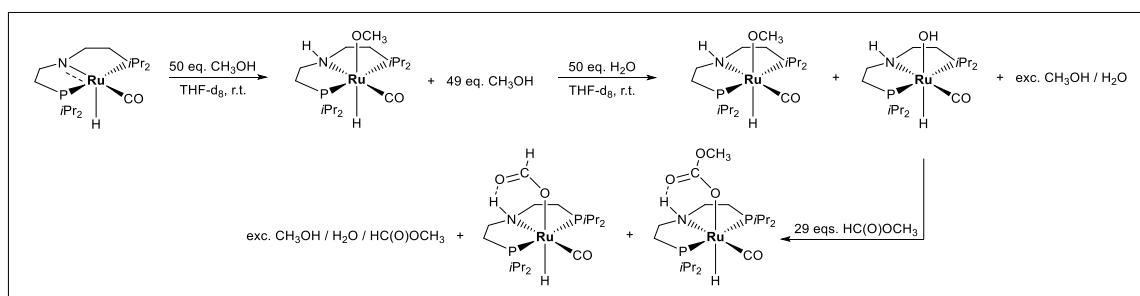
Supplementary Fig. 33 ^{13}C NMR (100 MHz, THF-d₈, 298K)



Supplementary Fig. 34 Comparison of ^1H and $^{31}\text{P}\{^1\text{H}\}$ NMR spectra in Supplementary Figs. 26-29 and 31-32

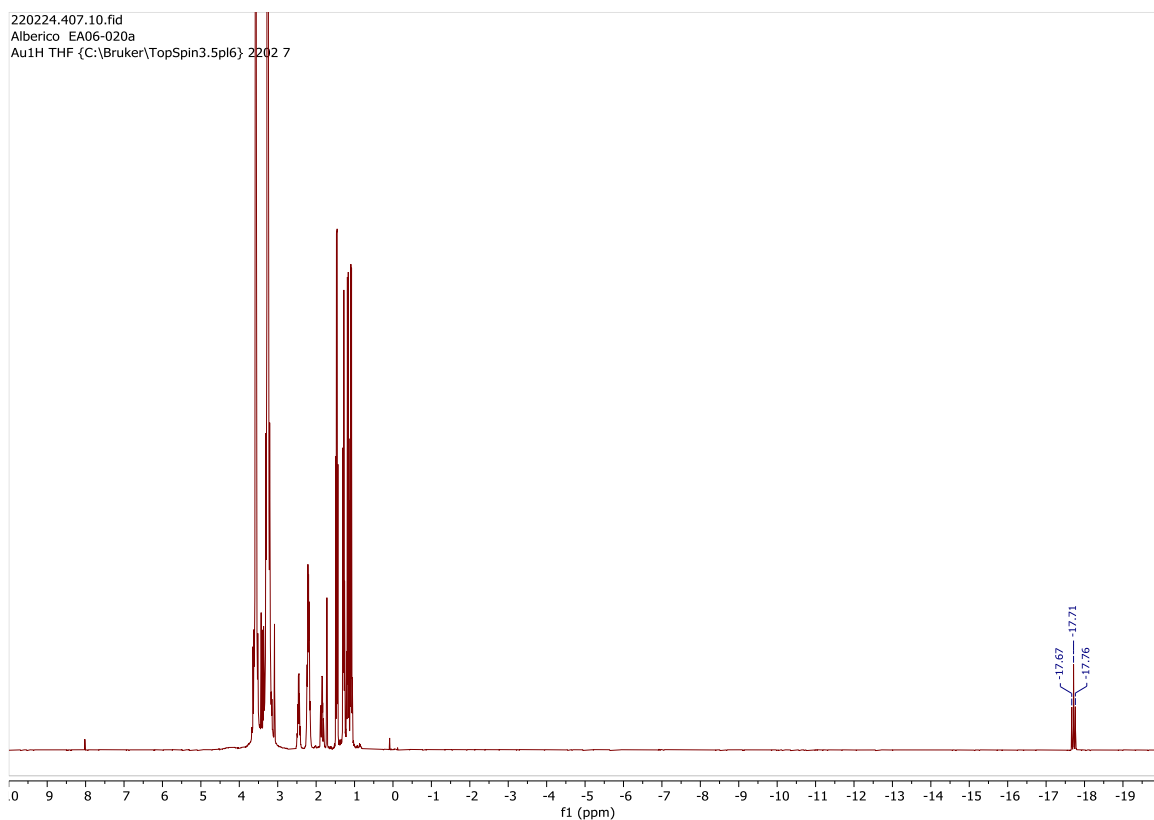
As shown in Supplementary Fig. 34, ^1H and $^{31}\text{P}\{^1\text{H}\}$ NMR spectra in Supplementary Figs. 26-29 and 31-32 are compared to show the correlation between the low field shifted NH signals (due to hydrogen bonding), the hydride signals and the ^{31}P signals of the detected species. The assignment of the species is based on the comparison of their NMR data with those reported in the reference.¹ The reference spectrum refers to a similar experiment in which an NMR spectrum was recorded before addition of methyl formate, which is shown here to highlight the presence of unreacted catalyst precursor Ru-PNPiPr **C1** and the full conversion of [RuH-PNPiPr-OH] upon reaction with methyl formate. And most importantly, both [RuH-PNPiPr-O $^{13}\text{C}(\text{O})\text{H}$] and [RuH-PNPiPr-O $^{13}\text{C}(\text{O})\text{OCH}_3$] were detected.

