

Supporting Information for

**Development of a Novel Secondary Phosphine Oxide-Ruthenium(II)
Catalyst and Its Application for Carbonyls Reduction**

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Content

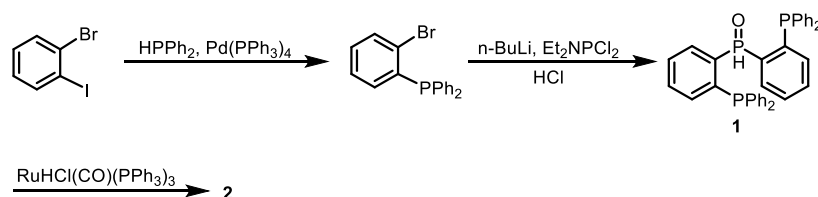
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General Information

Unless otherwise mentioned, all experiments were carried out under an atmosphere of argon or using standard Schlenk techniques. Solvents were dried with standard procedures and degassed with N₂. Flash column chromatography was performed using Tsingdao silica gel (60, particle size 300-400 mesh). NMR spectra were recorded on a Bruker DPX 400 spectrometer at 400 MHz for ¹H NMR, 100 MHz for ¹³C NMR and 161.7 MHz for ³¹P NMR in CDCl₃ with tetramethylsilane (TMS) as internal standard. Chemical shifts are reported in ppm and coupling constants are given in Hz. Chemical shifts were reported upfield to TMS (0.00 ppm) for ¹H NMR and relative to CDCl₃ (77.0 ppm) for ¹³C NMR. GC analysis was carried out on Angilent 1200 Series instrument using achiral capillary columns.

Synthetic Details

Synthesis of 2



Synthesis of (2-bromophenyl)diphenylphosphine¹

2-iodobromobenzene (24.1 g, 85.3 mmol), diphenylphosphine (15.9 g, 85.3 mmol), triethylamine (101 g, 100 mmol), and a catalytic amount of Pd(PPh₃)₄ (513.0 mg, 0.45 mmol) were dissolved in 15 mL of toluene to give a clear, bright yellow solution. The solution was heated at 80 °C with stirring for 16 hours in a sealed bomb, resulting in the precipitation of triethylammonium iodide. The resulting orange solution was dried in vacuo at 50 °C, extracted into diethyl ether (400 mL), and filtered through a pad of silica gel to give a clear, pale yellow solution, from which the volatiles were removed in vacuo to yield the phosphine as a creamy white powder (27.6 g, 95%). Characterization data matched those previously reported for this compound.

Synthesis of the ligand 1

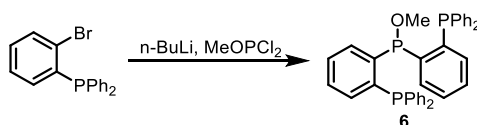
A solution of (2-bromophenyl)diphenylphosphine (1.71 g, 5 mmol) in 20 mL ethyl ether was cooled to -40 °C. Then a solution of n-butyl lithium in hexane (3.75 mL, 6 mmol) was added dropwise to the reaction mixture. The reaction was stirred under room temperature for 1 hour and then cooled to -40 °C again. A solution of 1,1-dichloro-N,N-diethylphosphanamine (0.435 g, 2.5 mmol) in ethyl ether (5 mL) was added dropwise and the solution was stirred at the same temperature for 1 hour. The reaction was warmed to room temperature slowly and stirred overnight. After cooling to 0 °C, 2 mL concentrated hydrochloric acid was added and the reaction

mixture was stirred for 3 hours. Saturated sodium bicarbonate (50 mL) was added cautiously. The reaction mixture was extracted with ethyl ester (30 mL x 3 times). The organic phase was combined and dried with sodium sulfate. Solvent was concentrated and the crude product was purified by column chromatography (hexane/ethyl ester = 3 : 1). ^1H NMR(400 MHz, CDCl_3): δ = 9.36 (dt, J^1 = 515 Hz, J^2 = 3.0 Hz, 1H), 7.80-7.90 (m, 2H), 7.23-7.38 (m, 12H), 7.06-7.21 (m, 14H); $^{13}\text{C}\{^1\text{H}\}$ NMR (126.2 MHz, CDCl_3) δ 140.3, 140.2, 140.1, 138.6, 138.3, 137.8, 137.5, 136.2, 136.1, 135.4, 135.3, 135.1, 135.1, 133.9, 133.8, 133.8, 133.7, 133.6, 133.5, 133.4, 133.3, 131.9, 131.9, 129.2, 129.1, 128.7, 128.6, 128.5, 128.5, 128.4, 128.3, 128.3, 128.3; $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, CDCl_3): δ = 11.3 (dt, J^1 = 77.6 Hz, J^2 = 515.8 Hz), 18.6 (d, J = 77.6 Hz). HRMS (ESI+), m/z 571.1489 ($[\text{M}+\text{H}]^+$), calcd for $\text{C}_{28}\text{H}_{31}\text{N}_2\text{P}_2^+$: 571.1504.

Synthesis of complex 2

Ligand **1** (0.57 g, 1 mmol) and $\text{RuHCl}(\text{CO})(\text{PPh}_3)_3$ (952 mg, 1 mmol) were suspended in toluene (10 mL) under an nitrogen atmosphere. The mixture was heated at reflux for 5 hours. After cooled to room temperature, ethyl ether (10 mL) was added and stirred for 5 min. The reaction mixture was filtered and washed with ethyl ether (5 mL $\times$ 3). The grey white solid was recognized as two compounds by TLC, and the mixed compounds were separated by column chromatography (dichloromethane/methanol, 50:1 to 20:1). Compound with less polarity was unidentified so far. The compound with higher polarity, however, was identified as **2** (light grey solid, 0.46 g, yield 46%). ^1H NMR(400 MHz, CDCl_3): δ = 8.26-8.50 (m, 2H), 7.29-7.38 (m, 2H), 6.91-7.23 (m, 21H), 6.55-6.87 (m, 18H), -7.94 (tdd, J^1 = 28 Hz, J^2 = 17.6 Hz, J^3 = 13.2 Hz, 1H); $^{13}\text{C}\{^1\text{H}\}$ NMR (126.2 MHz, CDCl_3) δ 135.9, 135.7, 133.8, 133.7, 133.7, 133.1, 132.3, 132.2, 132.1, 131.7, 131.5, 129.5, 129.3, 129.1, 128.8, 128.3, 128.2, 128.2, 127.5, 127.3; $^{31}\text{P}\{^1\text{H}\}$ NMR (161.7 MHz, CDCl_3): δ = 135.0 (dt, J^1 = 221.7 Hz, J^2 = 22.2 Hz), δ = 65.5 (dd, J^1 = 22.2 Hz, J^2 = 22.3 Hz), δ = 40.2 (dt, J^1 = 221.7 Hz, J^2 = 22.3 Hz). HRMS (ESI+), m/z 963.1396 ($[\text{M}]^+$), calcd for $\text{C}_{55}\text{H}_{45}\text{O}_2\text{P}_4\text{Ru}^+$: 963.1414.

Synthesis of 6



A solution of (2-bromophenyl)diphenylphosphane (1.36 g, 4 mmol) in 20 mL ethyl ether was cooled to -78°C . n-Butyllithium (1.7 mL of 2.4 M, 4 mmol) was added dropwise to the solution. The mixture was warmed to room temperature and stirred 2 hours and cooled to -78°C again. A solution of MeOPCl_2 (0.266 g, 2 mmol) in 1 mL ethyl ether was added dropwise to the above solution. The reaction was warmed to room temperature slowly and stirred at room temperature for 2 hours. The reaction mixture was concentrated and purified by neutral aluminum oxide column chromatography (eluted with PE/EA = 10). A white solid was obtained (0.65 g, yield 56%). ^1H NMR(400 MHz, CDCl_3): δ = 7.00-7.34 (m, 18H), 3.17-3.30 (d, 3H, J = 14 Hz); $^{13}\text{C}\{^1\text{H}\}$ NMR (126.2 MHz, CDCl_3) δ 148.1, 148.0, 147.8, 147.7, 141.1, 141.0,

140.8, 140.7, 138.0, 137.9, 137.9, 137.8, 136.8, 136.7, 136.7, 136.6, 134.2, 134.2, 134.0, 133.9, 133.9, 133.8, 133.8, 133.8, 133.7, 133.7, 133.6, 133.5, 130.8, 129.2, 129.1, 128.6, 128.4, 128.3, 128.3, 128.2, 128.1, 128.2, 128.1, 127.9, 127.9, 125.3, 57.3, 57.1; $^{31}\text{P}\{^1\text{H}\}$ NMR (161.7 MHz, CDCl_3): δ = 15.5 (d, J = 163.8 Hz), δ = 101.5 (t, J = 163.8 Hz). HRMS (ESI+), m/z 585.1647 ($[\text{M}]^+$), calcd for $\text{C}_{37}\text{H}_{32}\text{OP}_3^+$: 585.1661.

CCDC 1535463 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB21EZ, UK; fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

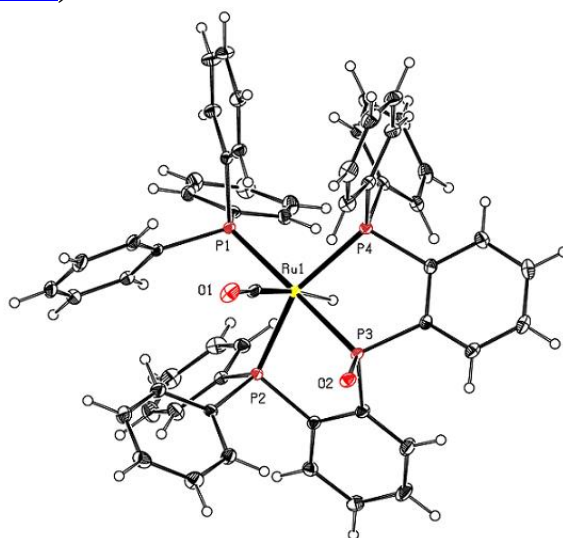


Figure S1. Crystal structure of complex 2.

Catalytic study details

In an argon glovebox, a 5 mL vial equipped with a magnetic stirring bar, was added the required amount of the catalyst (dissolved in relative solvent), substrates (5 mmol) and solvent (1.5 mL). The mixture was transferred to a stain-less autoclave and then was purged by three cycles of pressurization/venting with H_2 (10 atm). Then pressurized with H_2 (50 atm) and disconnected from the H_2 source. The autoclave was placed in an oil bath preheated to the desired temperature. After the desired reaction time, the autoclave was cooled in an ice bath, and the pressure was released slowly.

Table S1. Optimization of Reaction conditions of cinnamaldehyde reduction.^a

Entry	S/C	T (°C)	Solvent	3a / 4a / 5a ^b
1	5000	50	THF	74 26 <1
2	5000	50	Dioxane	73 27 <1
3	5000	50	DCM	76 24 <1
4	5000	50	Toluene	24 76 <1
5	5000	30	Toluene	93 6 <1
6	5000	70	Toluene	29 71 <1
7	5000	90	Toluene	<1 99 <1
8	10000	80	Toluene	2 98 <1
9	10000	100	Toluene	<1 98 2
10	20000	80	Toluene	53 47 <1
11	20000	100	Toluene	2 96 2
12	50000	100	Toluene	27 73 <1

^areaction conditions: substrates **3a** (5 mmol), toluene (1.5 mL), H₂ (50 bar), 80 °C, 20 h. ^bselectivities were determined by GC.

