Supplementary Information
for

Efficient Acceptorless Dehydrogenation of Secondary Alcohols to Ketones mediated by a PNN-Ru(II) Catalyst

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A. General Information

All experiments with metal complexes and phosphine ligands were carried out under an atmosphere of nitrogen. All solvents were reagent grade or better and were used after being distilled under nitrogen. Most of the chemicals used in the catalytic reactions were repurified according to standard procedures (*e.g.*, vacuum distillation). All ^{1}H NMR (500 MHz), ^{13}C NMR (125 MHz) and ^{31}P NMR spectra were recorded on a Bruker Bruker AV-III (500 MHz) spectrometer. GC analyses were carried out on an Agilent 6820 instrument using an OV-1701 column. GC conditions: Injector Temp: 250 ºC; Detector Temp: 250 ºC; column temperature 150 ºC. ESI-MS analysis was performed on a 3200 QTRAP 1200 infinity series instrument using a column C18, acetonitrile: water = 70:30, flow rate = 1 mL / min, electronic energy = 50 eV, Q1MS scan range = 100~1000.

B. Experimental

1 Syntheses and characterization of the catalyst

1.1. Complex **A** was synthesized and characterized according to the procedure reported by ourselves.[1]

1.2. Complex **B** was synthesized and characterized according to the procedure reported by ourselves.[2]

1.3 Synthesis of complex C[3]

$RuCl_2(PPh_3)_3$ (2.00 g, 2.087 mmol) and N-(2-(diphenylphosphino)ethyl)-5,6,7,8-tetrahydro-quinolin-8-amine (0.75 g, 2.087 mmol) were dissolved in toluene (100 mL) and stirred at 100 ºC for 3 h. After being cooled to room temperature, the resulting precipitate was filtered and washed with diethyl ether (3 × 10 mL). The title complex was obtained as pale yellow solid (1.08 g, 65%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 (q, *J* = 7.8, 7.2 Hz, 6H), 7.43 (t, *J* = 8.7 Hz, 2H), 7.39 – 7.18 (m, 10H), 7.17-7.06 (m, 8H), 6.97 (d, *J* = 7.8 Hz, 1H), 6.88 (t, *J* = 7.6 Hz, 1H), 5.35 (s, H, N-H), 3.54 (q, *J* = 48.6, 38.2 Hz, 1H), 2.86 – 2.57 (m, 4H), 2.39 – 2.29 (m, 2H), 2.17-1.98 (m, 3H), 1.78 – 1.62 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.21, 154.69, 138.71, 137.89, 137.17, 136.87, 136.77, 135.23, 135.18, 135.10, 135.07, 135.02, 134.90, 134.78, 134.71, 134.00, 133.93, 133.57, 131.42, 131.35, 129.07, 128.84, 128.78, 128.62, 128.26, 127.83, 127.76, 127.61, 127.54, 127.34, 127.29, 127.27, 127.21, 127.14, 127.08, 127.01, 125.34, 122.59, 61.22, 45.65, 44.78, 37.98 (d, *J* = 27.2 Hz), 28.96, 27.97, 21.50, 20.73 (CH_3-Toluene)

^{31}P NMR (202 MHz, $CDCl_3$) δ 55.68 (d, *J* = 27.6 Hz), 45.61 (d, *J* = 27.8 Hz).

ESI-MS (m/z) Calcd for $[C_{41}H_{41}Cl_2N_2RuP_2]$, 795.1; found: 795.4 [**C**+1]$^+$; Calcd for$[C_{41}H_{40}Cl_2N_2RuP_2]$, 759.1; found: 759.6 [**C**-Cl]$^+$.

Anal. Calcd for $C_{41}H_{40}Cl_2N_2RuP_2$: C, 61.96; H, 5.073; N, 3.52. Found: C, 61.77; H, 5,159; N, 3.34.

On standing in $CDCl_3$ for 4 h, complex **C** was obtained as a mixture of two isomers, **C**/**C'** 72:28. No free PPh_3 was detected after this time (NMR sample: 20 mg of **C** in 0.8 mL $CDCl_3$).

C and **C'**

^{13}C NMR (126 MHz, $CDCl_3$) δ 162.74 (**C'**), 161.21 (maj-C), 157.58 (**C'**), 154.69 (maj-C), 138.71, 137.89, 137.17, 136.87, 136.77, 135.23, 135.18, 135.10, 135.07, 135.02, 134.90, 134.78, 134.71, 134.00, 133.93, 133.57, 131.42, 131.35, 129.07, 128.84, 128.78, 128.62, 128.26, 127.83, 127.76, 127.61, 127.54, 127.34, 127.29, 127.27, 127.21, 127.14, 127.08, 127.01, 125.34, 122.59 (maj-C), 120.98 (**C'**), 61.93 (**C'**), 61.22 (**C**), 45.65 (maj-C), 44.78 (**C'**), 37.98 (d, *J* = 27.2 Hz, **C**), 35.11 (d, *J* = 27.6 Hz, **C'**), 28.96 (**C**), 28.27 (**C'**) 27.97 (**C**), 27.21 (**C'**), 21.50 (**C**), 21.21 (**C'**), 20.73 (CH_3-Toluene).

^{31}P{^{1}H} NMR (202 MHz, $CDCl_3$) **C**: δ 55.68 (d, *J* = 27.6 Hz), 45.61 (d, *J* = 27.8 Hz); **C'**: δ 48.12 (d, *J* = 27.7 Hz), 43.16 (d, *J* = 29.3 Hz).

1.4 Preparation of complex D

To a solution of **C** (0.50 g, 0.63 mmol) in toluene (10 mL) was added a solution of $NaBH_4$ (0.46 g, 12.6 mmol) in ethanol (10 mL). The reaction mixture was stirred for 30 min at 65 ºC and then for 30 min at room temperature to give a grey suspension. The suspension was filtered in the air, washed with diethylether (3 × 10 mL) affording the title complex as a grey solid that was dried under reduced pressure for 2 h (0.42 g, 90%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.76-6.14 (m, 28H, py+ph), 5.56 (s, H, N-H), 4.70 (d, *J* = 45.8 Hz, 1H,), 4.18 (m, 1H), 3.73-3.37 (m, 1H), 3.05-2.55 (m, 4H), 2.28-1.09 (m, 4H), -1.96 (br, *J* = 100.5 Hz, 4H, BH_3), -14.11 (t, *J* = 24.5 Hz, 1H). ^{13}C NMR ($CDCl_3$) δ 161.19, 154.69, 138.68, 138.42, 137.16, 136.86, 136.73, 135.22, 135.08, 135.00, 134.89, 133.99, 133.91, 133.80, 133.54, 132.16, 132.08, 131.92, 129.04, 128.81, 128.74, 128.59, 128.46, 128.23, 127.26, 127.18, 127.11, 127.05, 126.98, 125.31, 122.57, 61.20, 45.63, 37.97 (d, *J* = 27.0 Hz), 28.96, 27.95, 20.71.

^{31}P{^{1}H} NMR (202 MHz, $CDCl_3$) δ 47.68 (d, *J* = 29.4 Hz), 42.74 (d, *J* = 29.4 Hz).

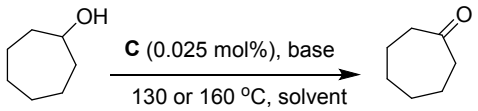
ESI-MS (m/z): Calculated for $[C_{41}H_{44}BN_2P_2Ru]$: 740.2; found: 740.7 $[M+1]^+$.

Anal. Calcd for $C_{41}H_{44}BN_2P_2Ru$: C, 66.67; H, 6.00; N, 3.79. Found: C, 66.43; H, 5.95; N, 3.53.

C. Catalyst optimization using C

1. Optimizing conditions

Table S1. Optimization of the reaction conditions for the acceptorless dehydrogenation of cycloheptanol using **C**.[a]



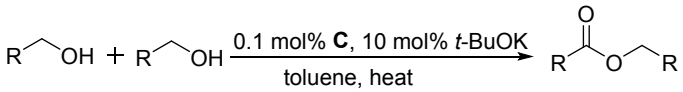
Entry	Base (mmol)	T (℃)	Time (h)	Conv.[c] (%)
1	NaOH (5)	130	16	18
			24	23
2	K_2CO_3 (5)	130	5	31
			24	39
3	$CsCO_3$ (2.5)	130	7	61
			24	63
4	$CsCO_3$ (1)	130	24	19
5	*t*-BuOK (5)	130	24	74
			48	81
6[b]	*t*-BuOK (5)	160	24	76
			36	94
7[b]	None	160	24	5

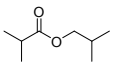
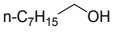
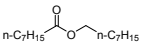
[a] Cycloheptanol (5 mmol), complex **C** (1.25×10^{-3} mmol), reaction temperature = 130 ºC (oil bath temperature), toluene (5 mL). [b] Reaction temperature = 160 ºC (oil bath temperature), *p*-xylene (5 mL). [c] The conversion was determined by GC using dodecane as an internal standard.