Reaction of [H-Ru-OCH₃] with H₂O and HC(O)OCH₃

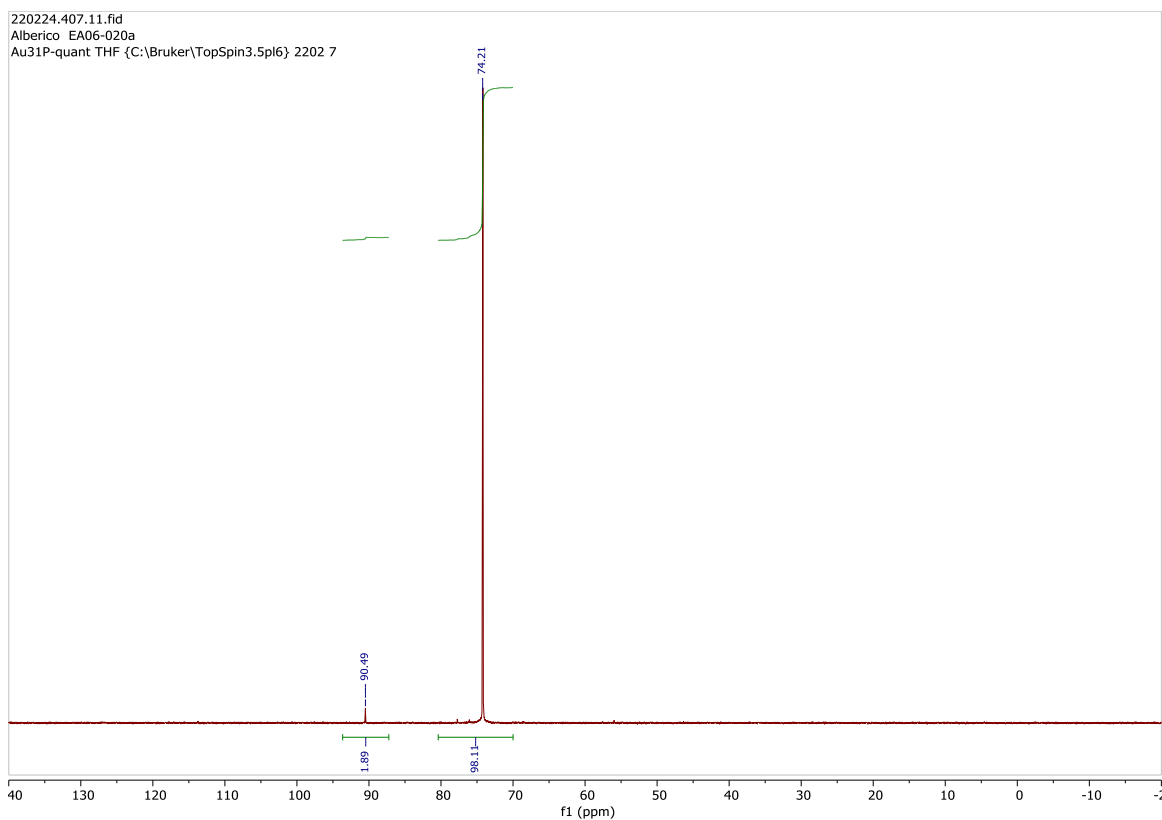


Supplementary Fig. 35 Reaction of [H-Ru-OCH₃] with H₂O and HC(O)OCH₃

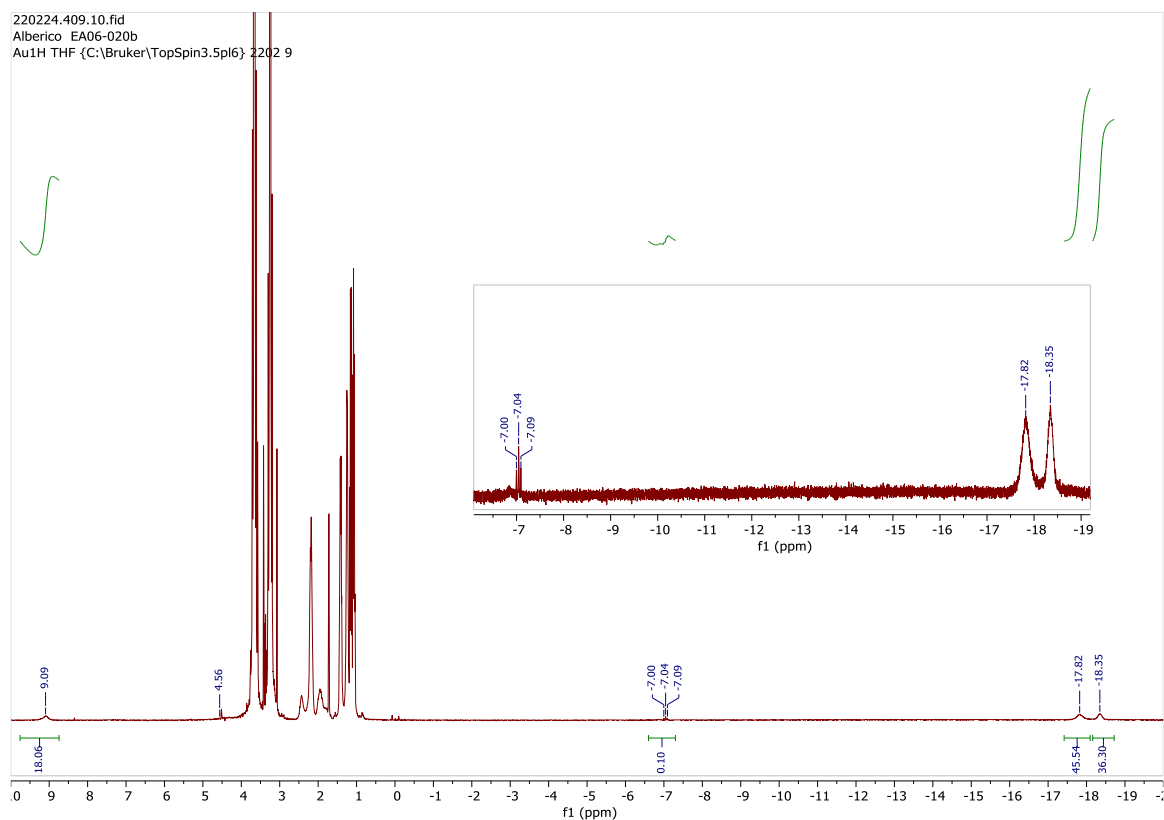
To a suspension of [RuHCl(CO)(HN(CH₂CH₂P(CH(CH₃)₂)₂)₂)] (60 mg, 0.127 mmol, 1 eq.) in diethyl ether (10 mL) *t*BuOK (17.2 mg, 0.153 mmol, 1.2 eq.) was added. The resulting orange suspension was stirred at room temperature for 1 hour and then filtered through a short pad of Celite S (pH ≈ 7) to remove KCl. Solvent was removed in vacuo and the orange residue redissolved in tetrahydrofuran-*d*₈ (3 mL) to give a clear orange solution. To the latter, CH₃OH (276 μL, 204 mg, 6.37 mmol, 50 eq.) was added, upon which the orange color faded. The resulting clear solution was stirred at room temperature for 15 minutes, after which a sample, 0.7 mL, was withdrawn for NMR analysis (Supplementary Figs. 36-37). To the rest of the solution (2.3 mL, 0.098 mmol [Ru]), H₂O (88 mL, 88 mg, 4.88 mmol, 50 eq.) was added. After stirring at room temperature for 15 minutes, 0.7 mL of the solution were transferred into a J-Young tube for NMR analysis (Supplementary Figs. 38-39). To the remaining solution, 1.6 mL, containing approximately 1.6 mL / 3.0 mL × 6.37 mmol = 3.40 mmol CH₃OH, HC(O)OCH₃ (120 mg, 123 mL, 2 mmol, 0.59 eq. to the remaining CH₃OH) was added. The solution was stirred at room temperature for 15 minutes and then a sample withdrawn for NMR analysis. (Supplementary Figs. 40-41).