Table S2. Additive effect on the reduction of acetophenone.^a

Entry	S/C	Additive	Solvent	Yield (%)
1	500	-	Toluene	30
2	500	KO ^t Bu	Toluene	72
3	500	KO ^t Bu	MeOH	98
4	500	KO ^t Bu	ⁱ PrOH	33
5	1000	NaH	Toluene	99

^areaction conditions: acetophenone (1 mmol), additive (0.02 mmol), solvent (1 mL), H₂ (50 bar), 80 °C, 18 h. ^byields were determined by ¹H NMR.

Table S3. Additive effect on the reduction of cinnamaldehyde.^a

Entry	Additive (1 mol%)	Yield (%)
1	-	91
2	CF ₃ COOH	26
3	PhCOOH	92
4	NaOAc	81
5	KOAc	69
6	CsOAc	82
7	KOTf	73

^areaction conditions: substrates **3a** (5 mmol), toluene (1.5 mL), H₂ (50 bar), 80 °C, 20 h.

Details of mechanistic study

Additive effect study

Acid additive: Trifluoroacetic acid (0.02 mmol, 0.1 mL, 0.2 mmol/mL in CDCl_3) was added into a solution of complex **2** (10 mg, 0.01 mmol) in toluene (0.5 mL) under nitrogen atmosphere. This solution was stirred at room temperature for 2 hours, and then concentrated under vacuum. The obtained solid was dissolved in d_6 -benzene for NMR test (CDCl_3 , 400 MHz for ^1H NMR and 161.7 MHz for ^{31}P NMR).

Base additive: KOMe (0.02 mmol, 0.1 mL, 0.2 mmol/mL in MeOH) was added into a solution of complex **2** (10 mg, 0.01 mmol) in MeOH under nitrogen atmosphere. This solution was stirred at room temperature for 2 hours. Solvent was concentrated under vacuum. The white solid was dissolved in CDCl_3 and then used to do NMR test (CDCl_3 , 400 MHz for ^1H NMR and 161.7 MHz for ^{31}P NMR).

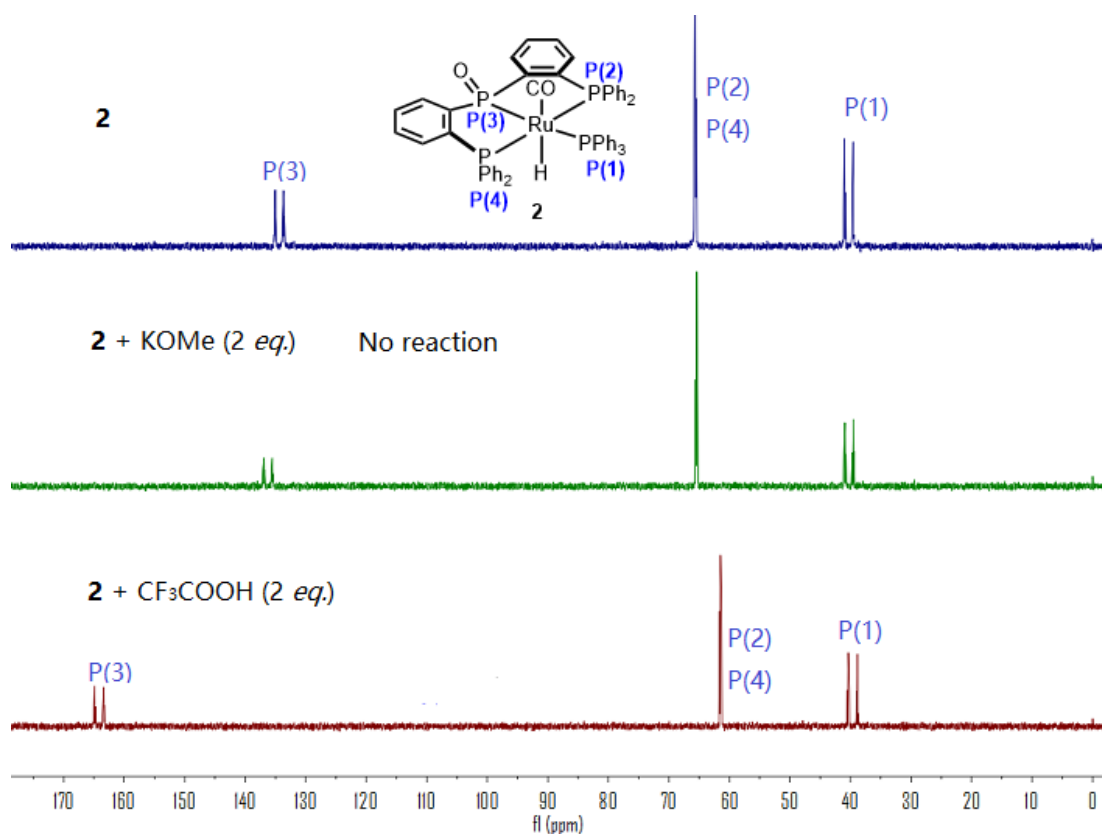


Figure S2. ^{31}P NMR of complex **2** with KOMe/ CF_3COOH as additives.

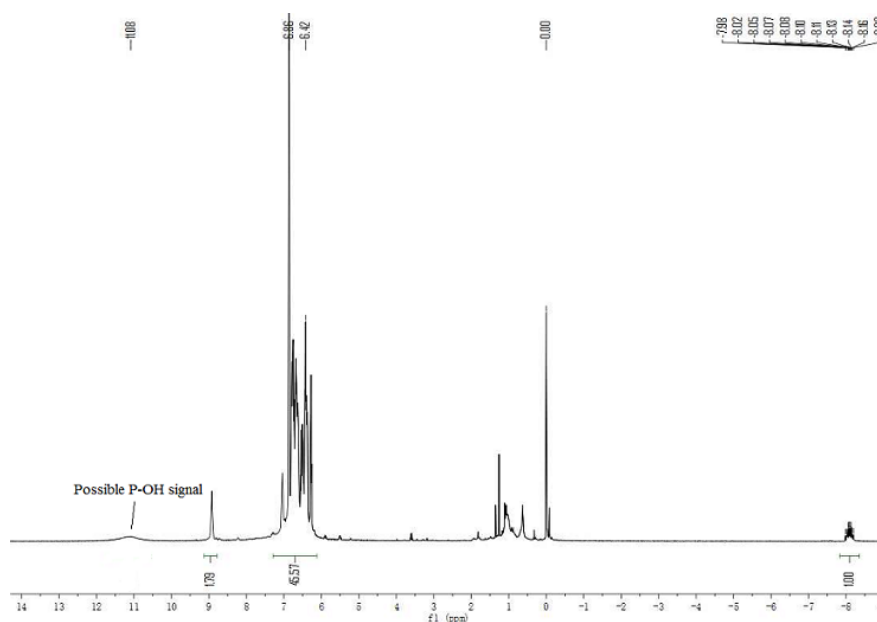
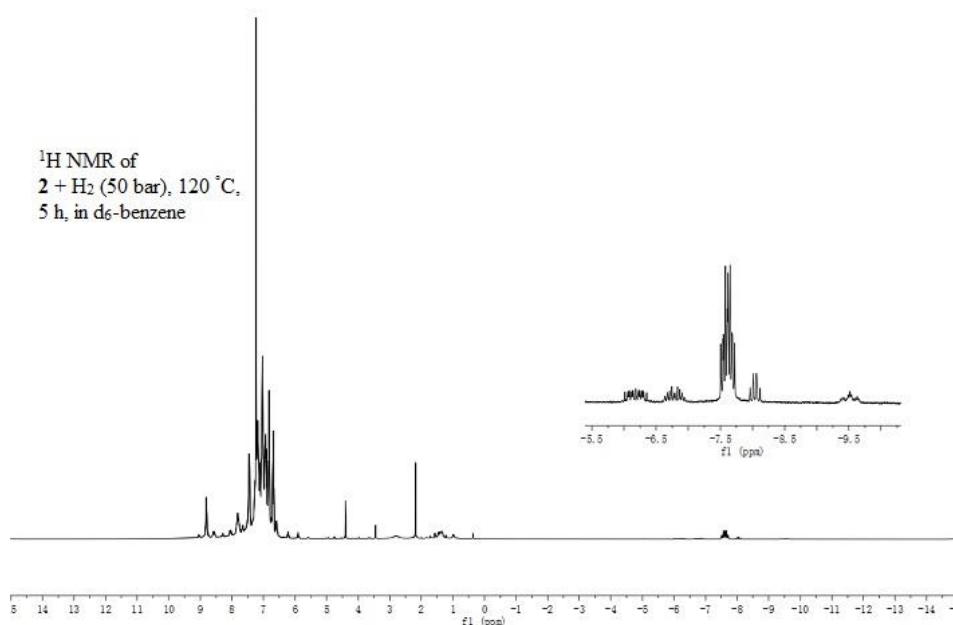


Figure S3. ^1H NMR of complex **2** reacted with CF_3COOH .

H_2 activation study:

(a) Stepwise NMR study

A solution of complex **2** (15 mg) in d_6 -benzene (0.5 mL) was exposed in H_2 (50 atm) at 120°C for 2 h. After cooled to room temperature and the H_2 pressure was released, a red solution was obtained. This solution was subjected to NMR study directly (d_6 -benzene, 400 MHz for ^1H NMR and 161.7 MHz for ^{31}P NMR). ^1H and ^{31}P NMR analysis revealed most of the complex **2** kept unreacted. ^1H NMR showed several kinds of hydride species formed. ^{31}P NMR showed that part of PPh_3 disassociated from the metal center. When prolonging the reaction time to 12 h, free PPh_3 did not accumulate to a higher level, implying that the H_2 activation step might be reversible and an equilibrium between the H-Ru-P-OH species and Ru-P=O species existed.