2. The primary alcohols in the AAD reaction by C

2. 1 Experimental: Under an atmosphere of argon, a Schlenk vessel equipped with a stir bar, was loaded with the ruthenium complex **C** (0.1 mmol), the corresponding alcohol (10 mmol) and *t*-BuOK (1 mmol) in toluene (5 mL). The reaction was then stirred and heated to 117 °C (oil-bath temperature), with the reaction vessel open to the bubbler. After the specified reaction time (40 - 72 h), the resultant solution was cooled to room temperature and the reaction mixture filtered through a plug of silica gel and then analyzed by GC using dodecane as an internal standard, employing an OV-1701 column column on Agilent 6820 instrument

Table S2.[5] Using primary alcohols in the acceptorless alcohol dehydrogenation with **C**.[a]



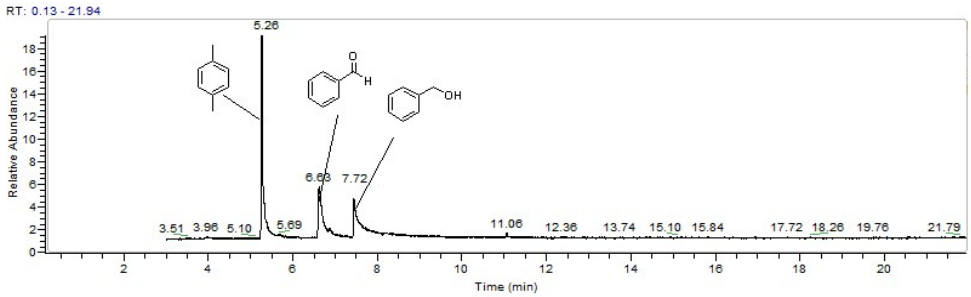
Entry	Alcohol	Product	t (h)	Conv. (%)[b]	TON
1			40	36	360
2			72	96	960
3			72	86	860
4			20	78	780

[a] Reaction conditions: alcohol (10 mmol), **C** (0.1 mmol) and *t*-BuOK (1 mmol) in toluene (5 mL) at 117 ºC (oil-bath temperature).

[b] The conversion was determined by GC using dodecane as an internal standard

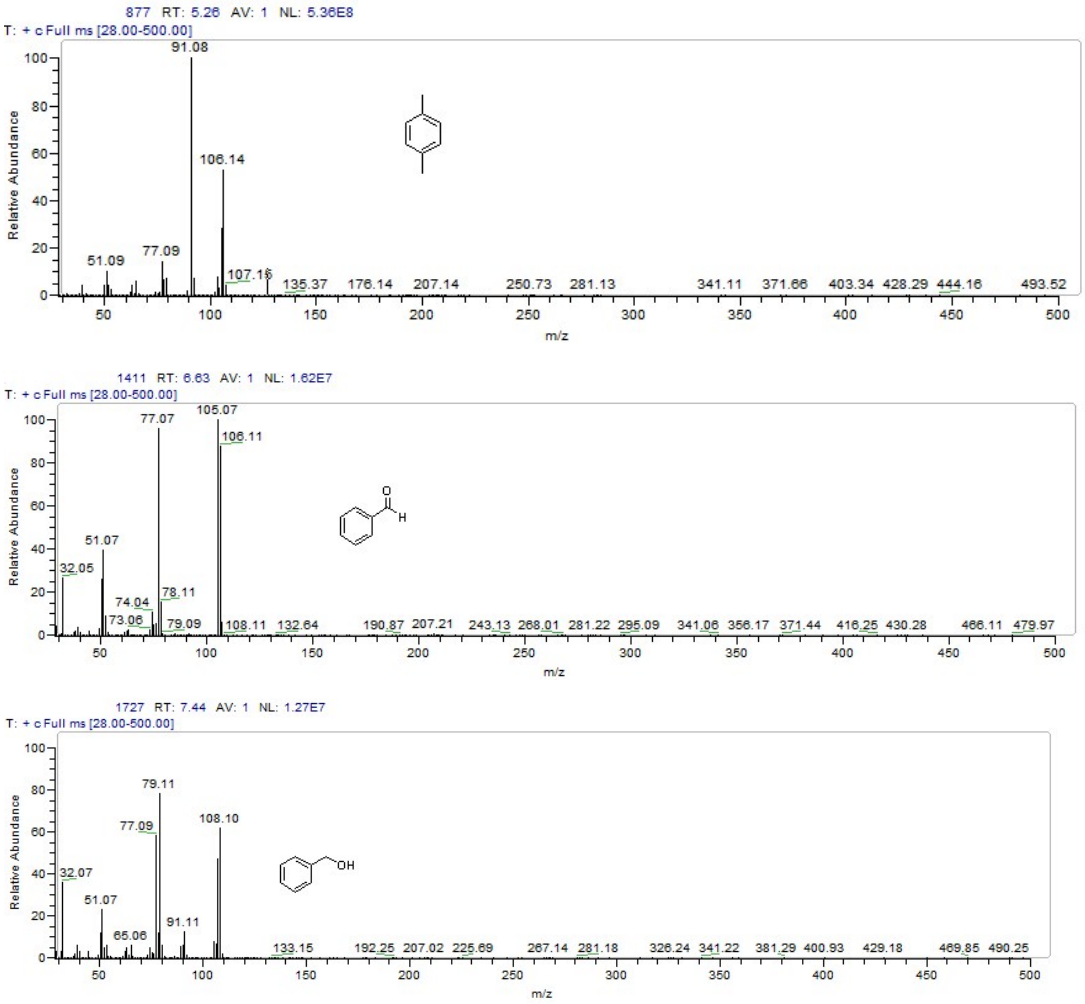
2.2 GC-MS spectra of the product of benzyl alcohol in AAD reaction

(a) GC-MS spectra of the product of benzyl alcohol in AAD reaction at 50 °C.

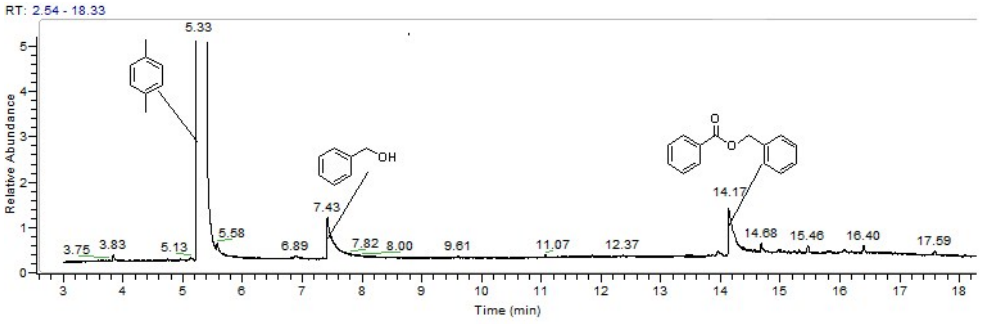


PEAK LIST
RT: 2.62 - 13.27
Number of detected peaks: 2

Apex RT	Start RT	End RT	Area	%Area	Height	%Height
6.63	6.58	6.8	4.27E+08	41.22	69481422	56
7.44	7.39	8.02	6.09E+08	58.78	54585071	44



(b) GC-MS spectra of the product of benzyl alcohol in AAD reaction at 160 °C.