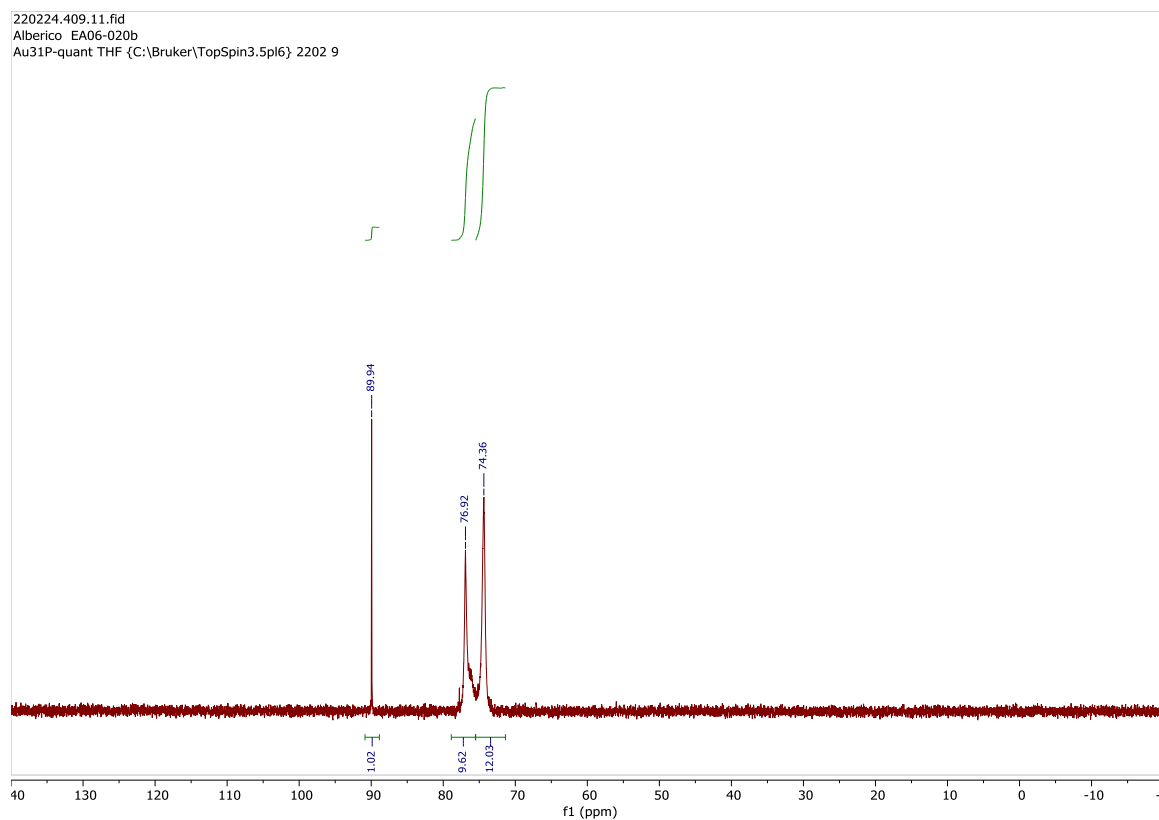
Supplementary Fig. 36 ^1H NMR (400 MHz, THF- d_8 , 298K)