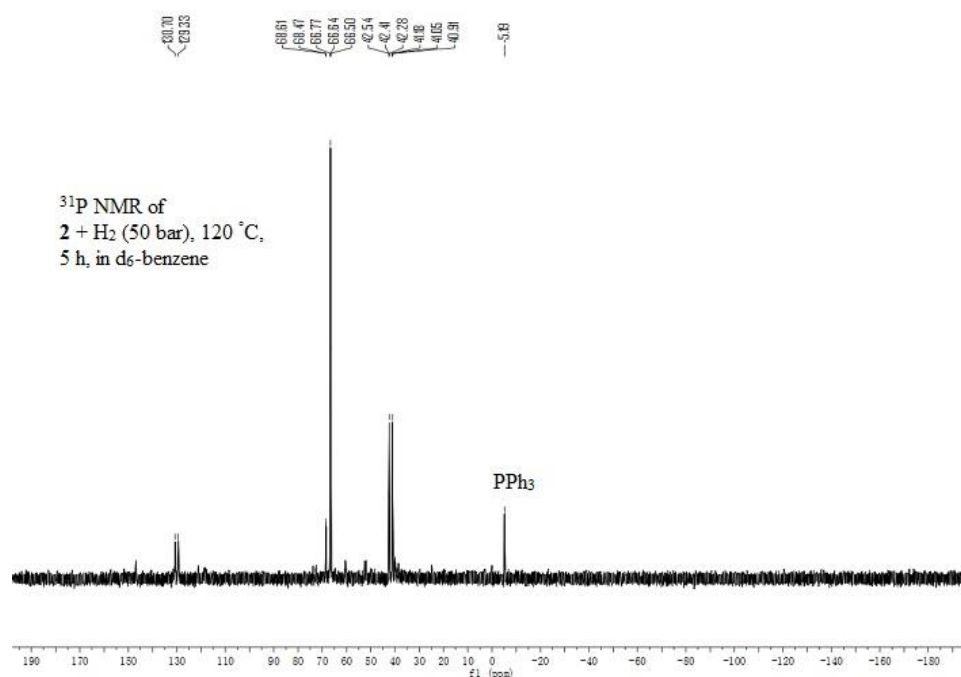


Figure S4. ¹H and ³¹P NMR of the reaction of complex **2** and H₂.

(b) In situ NMR study

We thought the dihydride species was unstable in room temperature without H₂ atmosphere. Hence, we carried out the in situ NMR experiments under H₂ atmosphere and high temperature. Limited by experimental conditions, only low pressure of H₂ can be achieved (by freeze-pump-thaw cycles with H₂ in liquid nitrogen and then warmed to 80 °C in a Young's NMR tube) in the d₈-toluene solution of catalyst **2**. Under this condition, 80 °C and near 4 atm H₂, ¹H NMR revealed the generation of two new hydrides in low concentration, which we were not sure whether it's the dihydride species we proposed, due to the weak signal and complexity of couplings.

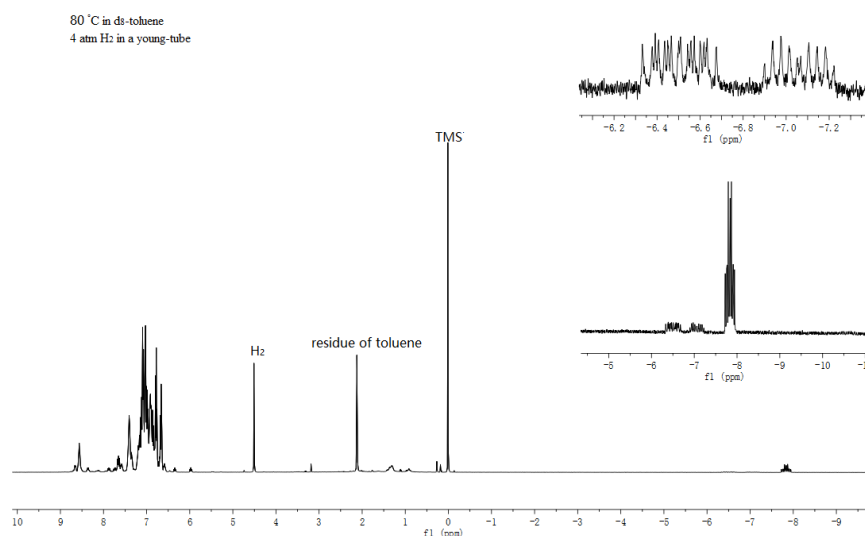


Figure S5. In situ ¹H NMR of complex **2** reacted with H₂.

Explanations

Based on the previous experiments, we proposed a new reaction pathway as illustrated in Figure S6. At first, when strong acid was mixed with catalyst **2**, the protonated species was inactive to aldehyde reduction, may be due to the big steric hindrance around the metal center. Then we suspect that one of the ligand disassociated from the ruthenium center to provide a vacant orbital for substrate coordination (inner-sphere mechanism, red part) or H₂ coordination (out-sphere mechanism, blue part). When we exposed the catalyst solution to H₂ (50 atm, 120 °C) for 2-12 hours, the color of catalyst changed from light yellow to deep red. ¹H NMR showed several kinds of hydride species were formed (Figure S4). ³¹P NMR showed that part of PPh₃ disassociated from the metal center. We were unable to see the P-OH proton in ¹H NMR no matter in chloroform-d or in d₆-benzene. We suspect that the H-Ru-P-OH intermediate was unstable in nitrogen atmosphere without high hydrogen pressure, releasing one molecule H₂ and regenerating the catalyst **2**. Hence, we carried out the in situ NMR experiments under H₂ atmosphere and high temperature. However, only two weak hydride signals can be seen in this low hydrogen pressure at 80 °C. Due to the existence of free PPh₃ in this system, we thought an equilibrium may be existed between the H₂ activation and H₂ generation. As all of the experiments were not so persuasive, we carried out a computational study to explore the reasonable reaction pathway. Computational results revealed a beneficial energy profile for the outer-sphere mechanism, which also explained well for the base effect. Under hydrogen pressure, the Ru-P-OH species can react with base to form the Ru-P-OX (X = Na or K) species (Figure S6, blue part), which was similar to the case of M-NH bifunctional catalyst.²

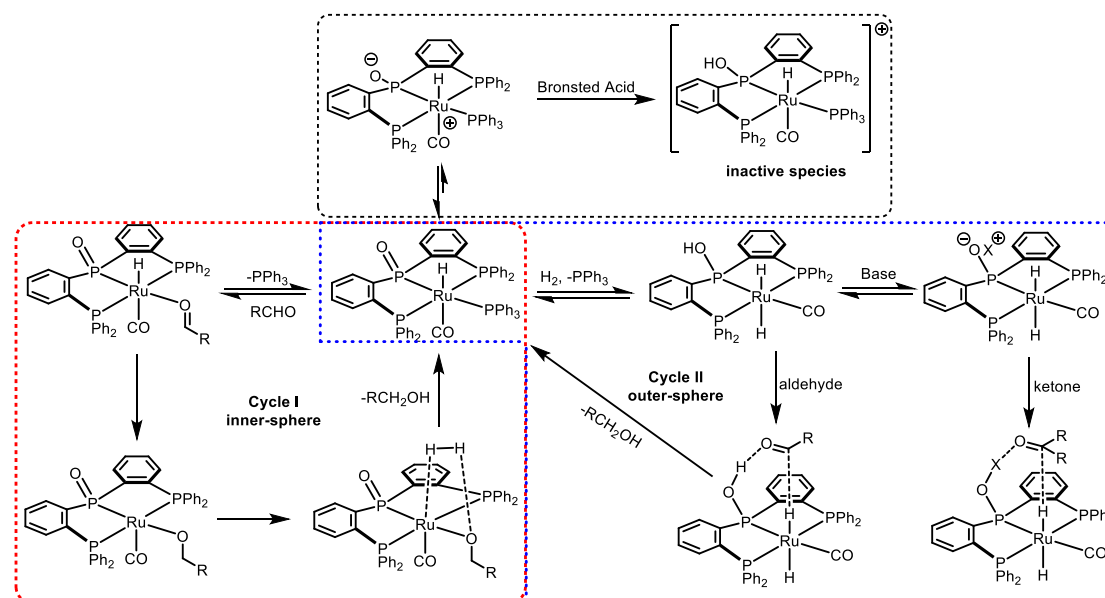


Figure S6. Proposed catalytic reaction pathways for the catalyst **2**.

Computational Details

Gaussian 09 package was employed to conduct density functional theory calculations in this work.³ All stationary points were fully optimized by M06-L⁴ functional (combined with 6-31G* basis set for the light atoms and SDD basis set plus its effective core potentials (ECPs)⁵ for Ru) in gas phase. The nature of each optimized structure was further characterized by harmonic vibration frequency calculations, i.e., reactants, intermediates and products having no imaginary frequency and transition states containing an imaginary frequency related to the reaction path. Thermodynamic data were computed at 353.15 K. To include the effect of the solvent, single-point energy calculations with an implicit SMD⁶ continuum model (using toluene as the solvent) at M06-L/6-311+G* + SDD level of theory. Optimization and energy calculations using B3LYP-D3⁷ were also carried out and found to give similar energies and geometries of the key step computed by the M06-L method.

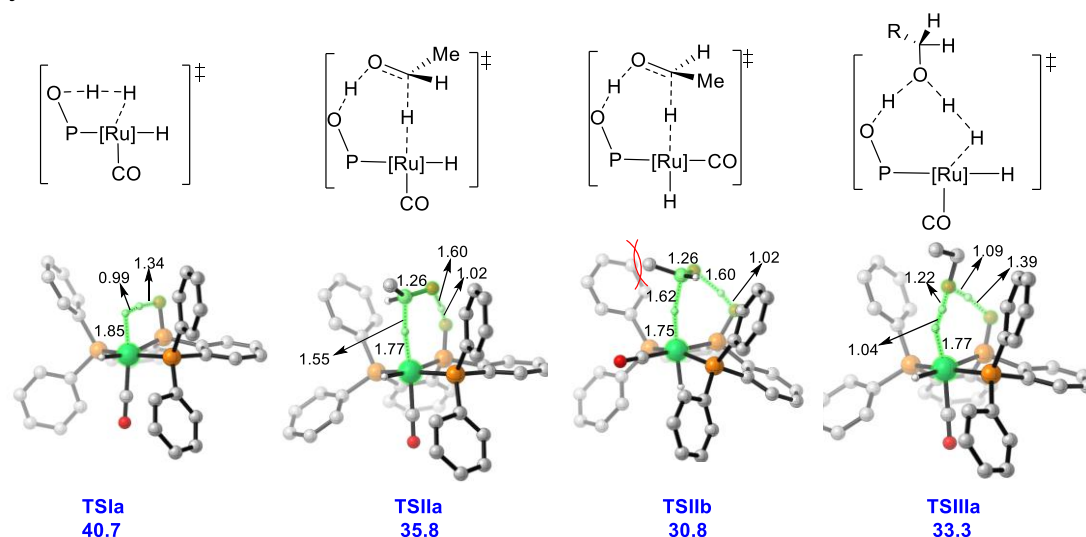


Figure S7. Calculated structures of the isomeric transition states **TS Ia**, **TS IIa**, **TS IIb** and **TS IIIa** for the outer-sphere mechanism by the M06-L/6-31G* + SDD method in gas phase. The relative free energies in toluene are given at 353 K at the M06-L/6-311+G* + SDD level based on the gas-phase-optimized geometries.

After the dissociation of the PPh₃ ligand, isomerization between the non-reacting hydride and CO ligands may take place. The non-reacting hydride locates in a *cis* position of the P-O-H group and CO ligand lies in the equatorial plane in **TSI** (Figure S7). When altering the coordination position of these hydride and CO ligands, the reaction barrier for the first H₂ cleavage step (induction process) via **TS Ia** is increased to 40.7 kcal/mol (Figure S7). Moreover, the hydrogenation process via the related isomeric 7-m-r transition state (**TS IIa**) is calculated to be 8.0 kcal/mol higher than **TS II**. Furthermore, the heterolytic cleavage of H₂ assisted by the alcohol also requires a higher barrier via **TS IIIa** (33.3 kcal/mol). Therefore, the non-reacting hydride ligand tends to retain as in the crystal structure of **2**: CO prefers to be *trans* to the P-O-H group in the whole reaction.