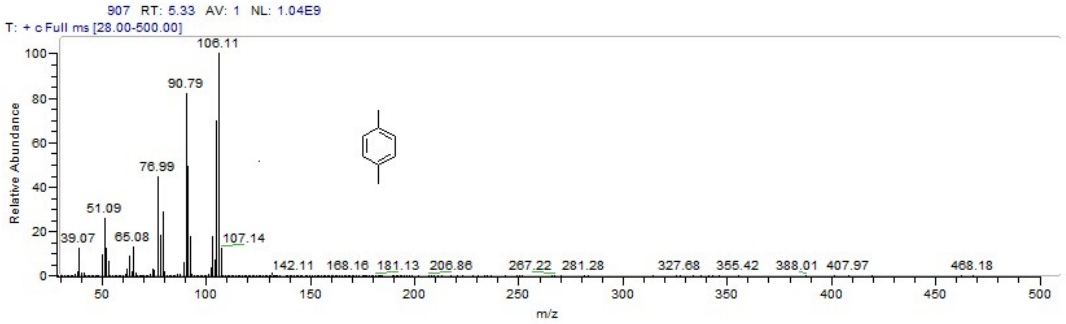


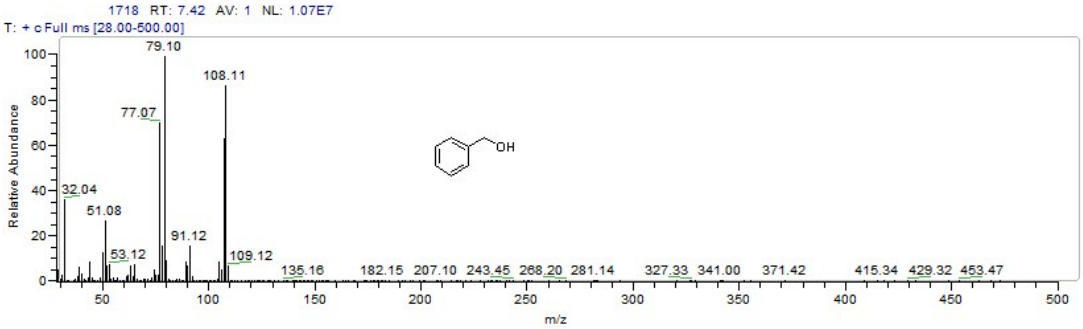
PEAK LIST

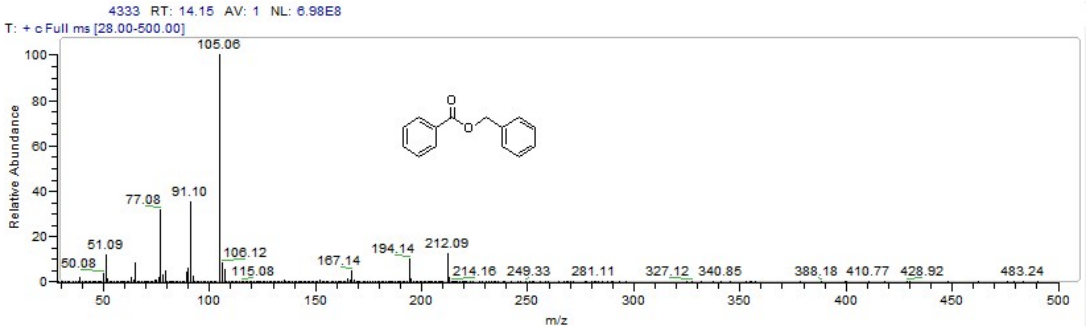
RT: 7.11 - 14.55

Number of detected peaks: 1

Apex RT	Start RT	End RT	Area	%Area	Height	%Height
7.43	7.39	7.81	3.82E+08	45.12	5.50E+07	49
14.17	14.11	14.34	4.65E+08	54.88	5.60E+07	50

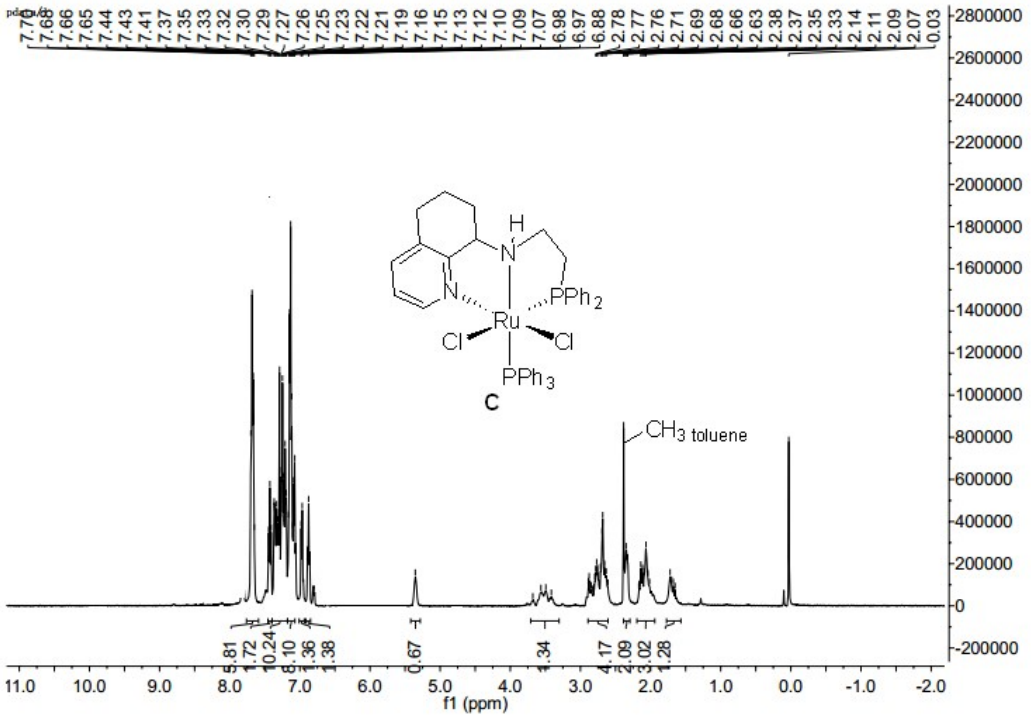

907 RT: 5.33 AV: 1 NL: 1.04E9
T: + c Full ms [28.00-500.00]
Relative Abundance
m/z
106.11
90.79
76.99
51.09
39.07
65.08
107.14
142.11 168.16 181.13 206.86 267.22 281.28 327.68 355.42 388.01 407.97 468.18


1718 RT: 7.42 AV: 1 NL: 1.07E7
T: + c Full ms [28.00-500.00]
Relative Abundance
m/z
79.10
108.11
77.07
OH
32.04
51.08
91.12
53.12
109.12
135.16 182.15 207.10 243.45 268.20 281.14 327.33 341.00 371.42 415.34 429.32 453.47

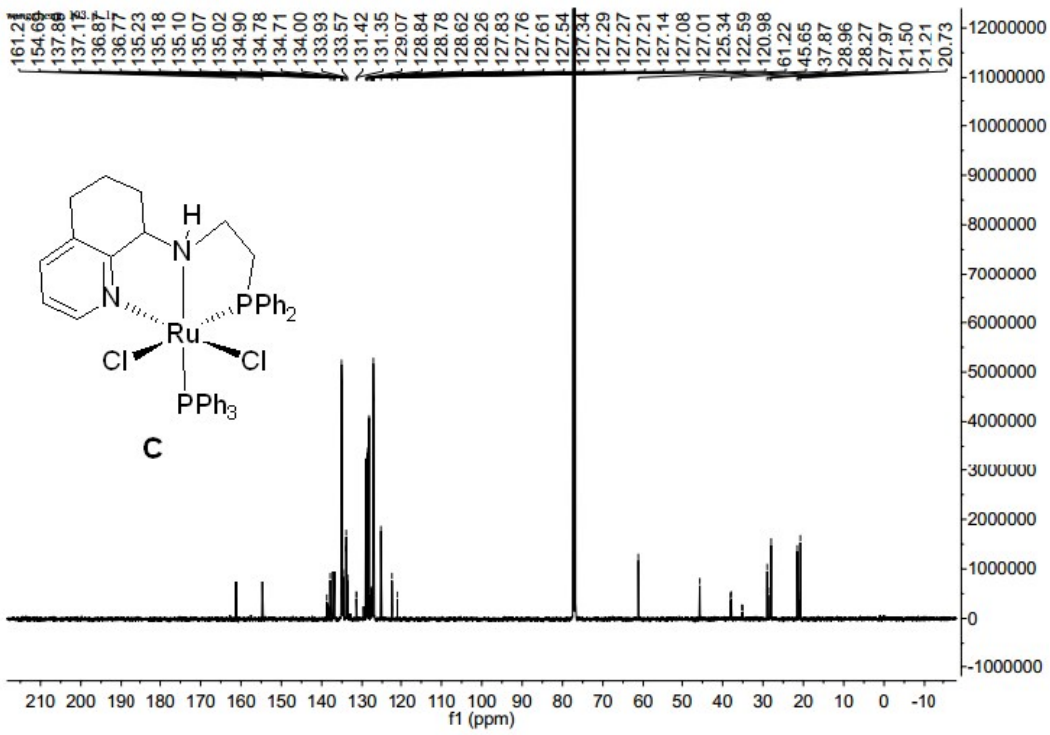

4333 RT: 14.15 AV: 1 NL: 6.98E8
T: + c Full ms [28.00-500.00]
Relative Abundance
m/z
105.06
O
O
77.08
91.10
51.09
50.08
106.12
115.08
167.14
194.14
212.09
214.16 249.33 281.11 327.12 340.85 388.18 410.77 428.92 483.24