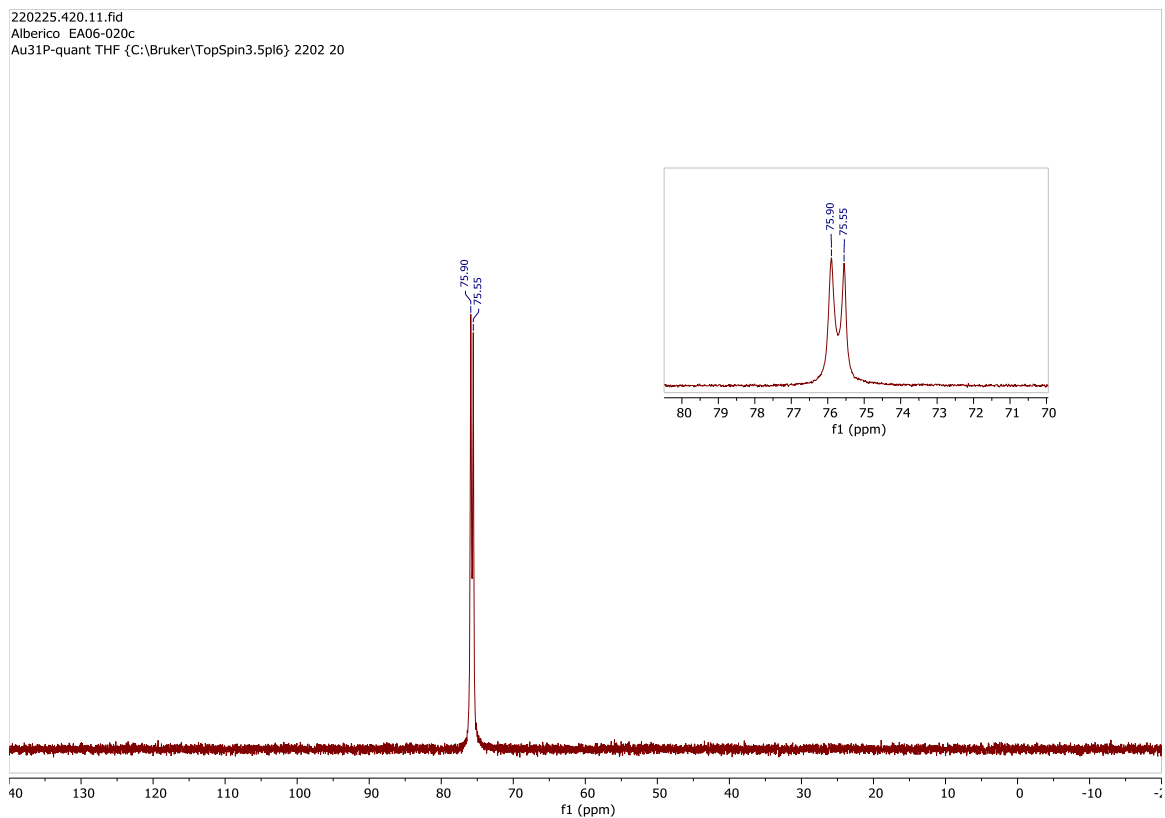
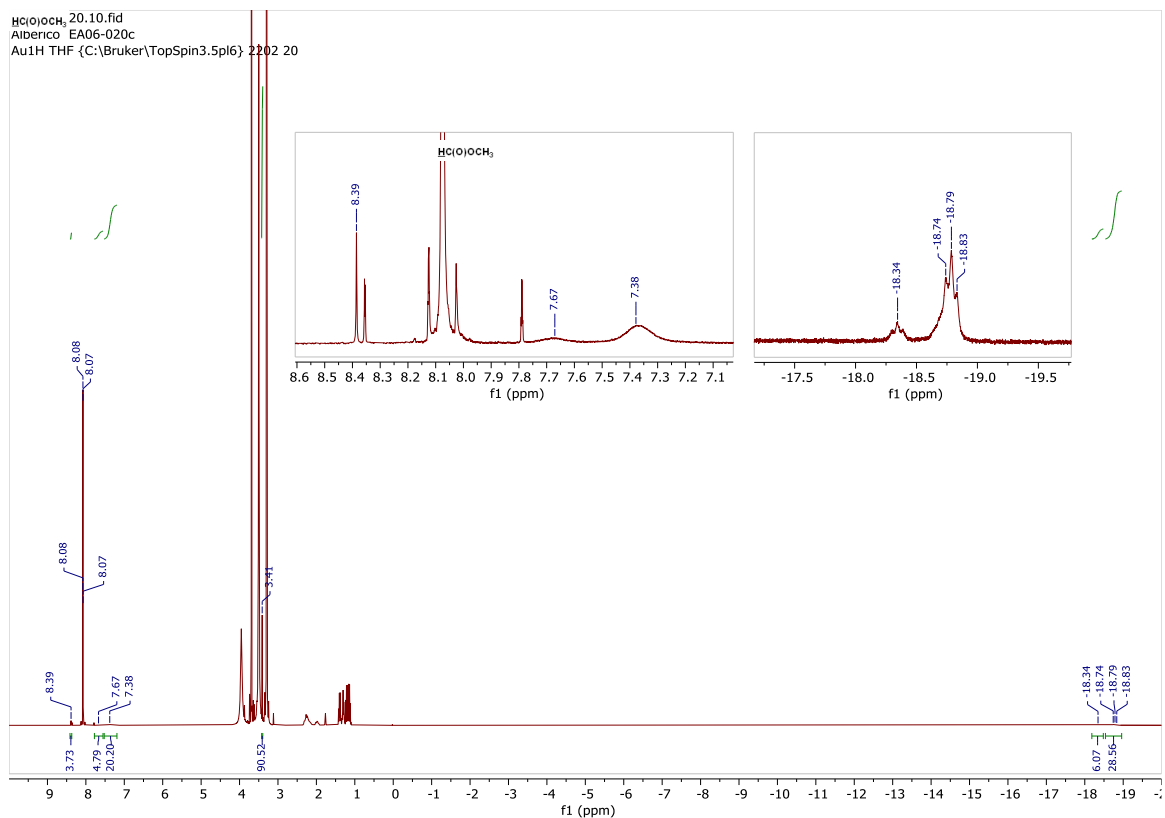
Supplementary Fig. 37 $^{31}\text{P}\{^1\text{H}\}$ NMR (131 MHz, THF- d_8 , 298K)

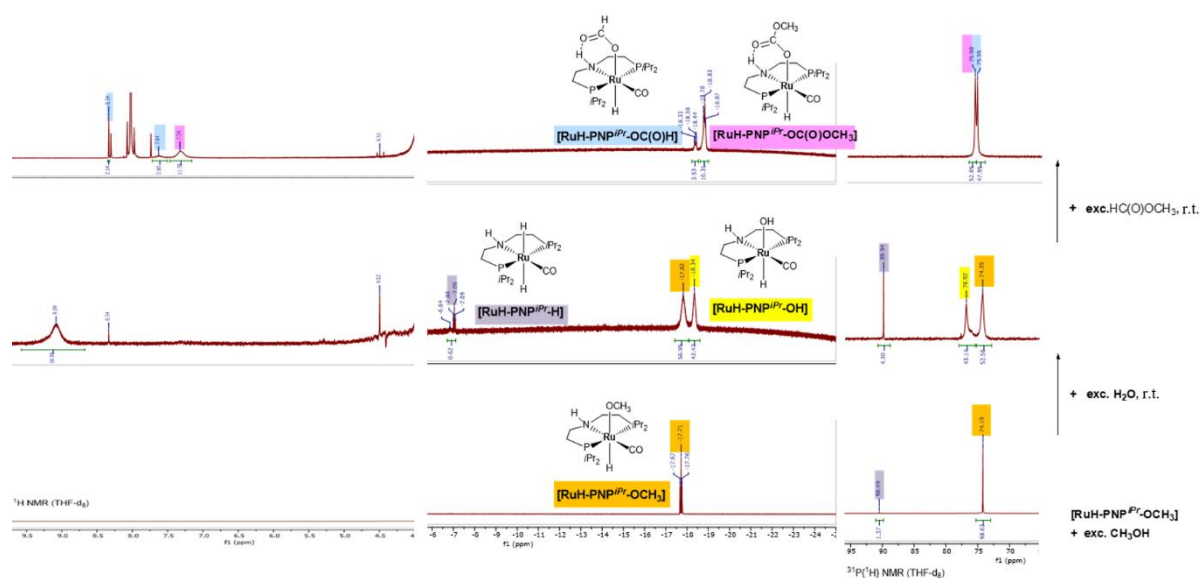


Supplementary Fig. 38 ^1H NMR (400 MHz, THF- d_8 , 298K)