In the hydrogenation step, there is another isomer (with different orientation of the methyl group of the substrate). The methyl group has no obvious steric contact between the methyl group and

the bulky phosphine ligand in **TSII**. However, isomeric **TSIIb**, in which the methyl group points towards to one side of the phosphine ligand, has a higher barrier of 30.8 kcal/mol, compared to **TSII**.

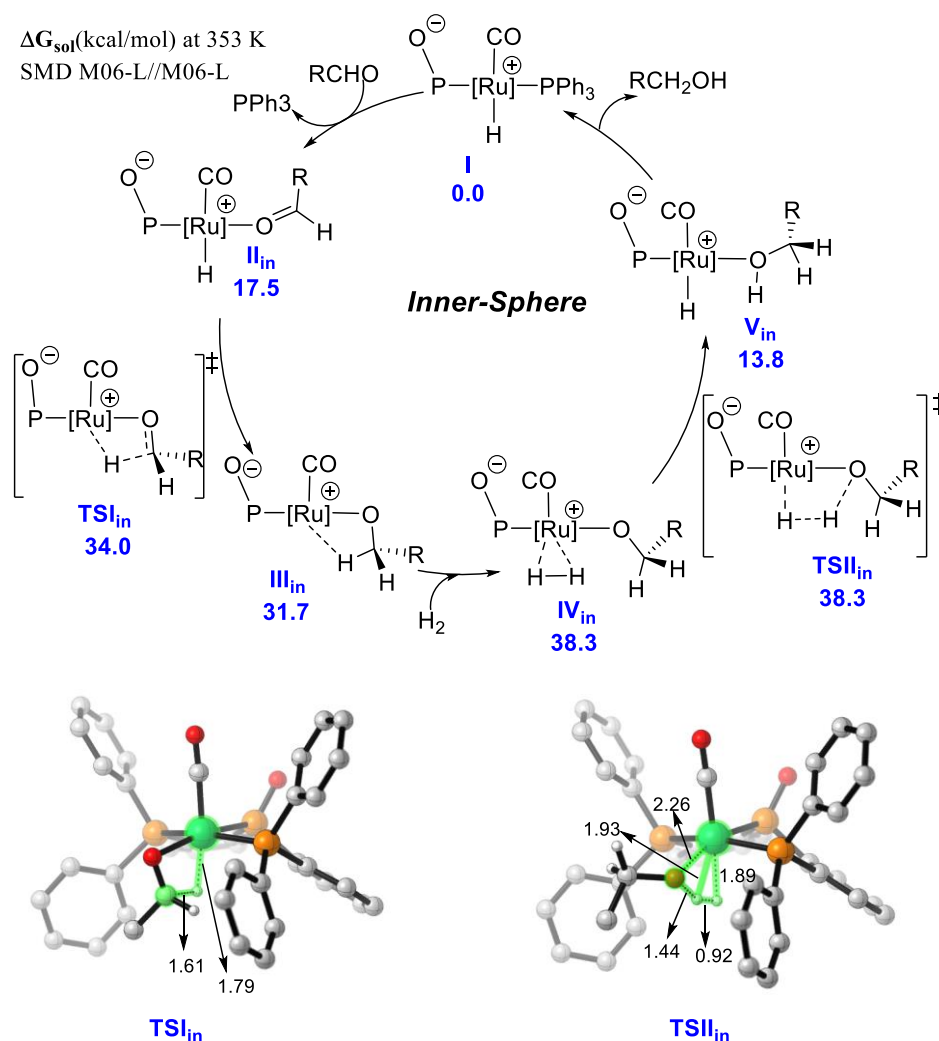


Figure S8. Computed reactions profile of the aldehyde reduction in the inner-sphere mechanism and computed geometries of **TSI_{in}** and **TSII_{in}** with bond lengths in Å by the M06-L/6-31G* + SDD method in gas phase. The relative free energies in toluene are given at 353 K at the M06-L/6-311+G* + SDD level based on the gas-phase-optimized geometries.

Besides the outer-sphere mechanism, we have also examined the hydrogenation through the inner-sphere mechanism (Figure S8). Different from the outer-sphere mechanism, the inner-sphere mechanism initiates with ligand replacement of PPh_3 by the aldehyde substrate to form an intermediate **II_{in}**. Then, the hydride transfers to the carbonyl carbon site via a four-membered-ring transition state **TSI_{in}** (34.0 kcal/mol), leading to an unstable intermediate **III_{in}**. Further coordination of H_2 gives an adduct **IV_{in}** followed by the subsequent cleavage transition state **TSII_{in}**, which is almost degenerate with **IV_{in}** in solution (while **TSII_{in}** is higher than **IV_{in}** by 2.7 kcal/mol in electronic energy at the M06-L/6-31G* + SDD level in gas phase). To conclude, the hydrogenation reaction *via* the inner-sphere mechanism has a larger reaction barrier and, thus, the

hydrogenation reaction should prefer to proceed through the outer-sphere mechanism.

Table S4. Relative free energies (kcal/mol, at 353.15 K) of the crucial transition states for the acetaldehyde reduction (ΔG_{smd}) in solution by the M06-L and B3LYP-D3 methods.

	ΔG_{smd}	
	M06-L	B3LYP-D3
I	0.0	0.0
TSI	34.1	34.8
TSIa	40.7	42.9
TSII	27.8	26.9
TSIIa	35.8	35.0
TSIIb	30.8	30.9
TSIII	25.2	20.6
TSIIIa	33.3	32.0
TSII_{in}	38.3	41.4

Additionally, B3LYP-D3 method was adopted to re-optimize the crucial transition states and calculate the free energy in solution. The B3LYP-D3 method gives a qualitatively similar energetic trend as the M06-L method (Table S4). In most cases, the free energy difference of the two methods is within 1.5 kcal/mol, except for **TSIII** (the B3LYP-D3 method predicts a much lower barrier (20.6 kcal/mol) than M06-L method (25.2 kcal/mol)).

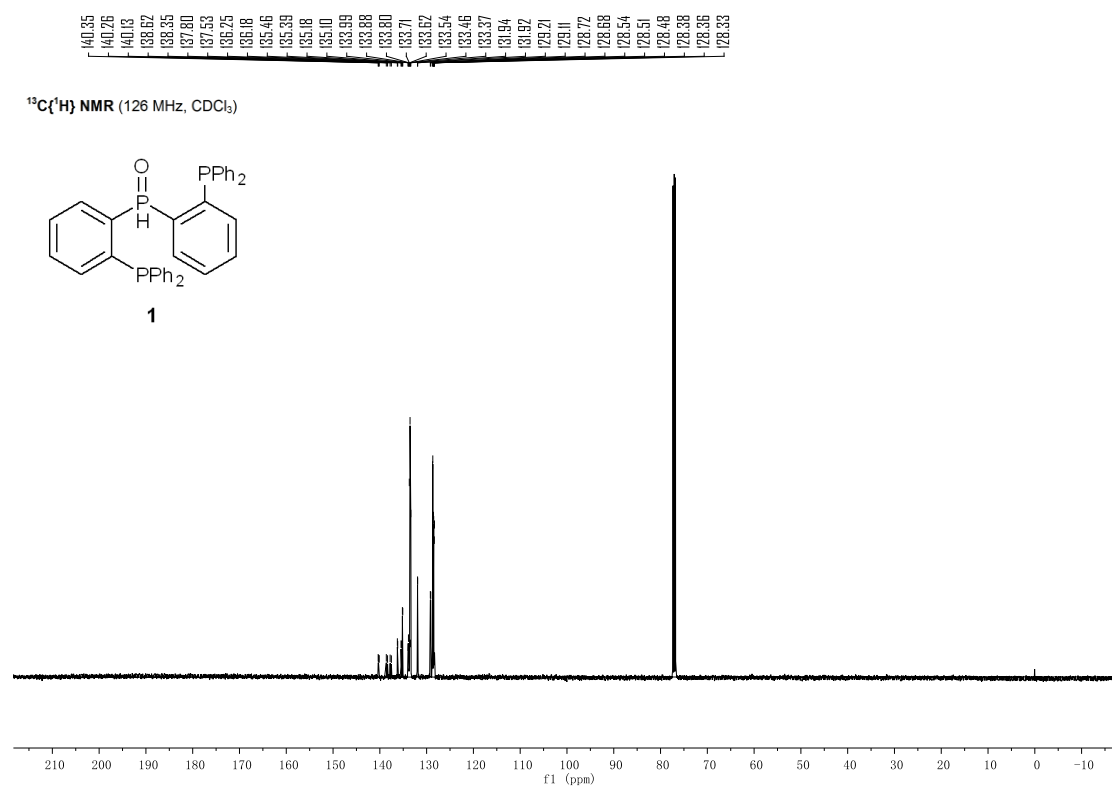
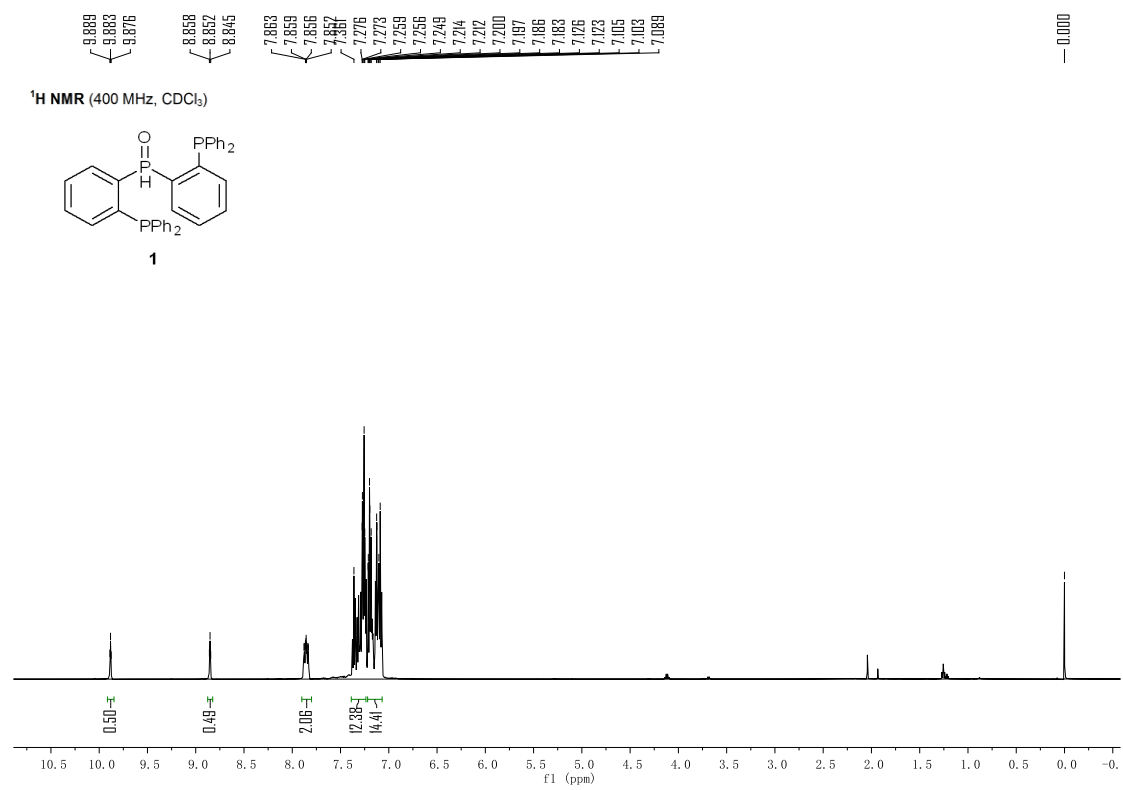
Table S5. Thermal correction to Gibbs free energy (G_{corr} , in au) at 353.15 K and absolute SMD energy $E(\text{SMD})$, in au) for all optimized structures by the M06-L method. Those for the crucial transition states by the B3LYP-D3 method are also provided.