D. ^{1}H, ^{13}C and ^{31}P NMR spectra of complexes C and D

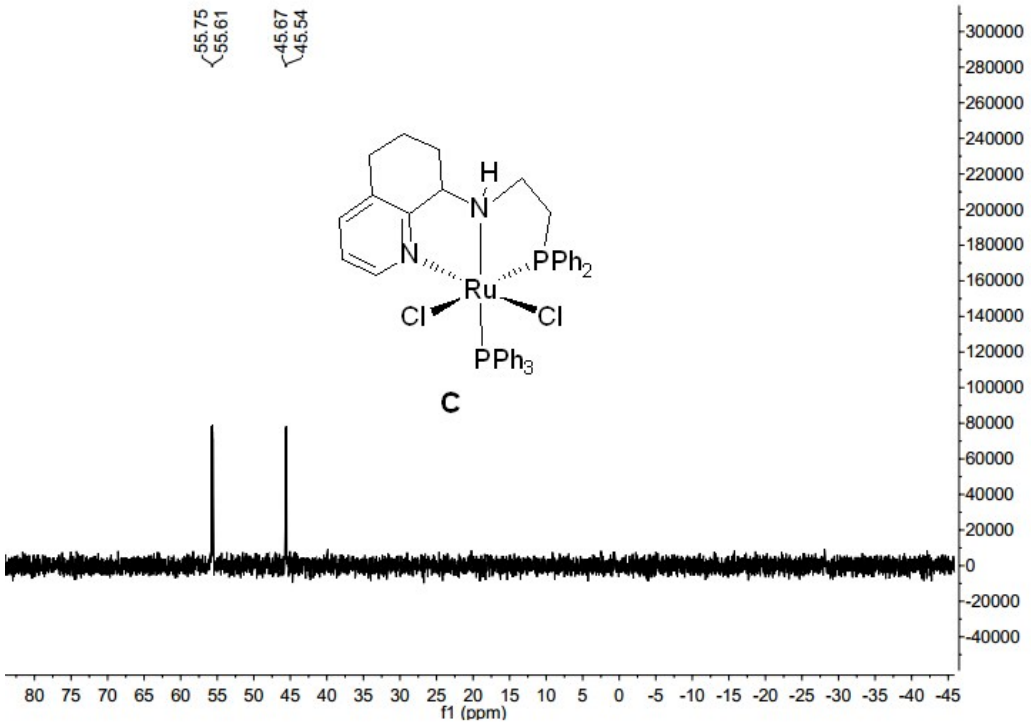
1. The ^{1}H NMR spectrum of C in $CDCl_3$



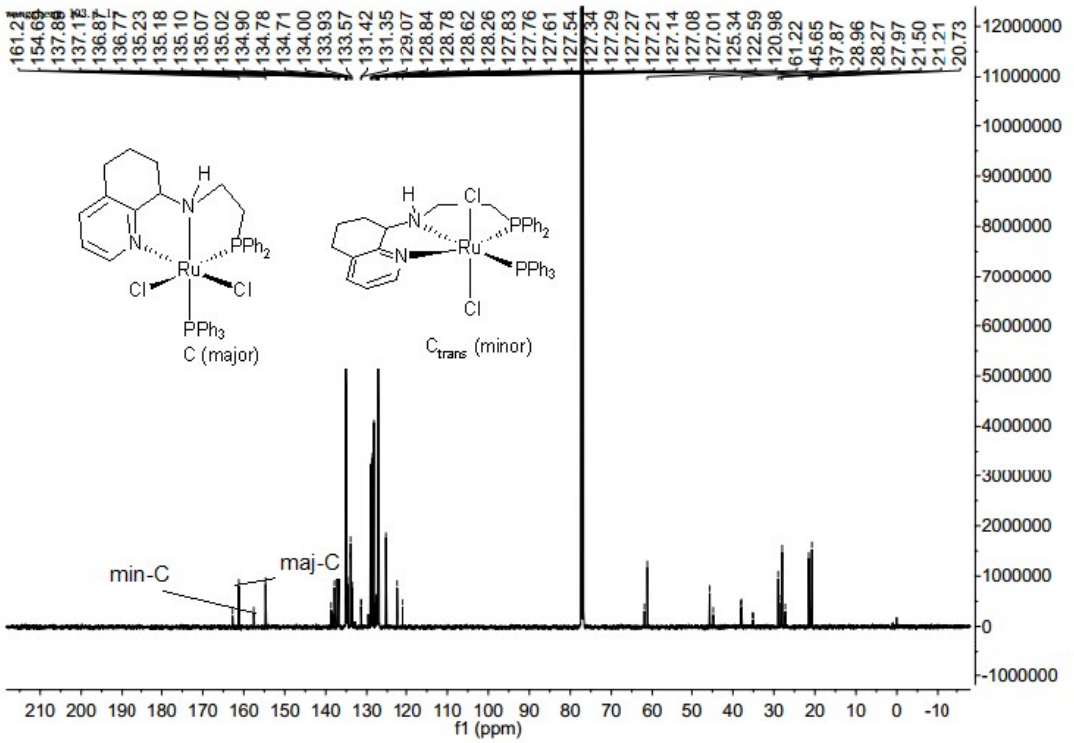
2. The $^{13}C\{^{1}H\}$ NMR spectrum of C in $CDCl_3$



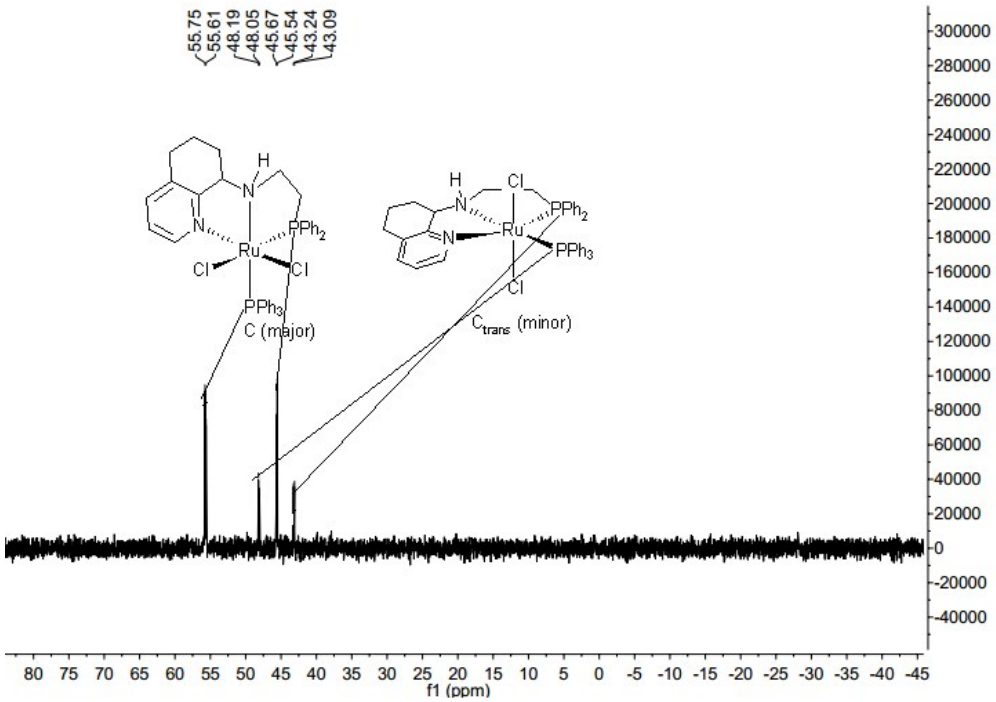
3. The $^{31}P\{^{1}H\}$ NMR spectrum of C in $CDCl_3$ recorded on dissolution