Supplementary Fig. 39 $^{31}\text{P}\{^1\text{H}\}$ NMR (131 MHz, THF- d_8 , 298K)



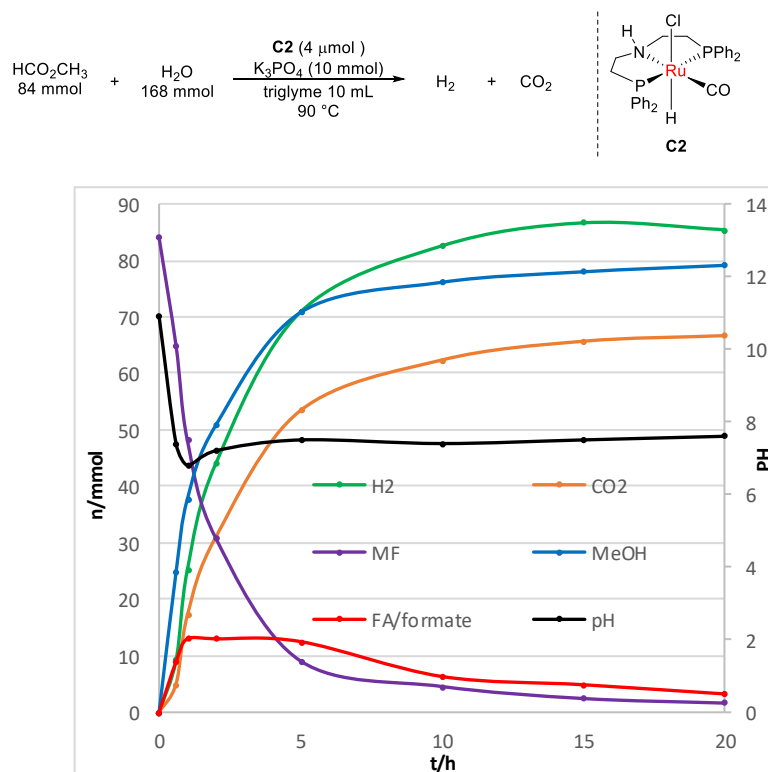


Supplementary Fig. 42 Comparison of selected chemical shift ranges of the ^1H and $^{31}\text{P}\{^1\text{H}\}$ NMR spectra in Supplementary Figs. 36-41

As shown in Supplementary Fig. 42, selected chemical shift ranges of the ^1H and $^{31}\text{P}\{^1\text{H}\}$ NMR spectra in Supplementary Figs. 36-41 are compared. The assignment of the various species is based on the comparison of their NMR data with those reported in reference.¹

Time course of Compounds distribution in MF dehydrogenation

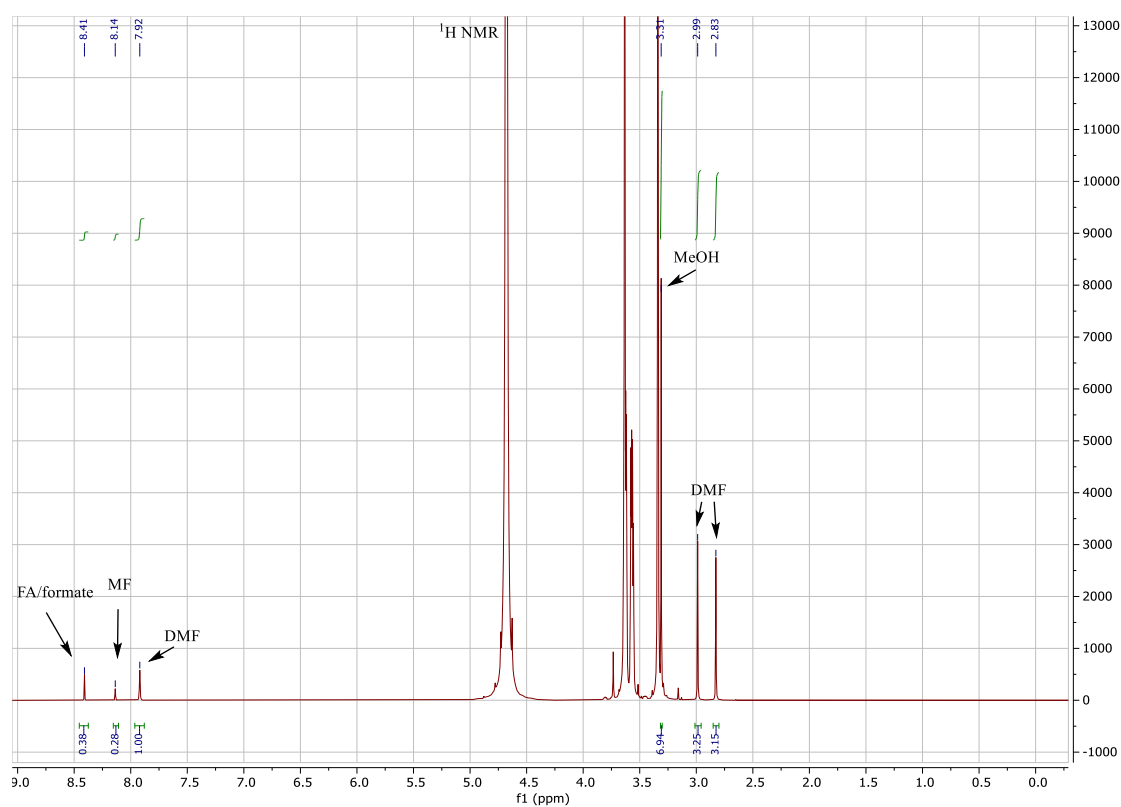
Supplementary Table 18. Time course of Compounds distribution in MF dehydrogenation.