	M06-L		B3LYP-D3	
	$E(\text{SMD})$	G_{corr}	$E(\text{SMD})$	G_{corr}
Acetaldehyde	-153.86046	0.02516	-153.891520	0.025253
H ₂	-1.1710	-0.00435	-1.17911795	-0.00411
PPh3	-1036.39455	0.21807	-1036.55766	0.21587
Benzaldehyde	-345.62732	0.07218		
I	-3733.70452	0.71676	-3734.22738	0.71792
II	-2698.438051	0.47535		
TSI	-2698.405079	0.47270	-2698.76727	0.47182
TSIa	-2698.395587	0.47382	-2698.75539	0.472883
<i>outer-sphere mechanism</i>				
III	-2698.433432	0.47564		
IV	-2852.306166	0.52670		
TSII	-2852.306368	0.52877	-2852.70487	0.53064
TSII_Ph	-3044.072665	0.578167		
TSIIa	-2852.295683	0.53070	-2852.69335	0.53195
TSIIb	-2852.301732	0.52880	-2852.69947	0.53162
V	-2852.335045	0.53485		
VI	-2853.527992	0.55133		
TSIII	-2853.503613	0.54649	-2853.9145	0.54695
TSIIIa	-2853.492782	0.54853	-2853.8975	0.54816
VII	-2853.524328	0.55078		
<i>inner-sphere mechanism</i>				
II_{in}	-2851.130391	0.51172		
TSI_{in}	-2851.106189	0.51376		
III_{in}	-2851.11352	0.51750		
IV_{in}	-2852.288522	0.52755		
TSII_{in}	-2852.292518	0.53152	-2852.68135	0.530202
V_{in}	-2852.335668	0.53567		

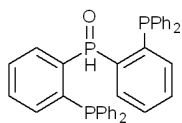
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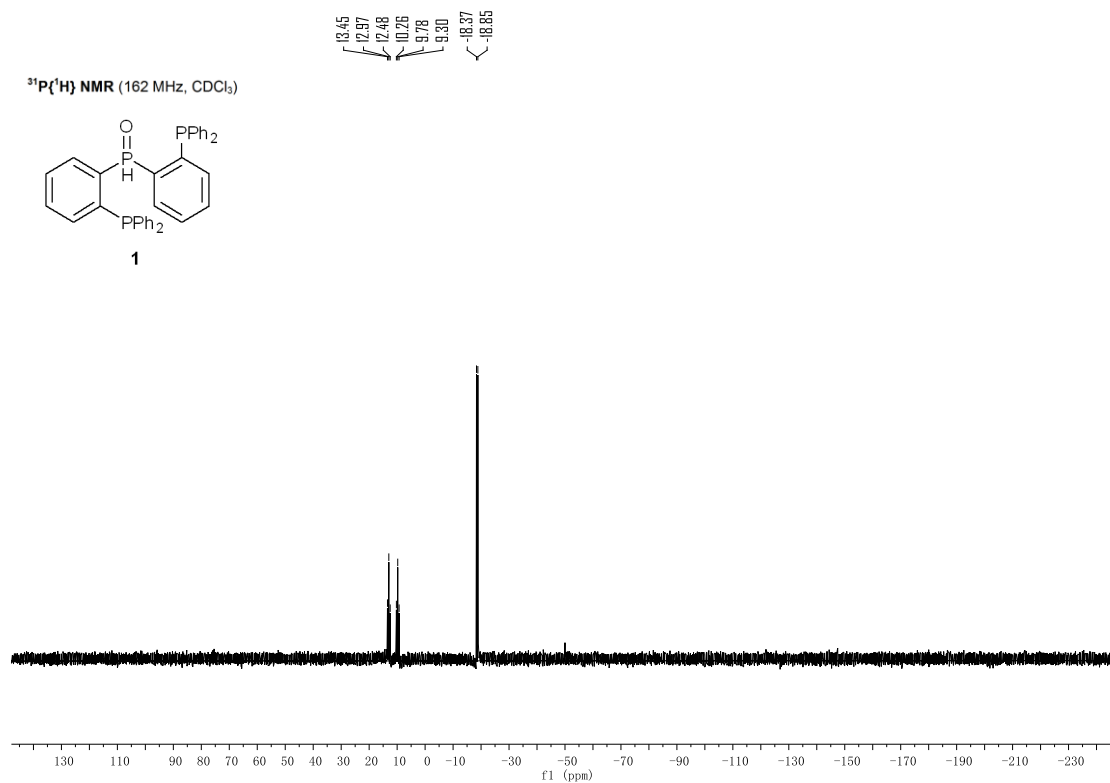
NMR Spectra



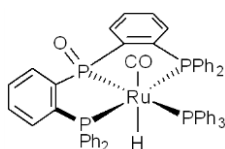
$^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, CDCl_3)



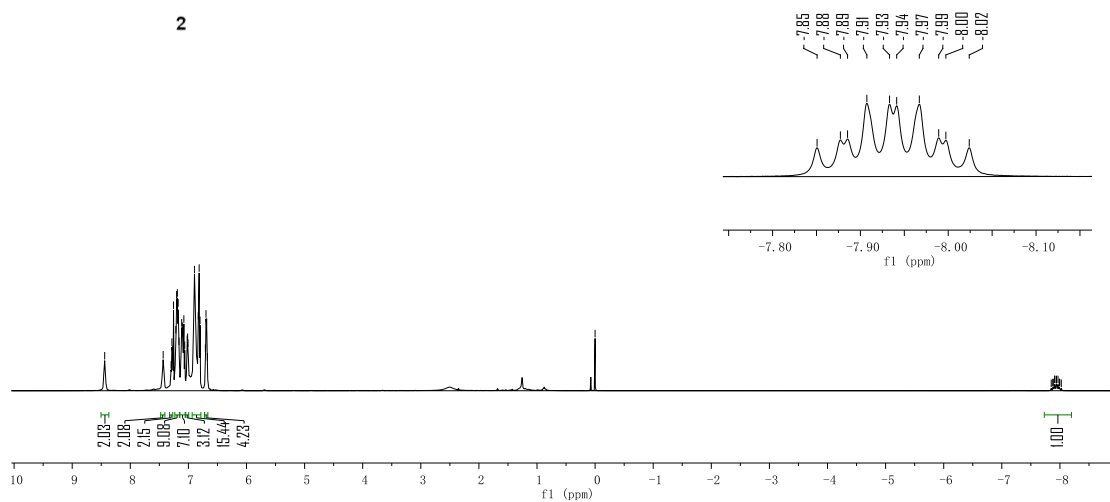
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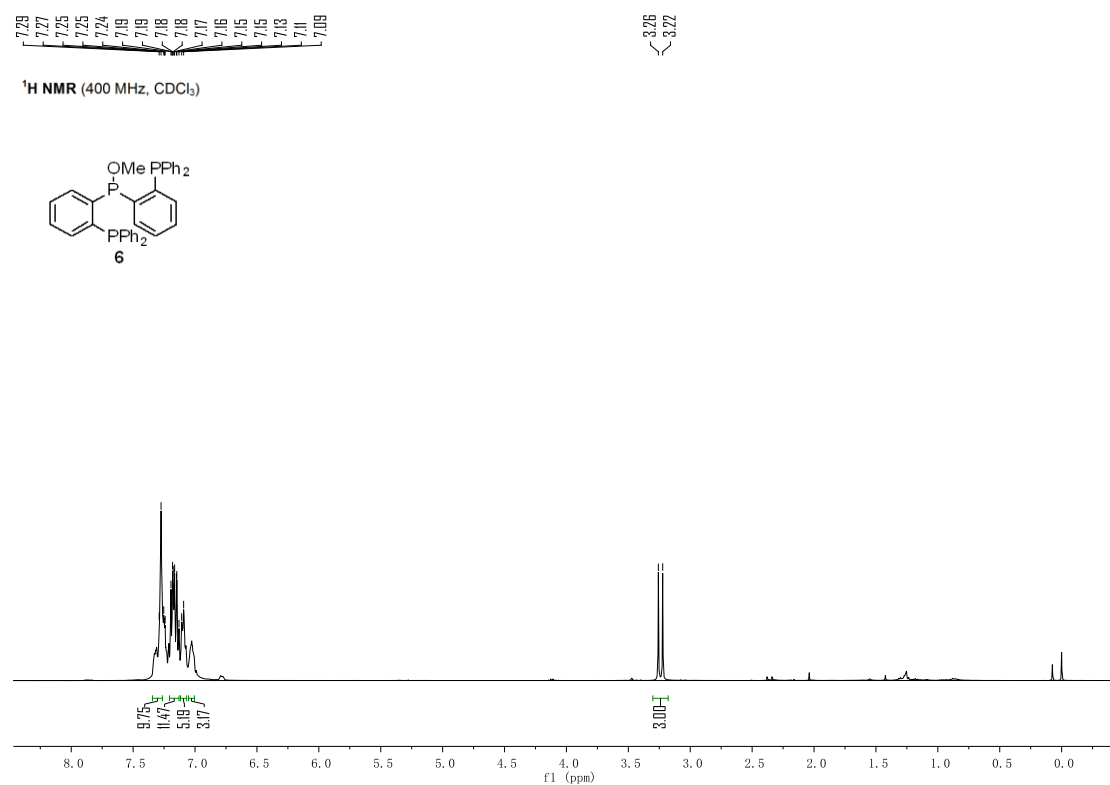
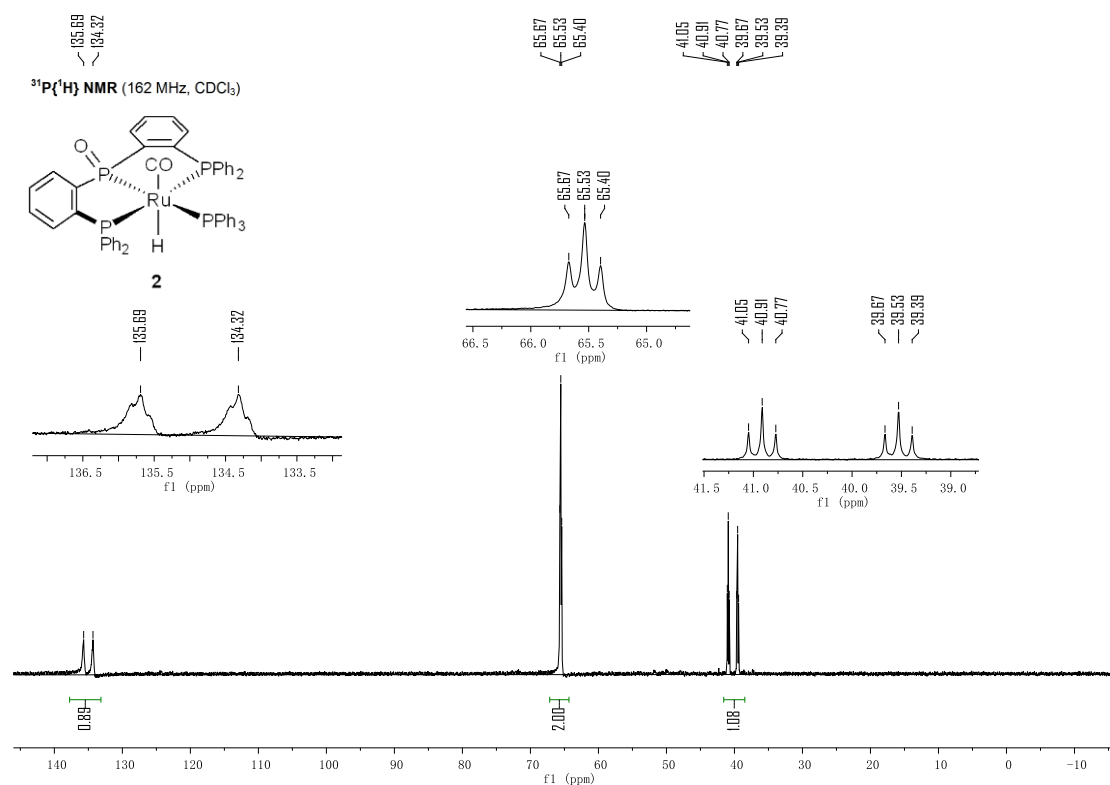