4. The $^{13}C\{^{1}H\}$ NMR spectrum of C in $CDCl_3$: spectrum recorded after 4 hours

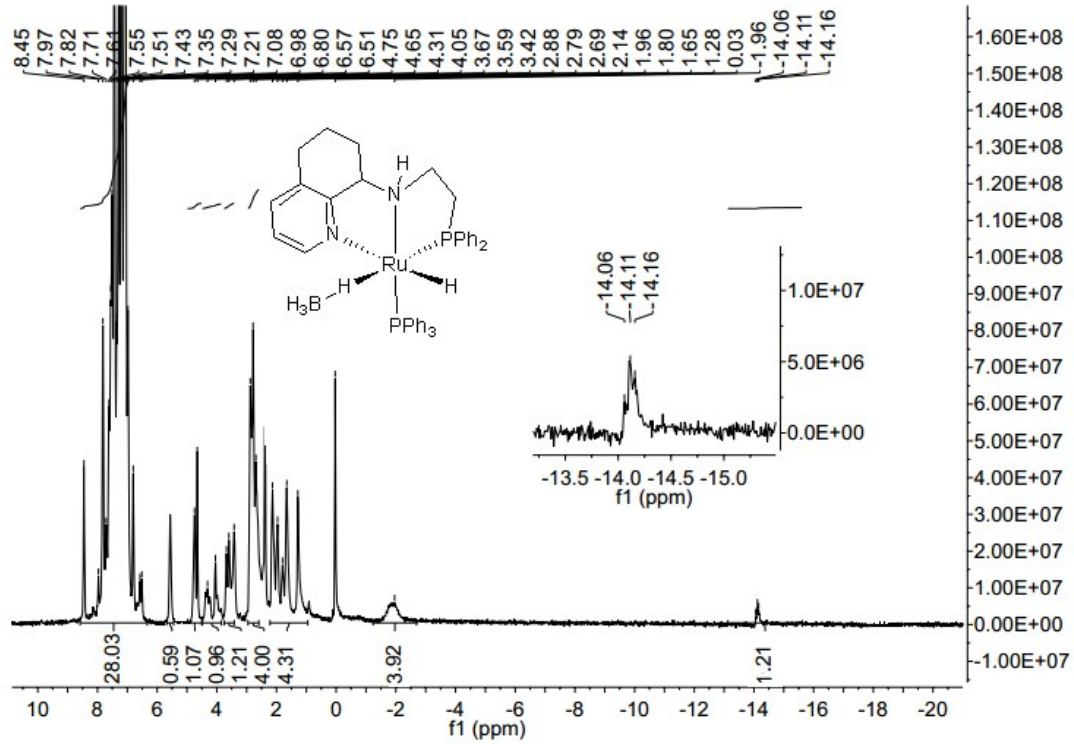


5. The $^{31}P\{^{1}H\}$ NMR spectrum of C in $CDCl_3$; spectrum recorded after 4 hours

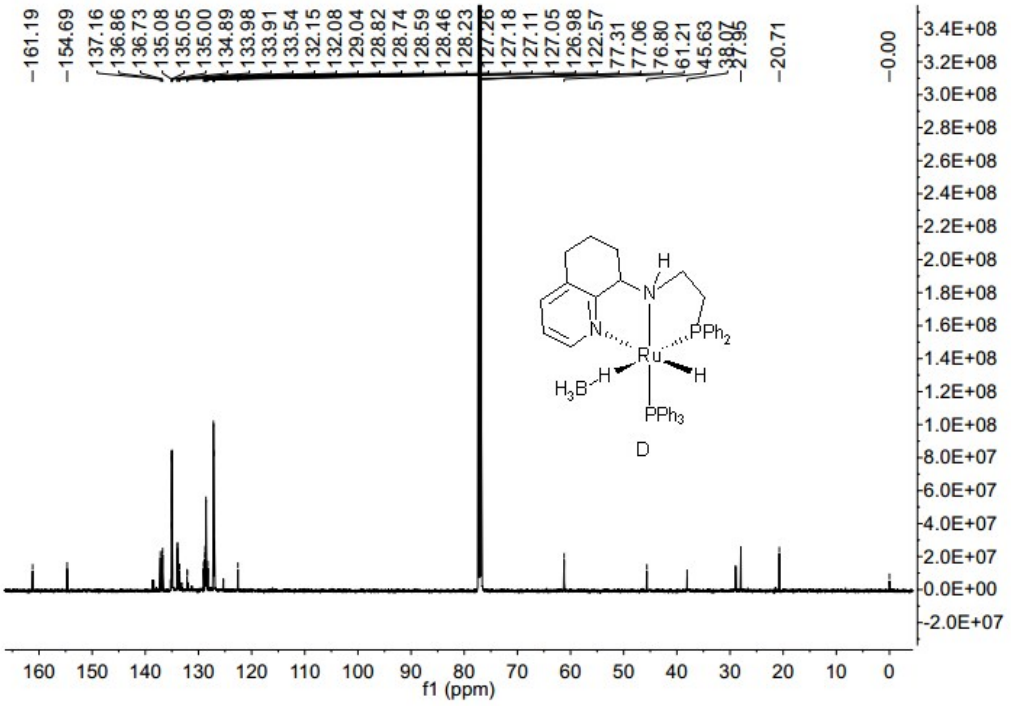


[$^{31}P\{^{1}H\}$ NMR (162 MHz, $CDCl_3$) spectrum recorded after four hours in $CDCl_3$ (ratio of **C**:**C'** = 78:28)]

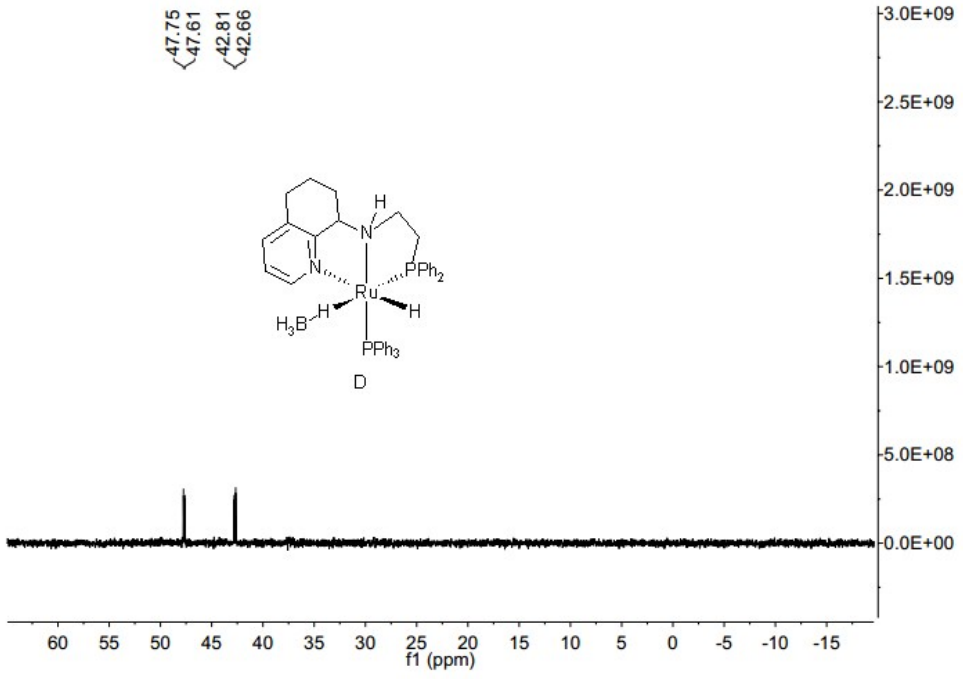
6. The ^{1}H NMR spectrum of D in $CDCl_3$



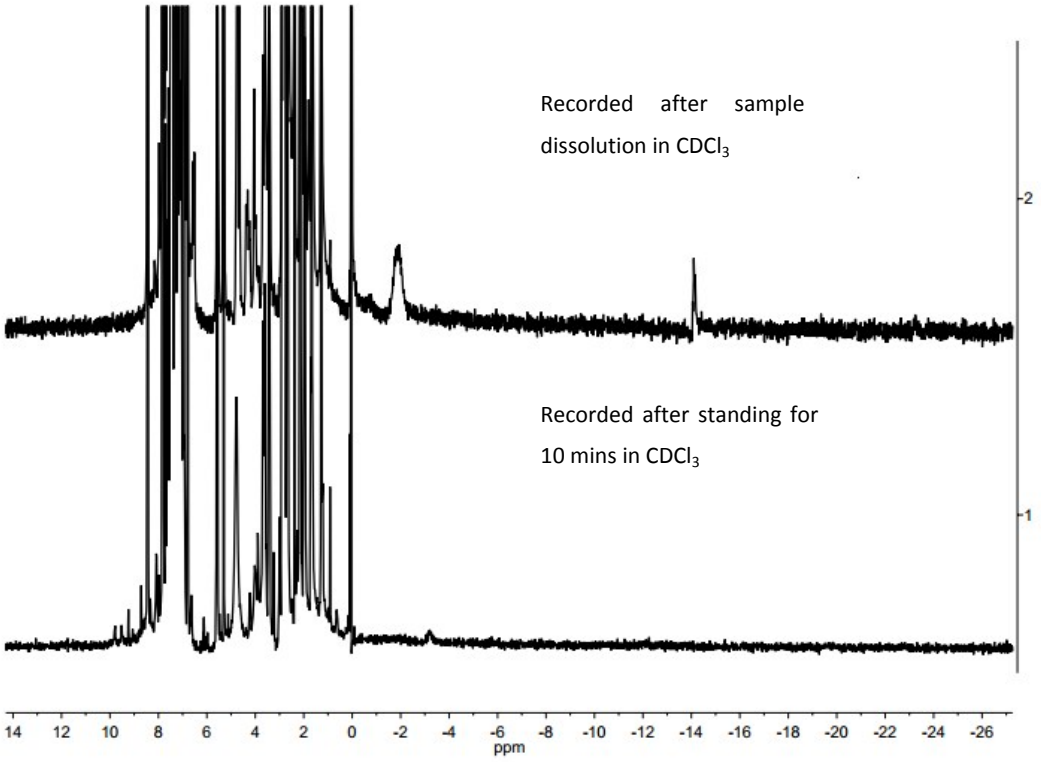
7. The $^{13}C\{^{1}H\}$ NMR spectrum of D in $CDCl_3$