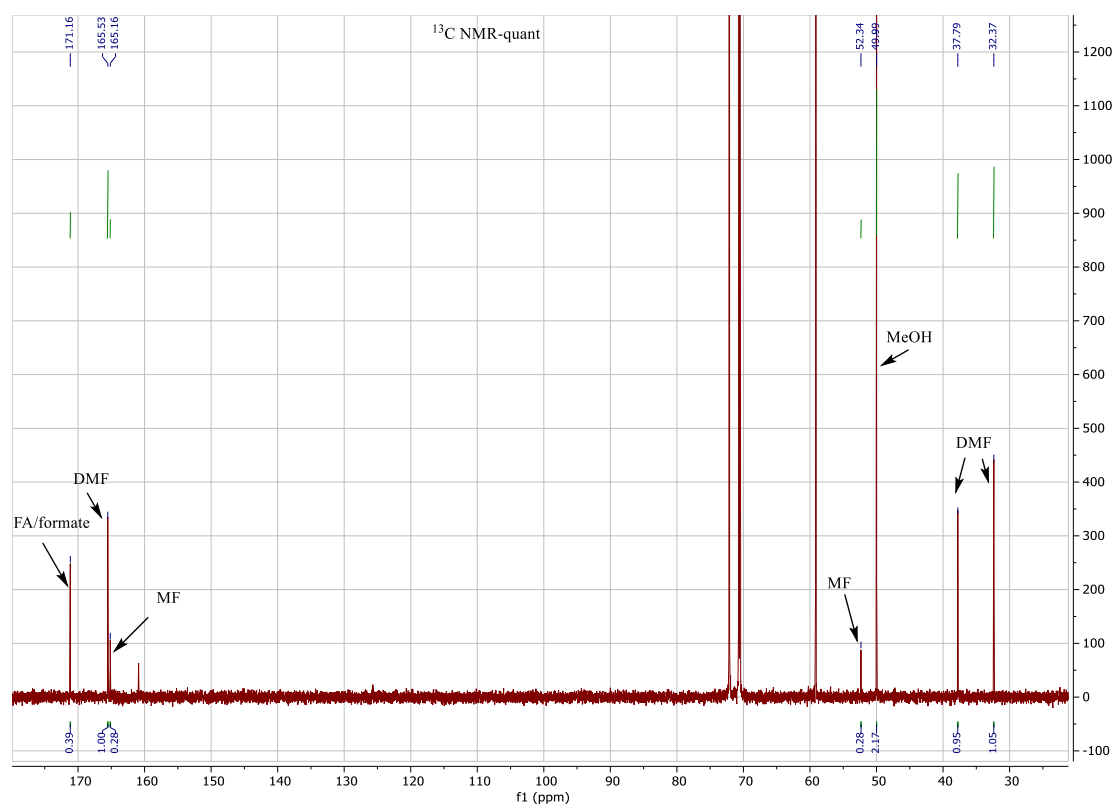
Entry	Time (h)	MF (mmol)	MeOH (mmol)	FA/formate (mmol)	V (mL)	H ₂ (mmol)	CO ₂ (mmol)	pH
1	0	84.0	0	0	0	0	0	10.9
2	0.6	64.9	24.8	8.9	347	9.2	5.0	7.4
3	1	48.2	37.7	13.0	1035	25.2	17.2	6.8
4	2	30.9	50.8	13.0	1830	44.0	31.0	7.2
5	5	9.1	70.8	12.5	3035	70.8	53.4	7.5
6	10	4.6	76.1	6.3	3540	82.6	62.4	7.4
7	15	2.4	78.0	4.9	3721	86.6	65.7	7.5
8	20	1.6	79.1	3.3	3715	85.4	66.7	7.6

Reaction conditions: under argon atmosphere 4 μmol **C2** catalyst (2.4 mg) and 10 mmol K_3PO_4 (2.12 g) were added to a 100 mL autoclave. Then 10.0 mL triglyme, 168 mmol H_2O (3.0 mL) and 84 mmol MF (5.3 mL) were injected by a syringe under ice-bath. After that, the autoclave was flushed with N_2 (5 bar) and the pressure was released three times. The reaction was performed at 90 $^\circ\text{C}$ for t h. After that the autoclave was cooled down using ice-bath and the pressure was carefully released through a room temperature (25 $^\circ\text{C}$) condenser (the water temperature was controlled by a thermostat) to a manual burette to get the gas volume. The gas was analyzed by GC. The pH values were measured on a laboratory digital pH meter (Mettler-Toledo AG, SevenEasy pH 8603). Later on, further triglyme and H_2O as well as internal standard DMF (2.5 mL, 32.5 mmol) were added to the reaction liquid phase. The amount of MF, methanol and FA/formate was determined by NMR with a few drops of D_2O . Additional CO_2 was collected via burette by adding HCl aqueous solution to the reaction liquid phase.

Example for NMR study to determine the amount of MF, MeOH, FA/formate



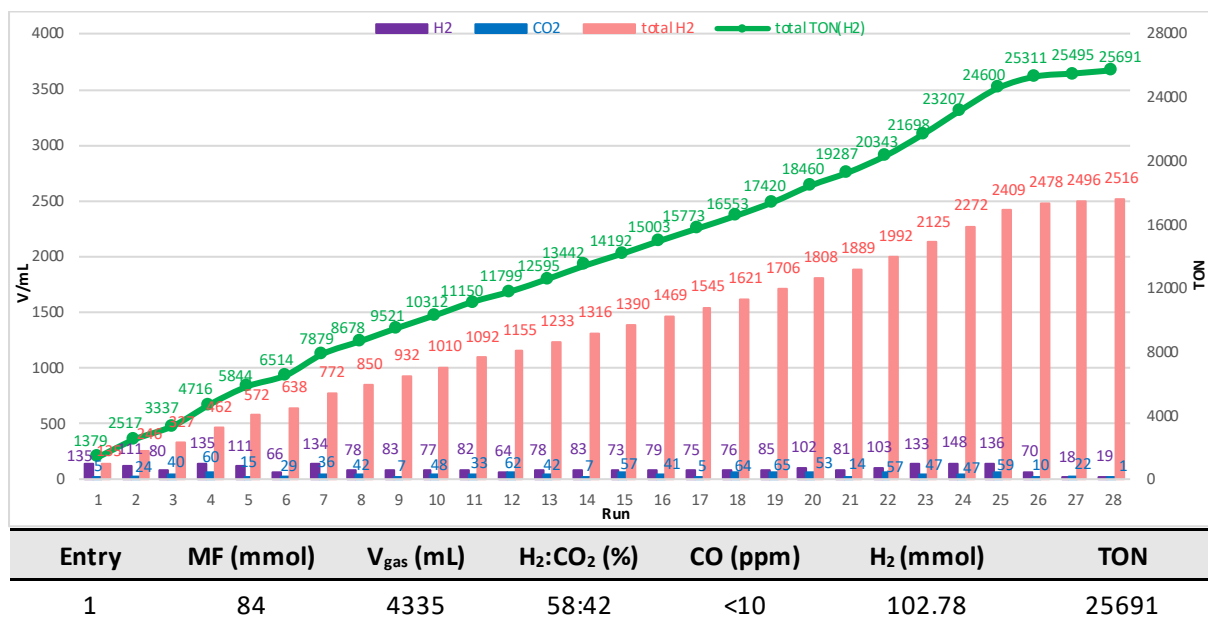
Supplementary Fig. 43 Example for ^1H NMR to determine the amount of MF, MeOH, FA/formate.