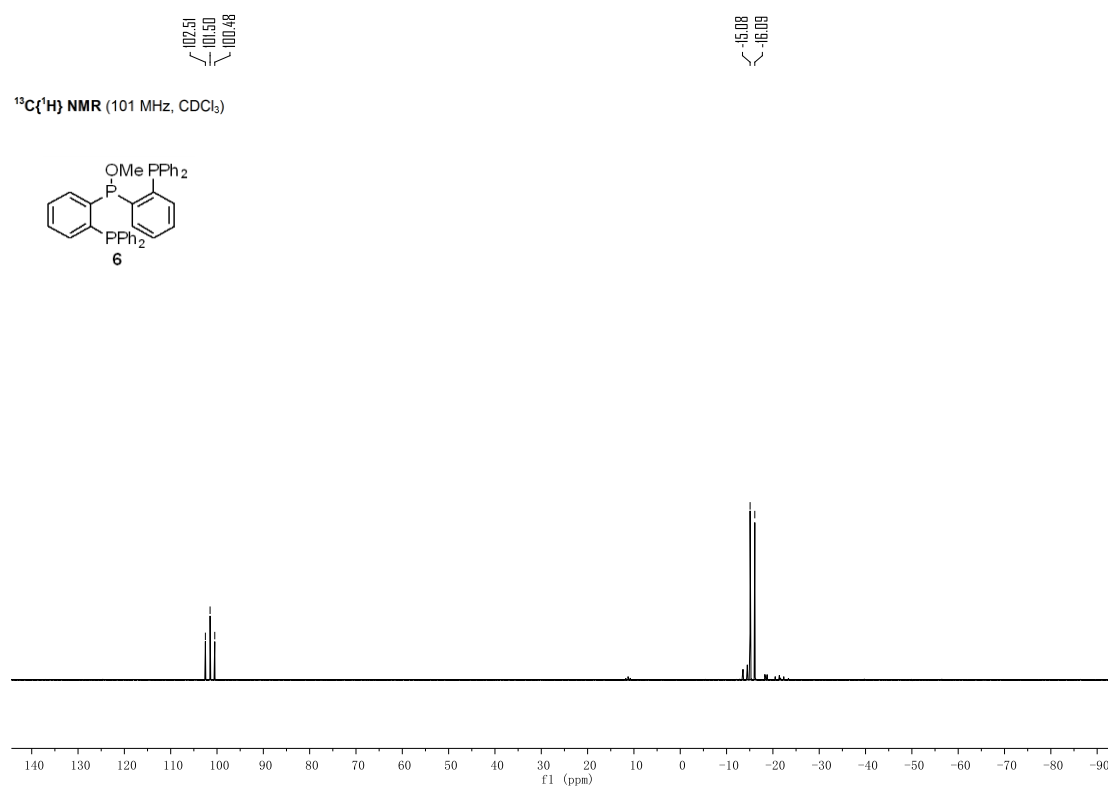
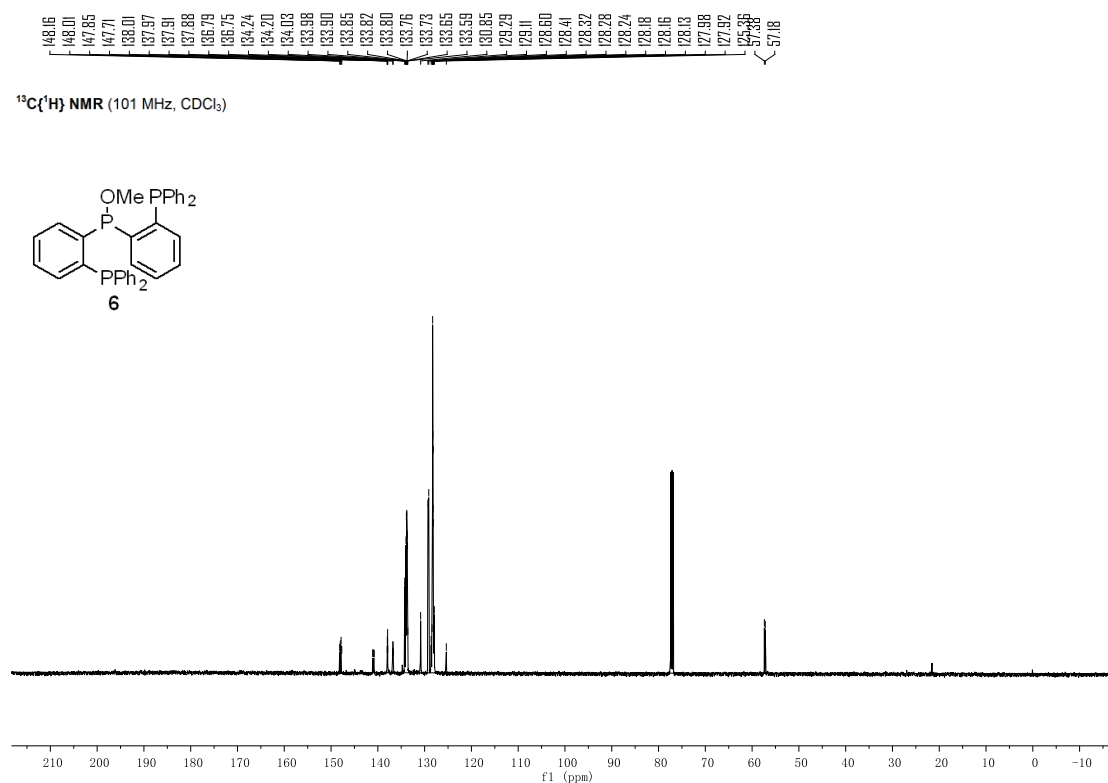
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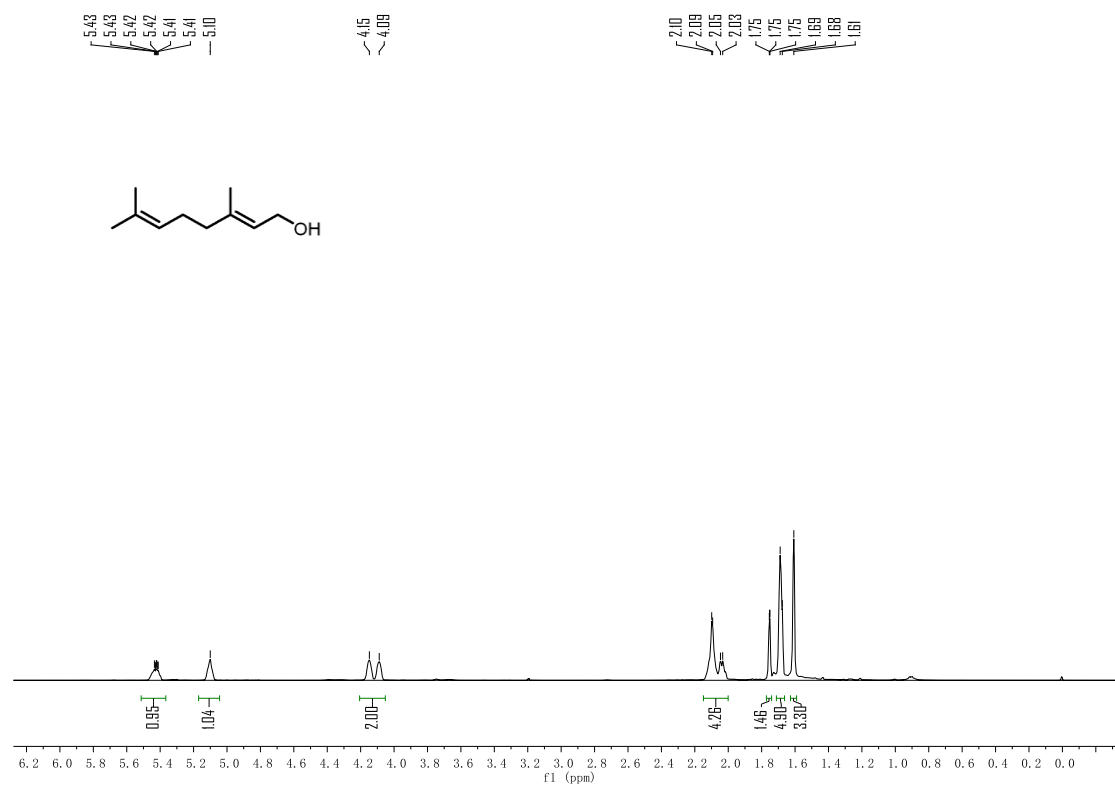
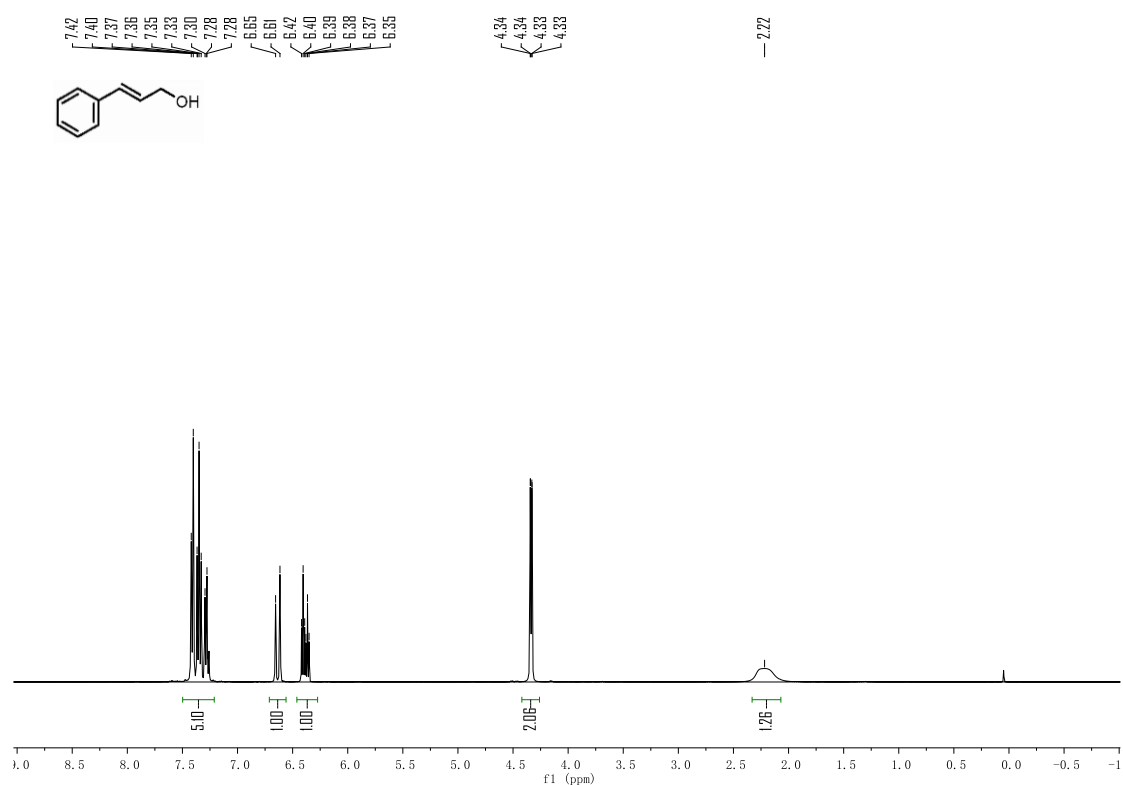