8. The $^{31}P\{^{1}H\}$ NMR spectrum of D in $CDCl_3$

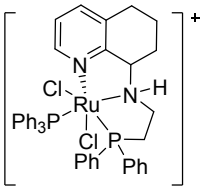
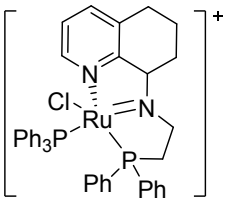
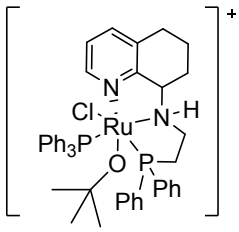
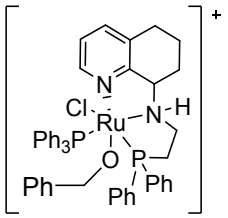
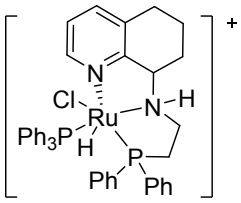


9. Comparison of the ^{1}H NMR spectra of D recorded over time in $CDCl_3$


Recorded after sample dissolution in CDCl3
Recorded after standing for 10 mins in CDCl3
2
1
14 12 10 8 6 4 2 0 -2 -4 -6 -8 -10 -12 -14 -16 -18 -20 -22 -24 -26
ppm

E. Identification of intermediate species detected using C as catalyst

Table S2. Species detected by ESI mass spectrometry under catalytic conditions using C as catalyst [4,6]

Intermediate	ESI detected species	*m/z* value	Structural assignment
Complex **C**	[**C**+1]$^+$	795.4	 **C**
M-1	[(**M-1**)+1]$^+$	759.1	 **M-1**
M-2	[(**M-2**)+1]$^+$	833.6	 **M-2**
M-2"	[(**M-2"**)+1]	867.8	 **M-2"**
M-3	[(**M-3**)+1]$^+$ [(**M-3**)+Na]$^+$	761.3 783.9	 **M-3**

1. ESI-MS (*m/z*) spectrum of C in $CDCl_3$

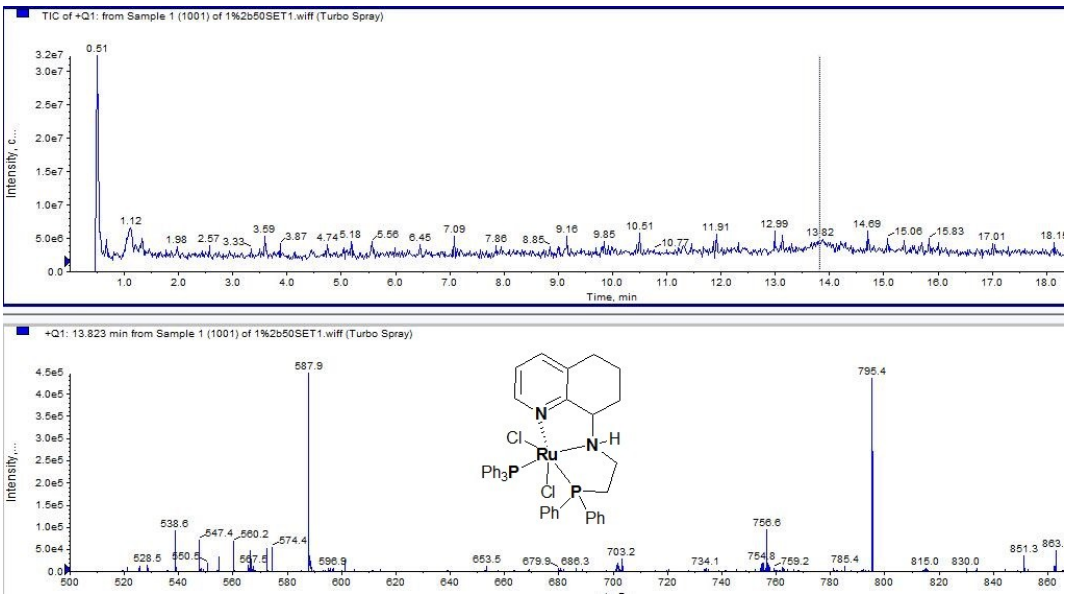


Figure S1. ESI mass spectra of **C** in $CDCl_3$ (1 mL) recorded using the 3200 QTRAP 1200 infinity series instrument. Acetonitrile:water = 70:30, flow rate = 1 ml / min, electronic energy = 50 eV, Q1MS scan range = 500~900. The base peak corresponds to [**C**+1]$^+$ at *m/z* 795.4.

2. ESI-MS (*m/z*) spectrum of C and benzyl alcohol in the presence of *t*-BuOK (1 eq.) in $CDCl_3$ at 45 ºC after 24 hours

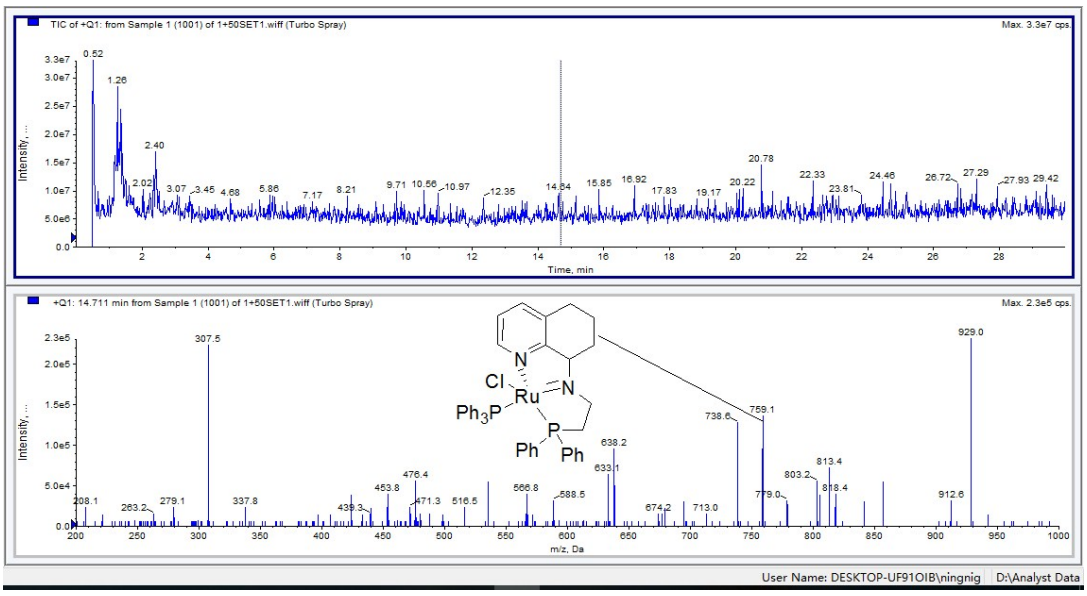


Figure S2. ESI mass spectra of **C** and benzyl alcohol in the presence of *t*-BuOK (1 eq.) in $CDCl_3$ at 45 ºC, recorded after 24 hours using the 3200 QTRAP 1200 infinity series instrument. Acetonitrile:water = 70:30, flow rate = 1 ml / min, electronic energy = 50eV, Q1MS scan range = 200~1000. The base peak corresponds to the intermediates [(M-1)+1]$^+$ at *m/z* 759.1