Supplementary Fig. 44 Example for ^{13}C NMR-quant to determine the amount of MF, MeOH, FA/formate. (Corresponding to ^1H NMR of Supplementary Fig. 43)

Controlled consecutive dehydrogenation of MF with 5 bar pressure limitation

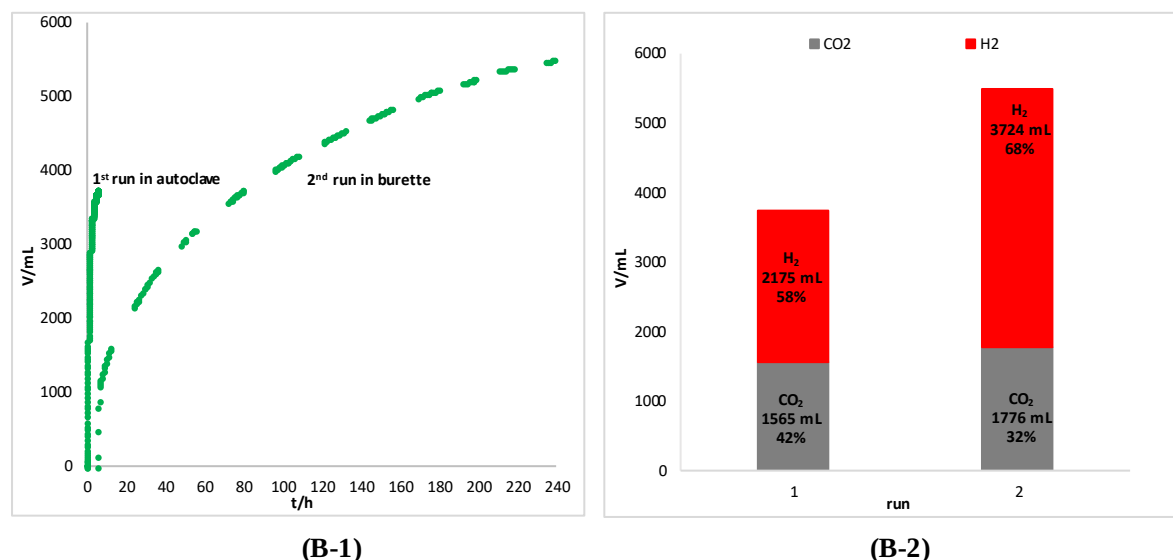
Supplementary Table 19. Consecutive runs of MF dehydrogenation and gas release (84 mmol MF)



Reaction conditions: under argon atmosphere 4 μmol C2 catalyst (2.4 mg) and 10 mmol K_3PO_4 (2.12 g) were added to a 100 mL autoclave. Then 10.0 mL triglyme, 168 mmol H_2O (3.1 mL) and 84 mmol MF (5.2 mL) were injected by a syringe under ice-bath. After that, the autoclave was flushed with N_2 (5 bar) and the pressure was released three times. The reaction was performed at 90 °C. Each time after the pressure in the autoclave reaches 5 bar, the reaction was stopped and cooled down using ice-bath. The pressure was carefully released through a room temperature (25 °C) condenser (the water temperature was controlled by a thermostat) to a manual burette to get the gas volume. The gas was analyzed by GC. After the gas was released, the reaction was set again.

MF dehydrogenation in consecutive runs applying autoclave and glass reactor/burette

Supplementary Table 20. MF dehydrogenation in consecutive runs applying autoclave and glass reactor/burette (100 mmol MF).

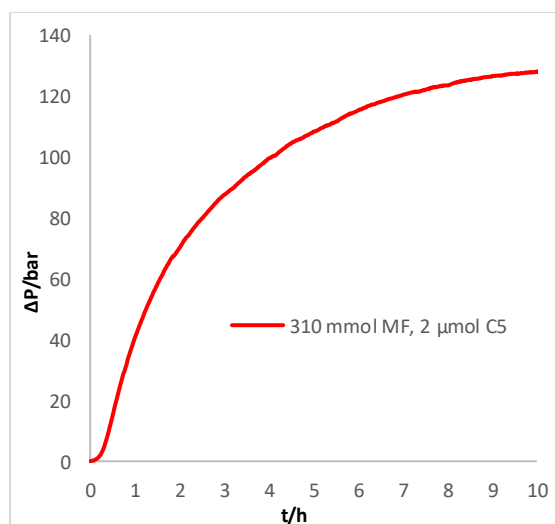


MF (mmol)	Gas (mL)	H ₂ (%)	CO ₂ (%)	CO (ppm)	H ₂ (mmol)	CO ₂ (mmol)
100	9470	62.3	37.7	<10	241.0	146.6

Reaction conditions: under argon atmosphere 0.1 mmol **C2** catalyst (60.7 mg) and 10 mmol K₃PO₄ (2.12 g) were added to a 100 mL autoclave. Then 20.0 mL triglyme, 400 mmol water (7.2 mL) and 100 mmol MF (6.1 mL) were injected by a syringe under ice-bath. After that, the autoclave was flushed with N₂ (5 bar), and the pressure was released three times. The reaction was performed at 90 °C for 6 h. The reaction was stopped and cooled down using ice-bath. The pressure was carefully released through a room temperature (25 °C) condenser (the water temperature was controlled by a thermostat) to a manual burette to get the gas volume. After the gas was released, the reaction solution was transferred to a glass reactor which was connected to a condenser and a manual burette. The reaction was performed at 90 °C. The generated gas was analyzed by GC.