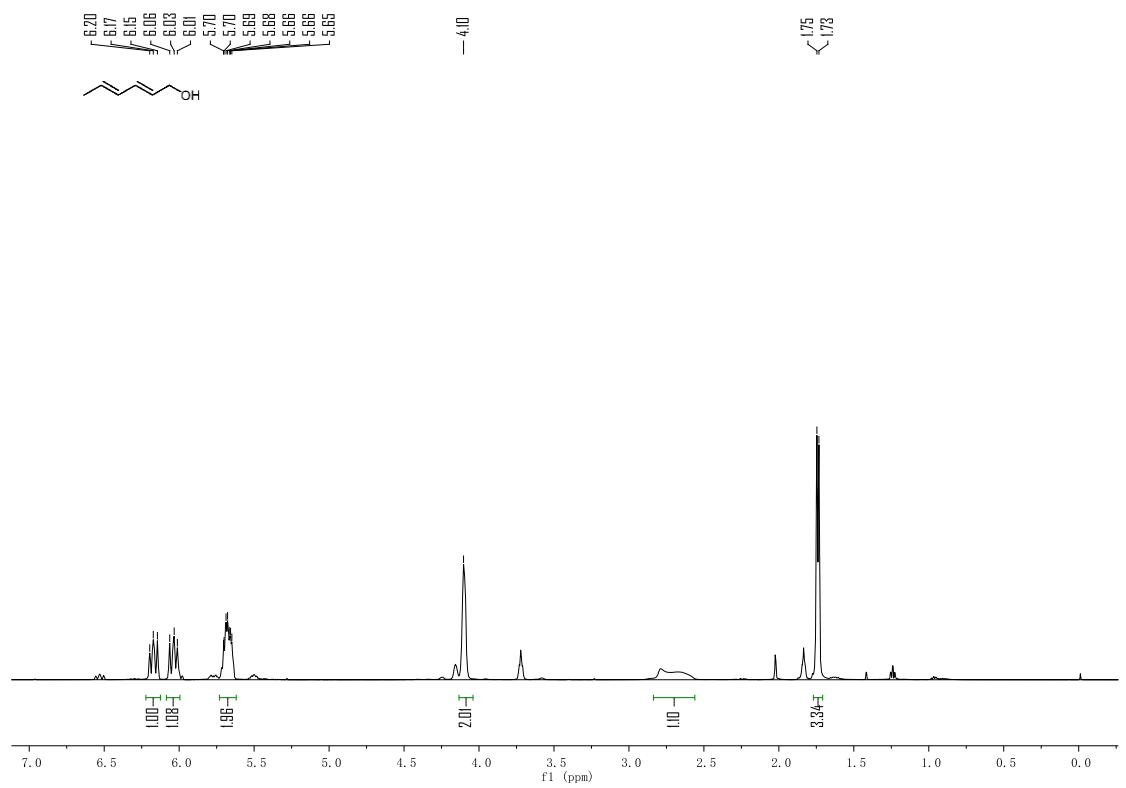
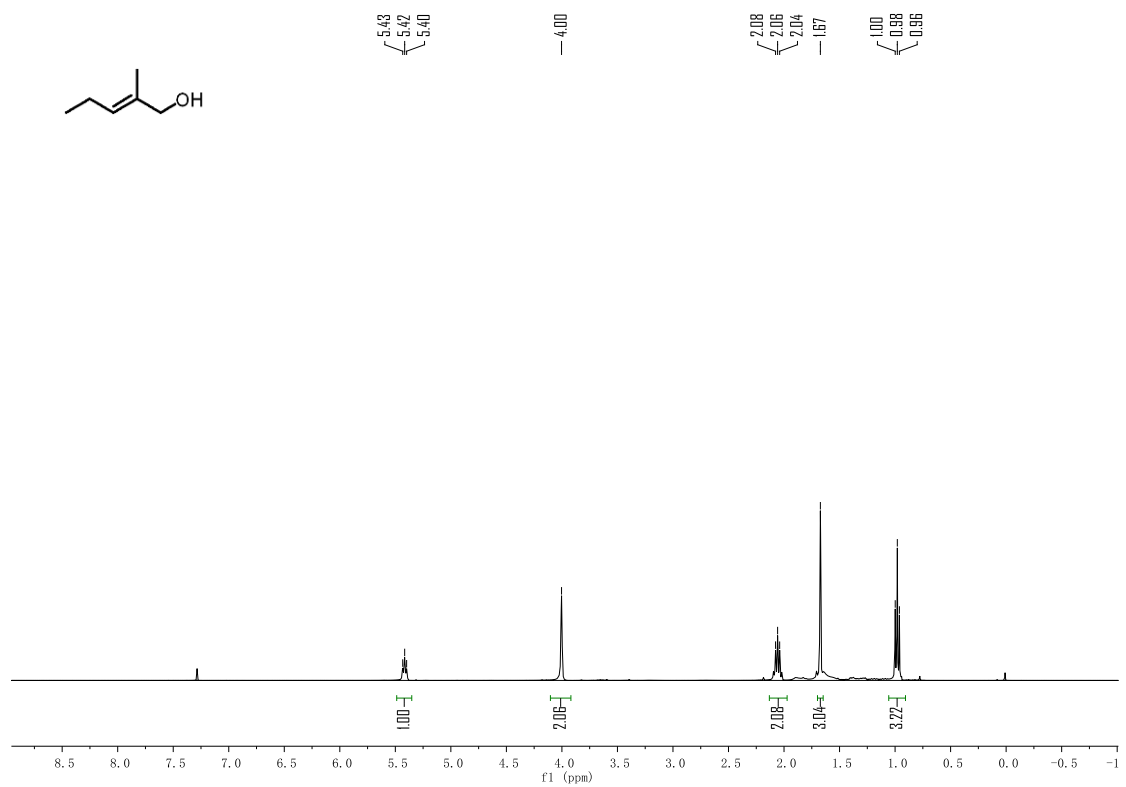
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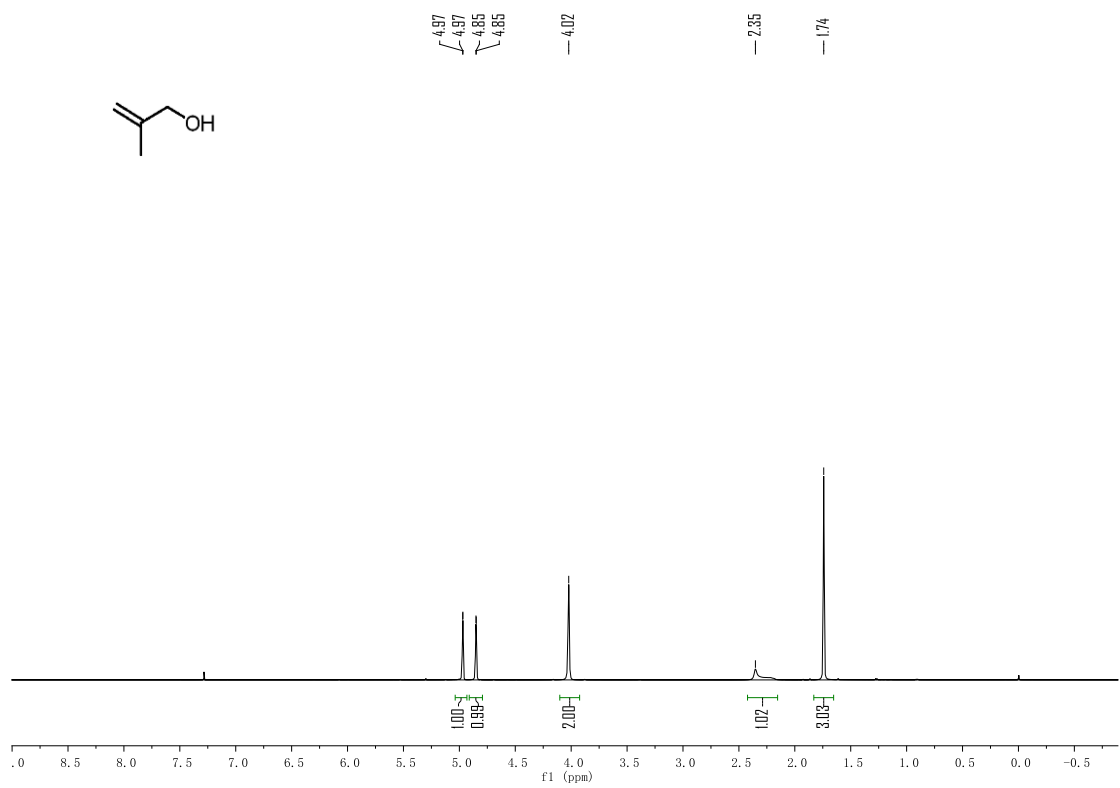
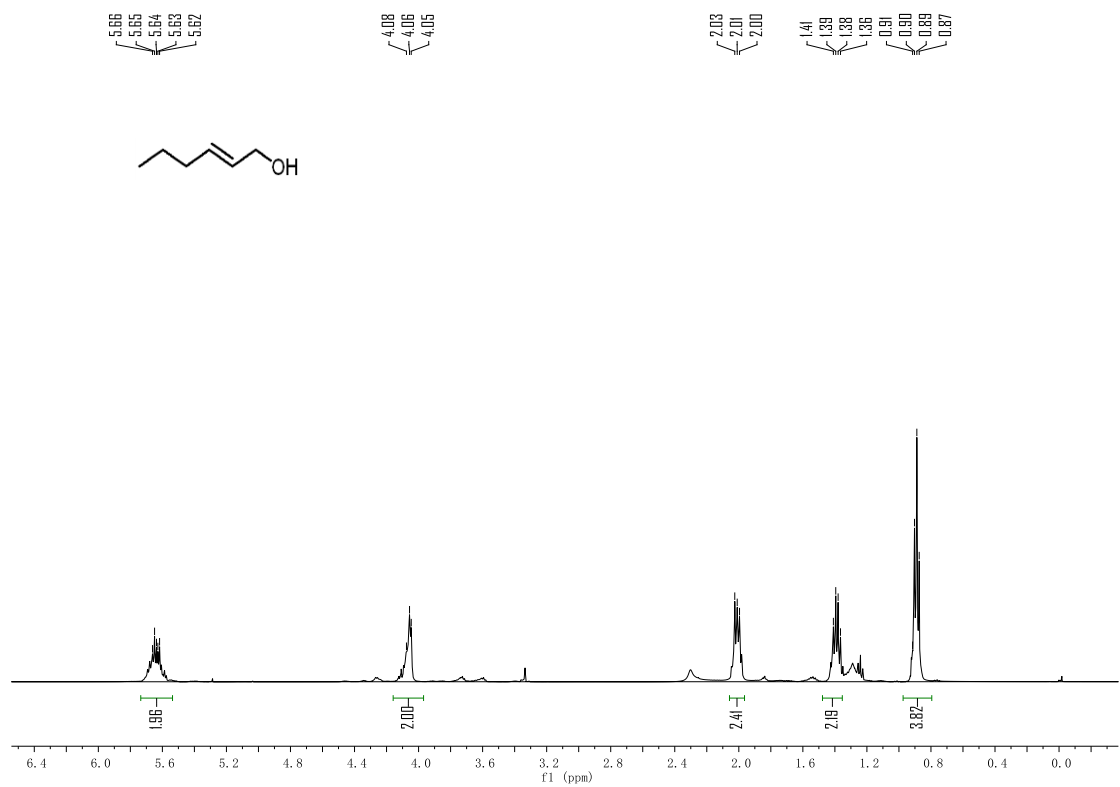