3. ESI-MS (*m/z*) spectrum of C and benzyl alcohol in the presence of *t*-BuOK (1 eq.) in $CDCl_3$ at 45 ºC after 24 hours

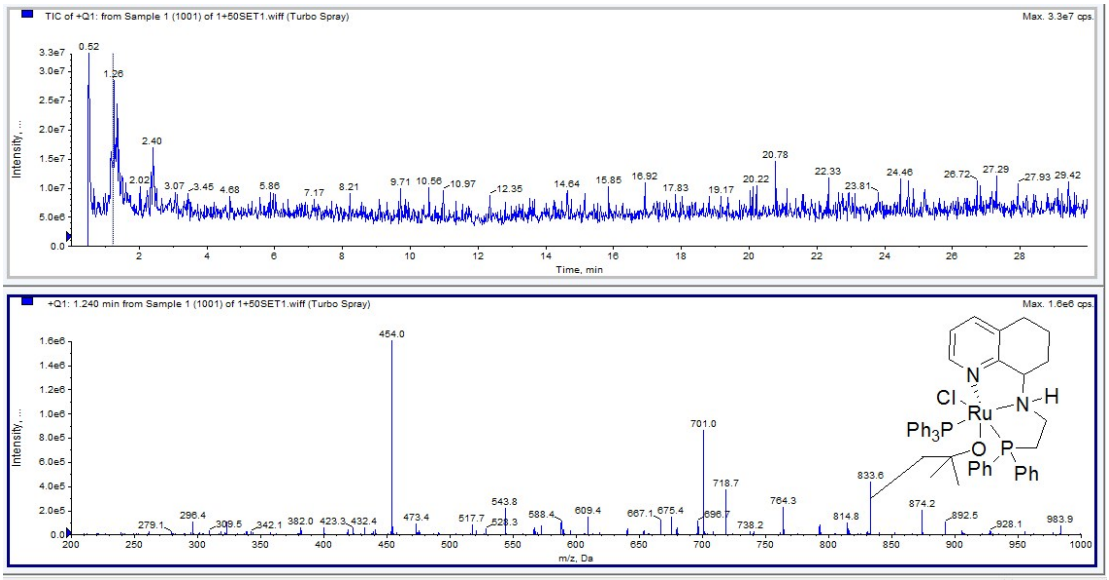


Figure S3. ESI mass spectra of **C** and benzyl alcohol in the presence of KOtBu (1 eq.) in $CDCl_3$ at 45 ºC, recorded after 24 hours using the 3200 QTRAP 1200 infinity series instrument. Acetonitrile:water = 70:30, flow rate = 1ml / min, electronic energy = 50 eV, Q1MS scan range = 200~1000. The base peak corresponds to the intermediate $[(M-2)+1]^+$ at *m/z* 833.6.

4. ESI-MS (m/z) spectrum of C and benzyl alcohol in the presence of *t*-BuOK (1 eq.) in $CDCl_3$ at 45 ºC after 24 hours

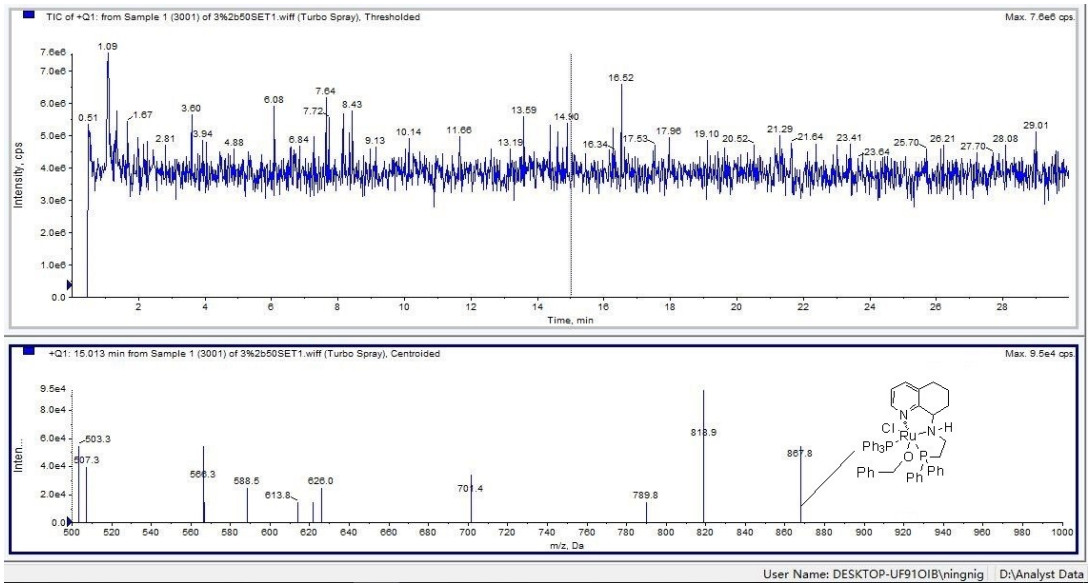


Figure S4： ESI mass spectra of **C** and benzyl alcohol in the presence of *t*-BuOK (1 eq.) in $CDCl_3$ at 45 ºC, recorded after 24 hours using the 3200 QTRAP 1200 infinity series instrument. Acetonitrile:water = 70:30, flow rate = 1 ml / min, electronic energy =5 0eV, Q1MS scan range = 500~1000. The base peak corresponds to the intermediates [(M-2")+1] at *m/z* 867.8.

5. ESI-MS (m/z) spectrum of C and benzyl alcohol in the presence of *t*-BuOK (1 eq.) in $CDCl_3$ at 45 ºC after 24 hours

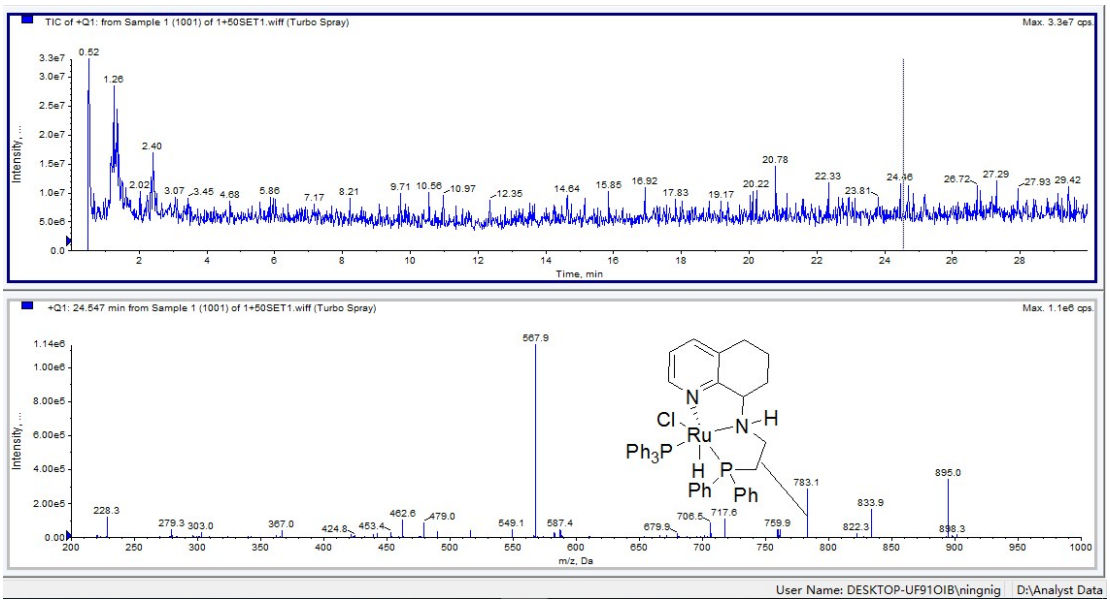


Figure S5. ESI mass spectra of **C** and benzyl alcohol in the presence of *t*-BuOK (1 eq.) in $CDCl_3$ at 45 ºC, recorded after 24 hours using the 3200 QTRAP 1200 infinity series instrument. Acetonitrile:water = 70:30, flow rate = 1 ml / min, electronic energy = 50 eV, Q1MS scan range = 200~1000. The base peak corresponds to the intermediates $[(M-3)+1]^+$ at *m/z* 761.3 and $[(M-3)+Na]^+$ at *m/z* 823.9.

F. Crystal data and structure refinement for C

Table S3. Crystallographic and data processing parameters for **C**.