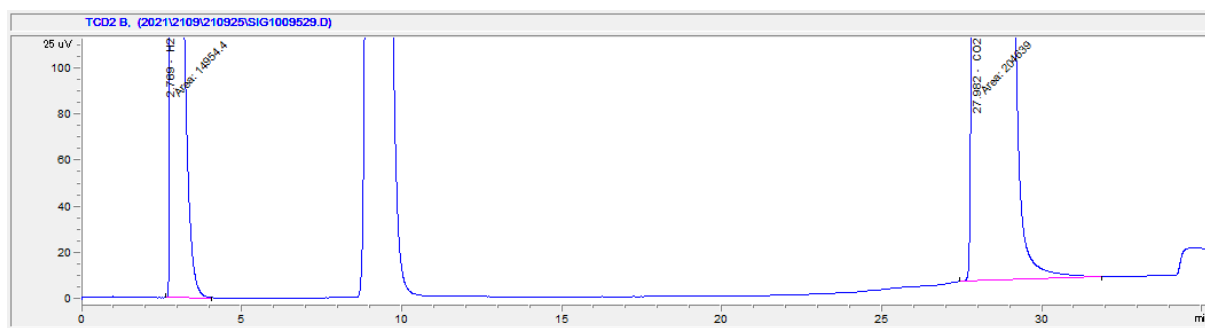
Scaled-up reaction of MF dehydrogenation in autoclave

Supplementary Table 21. Multiplicative reaction of Ru-catalyzed dehydrogenation of methyl formate



MF (mmol)	Cat. (μmol)	P (bar)	V (mL)	H ₂ (%)	CO ₂ (%)	CO (ppm)	H ₂ (mmol)	TON	TOF _{max} (h ⁻¹)
310	2	128.1	10025	52.3	47.7	undetectable	214.2	107100	44140

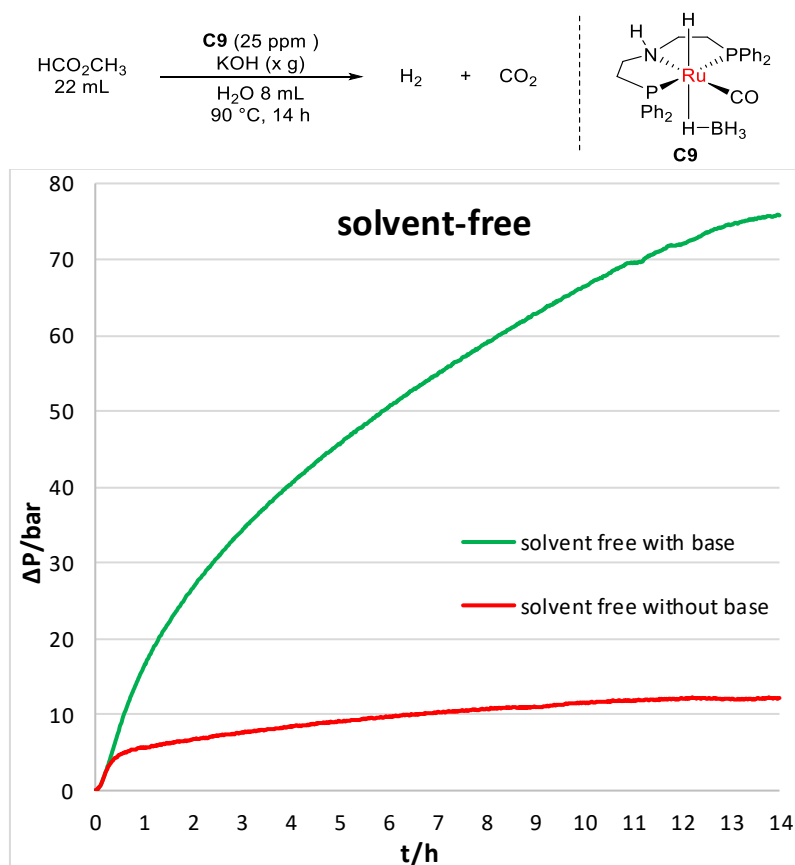
Reaction conditions: under argon atmosphere 2 μmol **C5** catalyst (6.5 ppm) and 20 mmol K₃PO₄ were added to a 100 mL autoclave. Then 20.0 mL triglyme, 620 mmol H₂O and 310 mmol MF were injected by a syringe under ice-bath. After that, the autoclave was flushed with N₂ (5 bar) and the pressure was released three times. The reaction was performed at 90 °C for t h. After that the autoclave was cooled down using ice-bath and the pressure was carefully released through a room temperature (25 °C) condenser (the water temperature was controlled by a thermostat) to a manual burette to get the gas volume. The gas was analyzed by GC. Additional CO₂ was collected via burette by adding HCl aqueous solution to the reaction liquid phase.



Supplementary Fig. 45. Multiplicative reaction of Ru-catalyzed dehydrogenation of methyl formate without CO detected (GC with CO quantification limit of 10 ppm)

Solvent-free reaction of MF dehydrogenation in autoclave

Supplementary Table 22. Solvent-free reaction of MF dehydrogenation.



Entry	KOH (g)	Δp (bar)	V (mL)	H ₂ :CO ₂ (%)	CO (ppm)	TON
1	0.3	75.8	7,148	52:48	<10	16,871
2	0	12.2	860	57:43	18	2,225

Reaction conditions: under argon atmosphere KOH (x g) were added to a 100 mL autoclave. Then 8 mL H₂O, 22 mL MF with 25 ppm cat. **C9** were added under cooling in an ice-bath. After that, the autoclave was flushed with N₂ (5 bar) and the pressure was released three times. The reaction was performed at 90 °C for 14 h. After that the autoclave was cooled down using an ice-bath and the pressure was carefully released through a condenser (25 °C, the water temperature was controlled by a thermostat) to a manual burette to measure the gas volume. The gas constitution was analyzed by GC. Additional CO₂ was collected via burette after adding aqueous HCl solution to the reaction solution.

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