Empirical formula	$C_{41}H_{40}Cl_2N_2P_2Ru$
Formula weight	794.66
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 11.188(2) Å alpha = 90 deg. b = 25.322(5) Å beta = 93.32(3) deg. c = 16.401(3) Å gamma = 90 deg.
Volume	4638.6(16) $Å^3$
Z, Calculated density	4,1.138 Mg/m^3
Absorption coefficient	0.548 mm^{-1}
F(000)	1632
Crystal size	0.14 x 0.10 x 0.08 mm
Theta range for data collection	2.03 to 25.00 deg.
Limiting indices	-13<=h<=10, -29<=k<=29, -19<=l<=18
Reflections collected / unique	26111 / 8142 [R(int) = 0.1055]
Completeness to theta = 25.00	99.7 %

Absorption correction	None
Max. and min. transmission	0.9590 and 0.9253
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8142 / 0 / 433
Goodness-of-fit on F^2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0736, wR2 = 0.1795
R indices (all data)	R1 = 0.0981, wR2 = 0.1921
Largest diff. peak and hole	0.519 and -0.591 e.$Å^{-3}$

Table S4. Bond lengths [Å] and angles [deg] for **C**

Ru(1)-N(2)	2.089(5)	C(9)-C(8)	1.524(8)
Ru(1)-N(1)	2.162(5)	C(8)-C(7)	1.526(10)
Ru(1)-P(1)	2.2622(17)	C(23)-C(24)	1.404(10)
Ru(1)-P(2)	2.3249(17)	C(23)-C(28)	1.406(10)
Ru(1)-Cl(1)	2.4275(17)	C(10)-C(11)	1.542(9)
Ru(1)-Cl(2)	2.5013(16)	C(19)-C(20)	1.402(11)
P(2)-C(35)	1.847(7)	C(39)-C(38)	1.400(10)
P(2)-C(23)	1.853(7)	C(28)-C(27)	1.410(9)
P(2)-C(29)	1.859(7)	C(38)-C(37)	1.309(11)
P(1)-C(12)	1.835(7)	C(24)-C(25)	1.366(10)
P(1)-C(11)	1.846(6)	C(26)-C(25)	1.335(11)
P(1)-C(18)	1.856(7)	C(26)-C(27)	1.390(11)
N(1)-C(9)	1.503(8)	C(2)-C(3)	1.380(10)
N(1)-C(10)	1.519(8)	C(2)-C(1)	1.389(10)
N(2)-C(1)	1.349(8)	C(34)-C(33)	1.386(10)
N(2)-C(5)	1.377(8)	C(7)-C(6)	1.505(10)
C(4)-C(3)	1.385(9)	C(13)-C(14)	1.375(11)
C(4)-C(5)	1.398(9)	C(33)-C(32)	1.389(11)
C(4)-C(6)	1.506(9)	C(32)-C(31)	1.439(12)
C(35)-C(36)	1.389(9)	C(17)-C(16)	1.381(11)
C(35)-C(40)	1.438(10)	C(36)-C(37)	1.397(10)
C(5)-C(9)	1.504(8)	C(14)-C(15)	1.393(11)
C(40)-C(39)	1.404(9)	C(21)-C(20)	1.386(10)
C(29)-C(34)	1.379(9)	C(21)-C(22)	1.404(11)
C(29)-C(30)	1.396(9)	C(30)-C(31)	1.308(10)
C(18)-C(69)	1.380(9)	C(15)-C(16)	1.360(11)
C(18)-C(19)	1.390(9)	C(22)-C(69)	1.339(10)
C(12)-C(13)	1.393(10)	C(12)-C(17)	1.416(10)
N(2)-Ru(1)-N(1)	78.61(19)	C(69)-C(18)-P(1)	124.8(5)
N(2)-Ru(1)-P(1)	90.62(14)	C(19)-C(18)-P(1)	116.5(5)
N(1)-Ru(1)-P(1)	84.06(14)	C(13)-C(12)-C(17)	118.1(7)

N(2)-Ru(1)-P(2)	98.90(15)	C(13)-C(12)-P(1)	121.7(5)
N(1)-Ru(1)-P(2)	173.39(14)	C(17)-C(12)-P(1)	120.0(6)
P(1)-Ru(1)-P(2)	102.16(6)	N(1)-C(9)-C(5)	108.8(5)
N(2)-Ru(1)-Cl(1)	165.34(14)	N(1)-C(9)-C(8)	116.5(5)
N(1)-Ru(1)-Cl(1)	86.84(14)	C(5)-C(9)-C(8)	113.5(5)
P(1)-Ru(1)-Cl(1)	89.63(6)	C(9)-C(8)-C(7)	109.1(6)
P(2)-Ru(1)-Cl(1)	95.37(6)	C(24)-C(23)-C(28)	118.4(6)
N(2)-Ru(1)-Cl(2)	92.35(14)	C(24)-C(23)-P(2)	119.3(5)
N(1)-Ru(1)-Cl(2)	84.61(13)	C(28)-C(23)-P(2)	122.1(5)
P(1)-Ru(1)-Cl(2)	167.48(6)	N(1)-C(10)-C(11)	111.9(5)
P(2)-Ru(1)-Cl(2)	89.40(6)	C(18)-C(19)-C(20)	119.7(7)
Cl(1)-Ru(1)-Cl(2)	84.44(6)	C(38)-C(39)-C(40)	120.4(7)
C(35)-P(2)-C(23)	99.8(3)	C(23)-C(28)-C(27)	119.7(7)
C(35)-P(2)-C(29)	98.0(3)	C(37)-C(38)-C(39)	121.2(7)
C(23)-P(2)-C(29)	101.7(3)	C(25)-C(24)-C(23)	119.5(7)
C(35)-P(2)-Ru(1)	115.9(2)	C(25)-C(26)-C(27)	119.5(6)
C(23)-P(2)-Ru(1)	119.0(2)	C(3)-C(2)-C(1)	119.4(6)
C(29)-P(2)-Ru(1)	118.8(2)	C(29)-C(34)-C(33)	119.2(7)
C(12)-P(1)-C(11)	100.2(3)	C(6)-C(7)-C(8)	111.6(6)
C(12)-P(1)-C(18)	102.4(3)	C(7)-C(6)-C(4)	112.5(6)
C(11)-P(1)-C(18)	105.1(3)	N(2)-C(1)-C(2)	121.3(6)
C(12)-P(1)-Ru(1)	128.0(2)	C(14)-C(13)-C(12)	122.1(7)
C(11)-P(1)-Ru(1)	101.3(2)	C(26)-C(27)-C(28)	119.6(7)
C(18)-P(1)-Ru(1)	116.5(2)	C(2)-C(3)-C(4)	121.0(7)
C(9)-N(1)-C(10)	110.6(5)	C(34)-C(33)-C(32)	122.9(7)
C(9)-N(1)-Ru(1)	106.5(3)	C(33)-C(32)-C(31)	114.8(7)
C(10)-N(1)-Ru(1)	116.3(4)	C(16)-C(17)-C(12)	118.1(8)
C(1)-N(2)-C(5)	118.6(5)	C(35)-C(36)-C(37)	121.5(7)
C(1)-N(2)-Ru(1)	126.4(4)	C(26)-C(25)-C(24)	123.4(7)
C(5)-N(2)-Ru(1)	114.9(4)	C(13)-C(14)-C(15)	119.3(7)
C(3)-C(4)-C(5)	117.0(6)	C(20)-C(21)-C(22)	119.0(7)
C(3)-C(4)-C(6)	121.4(6)	C(31)-C(30)-C(29)	121.6(7)
C(5)-C(4)-C(6)	121.6(6)	C(16)-C(15)-C(14)	118.9(7)
C(36)-C(35)-C(40)	117.8(6)	C(69)-C(22)-C(21)	120.1(7)
C(36)-C(35)-P(2)	121.5(6)	C(15)-C(16)-C(17)	123.4(8)
C(40)-C(35)-P(2)	120.7(5)	C(38)-C(37)-C(36)	120.9(7)
N(2)-C(5)-C(4)	122.6(6)	C(10)-C(11)-P(1)	108.1(4)
N(2)-C(5)-C(9)	115.8(5)	C(22)-C(69)-C(18)	122.3(7)
C(4)-C(5)-C(9)	121.6(5)	C(21)-C(20)-C(19)	119.9(7)
C(39)-C(40)-C(35)	118.3(6)	C(30)-C(31)-C(32)	122.5(7)
C(34)-C(29)-C(30)	118.8(6)	C(30)-C(29)-P(2)	125.1(5)
C(34)-C(29)-P(2)	115.8(5)	C(69)-C(18)-C(19)	118.7(6)

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