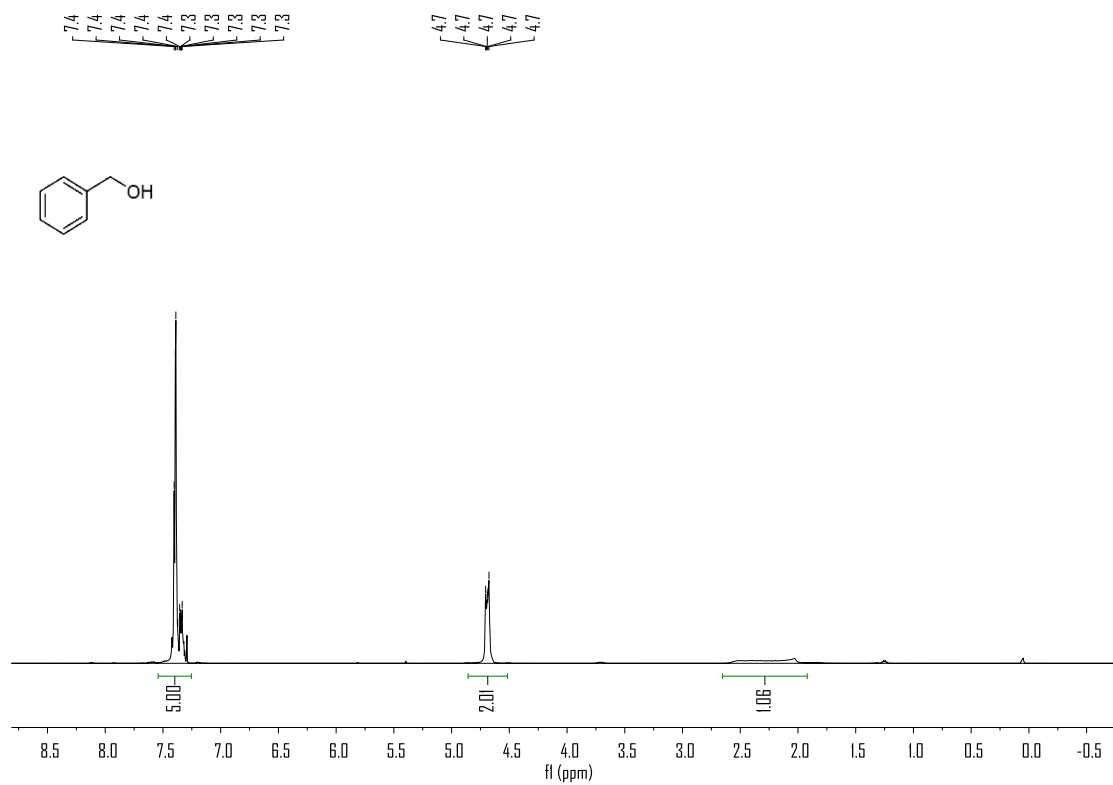
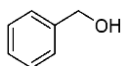
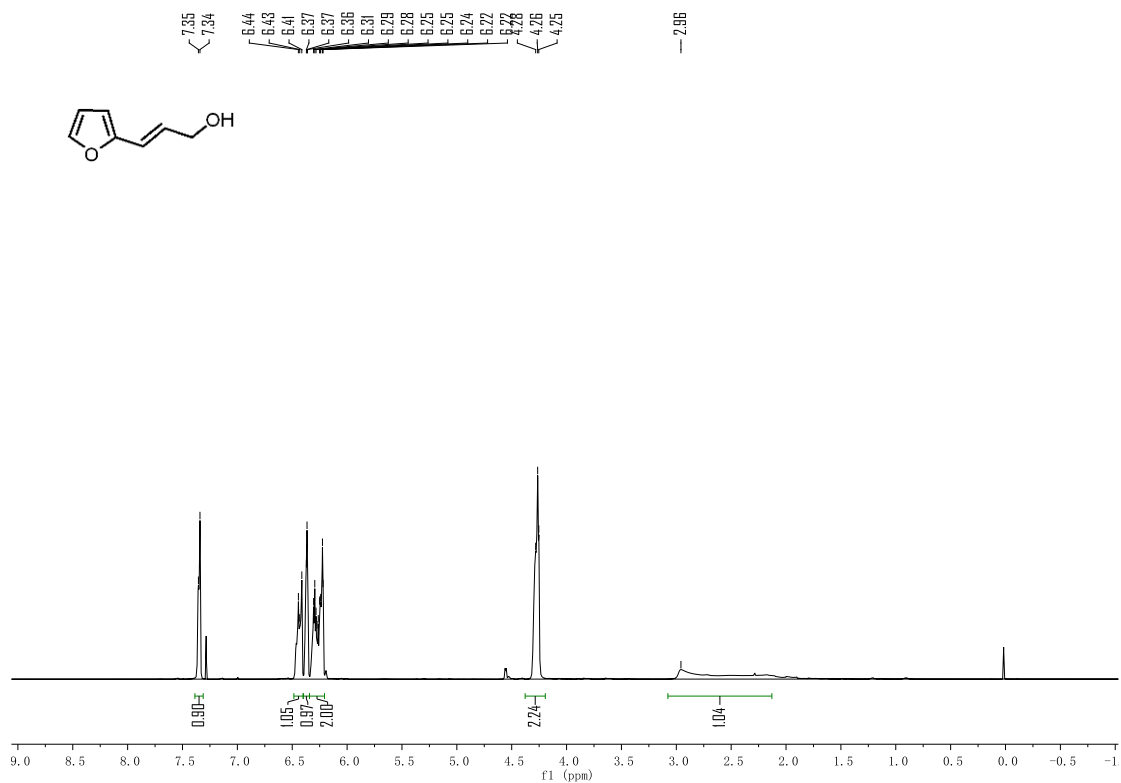
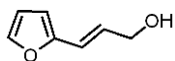


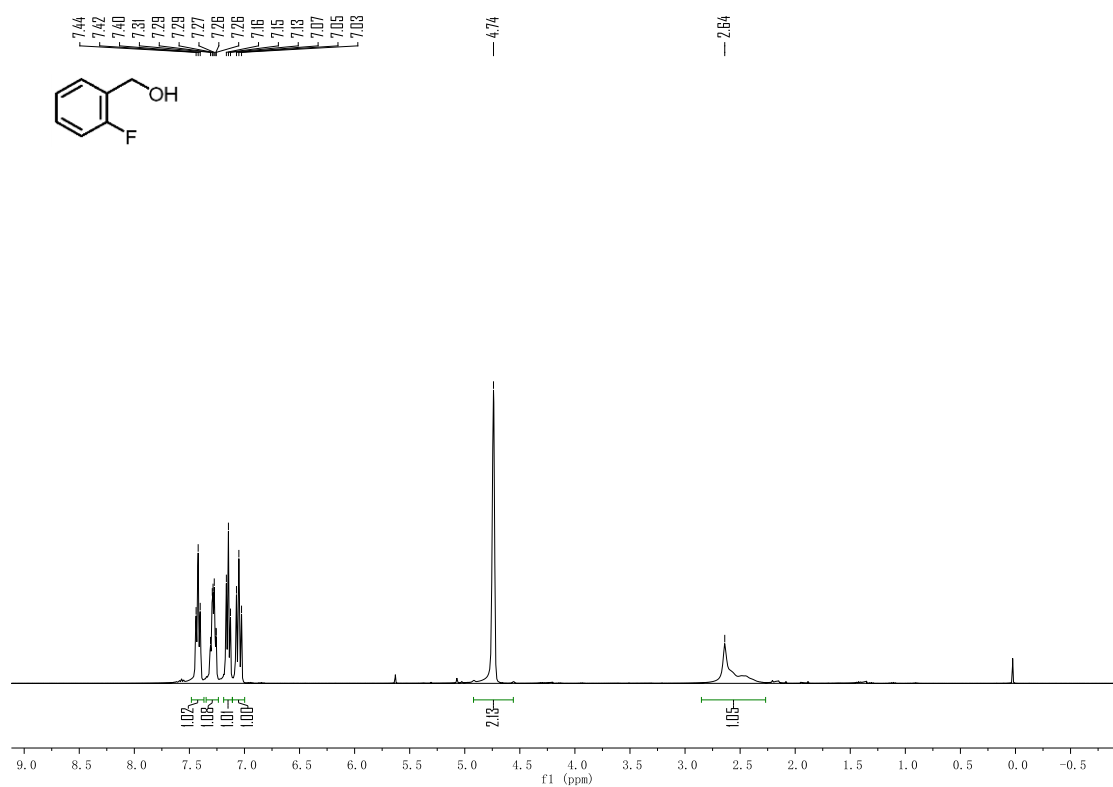
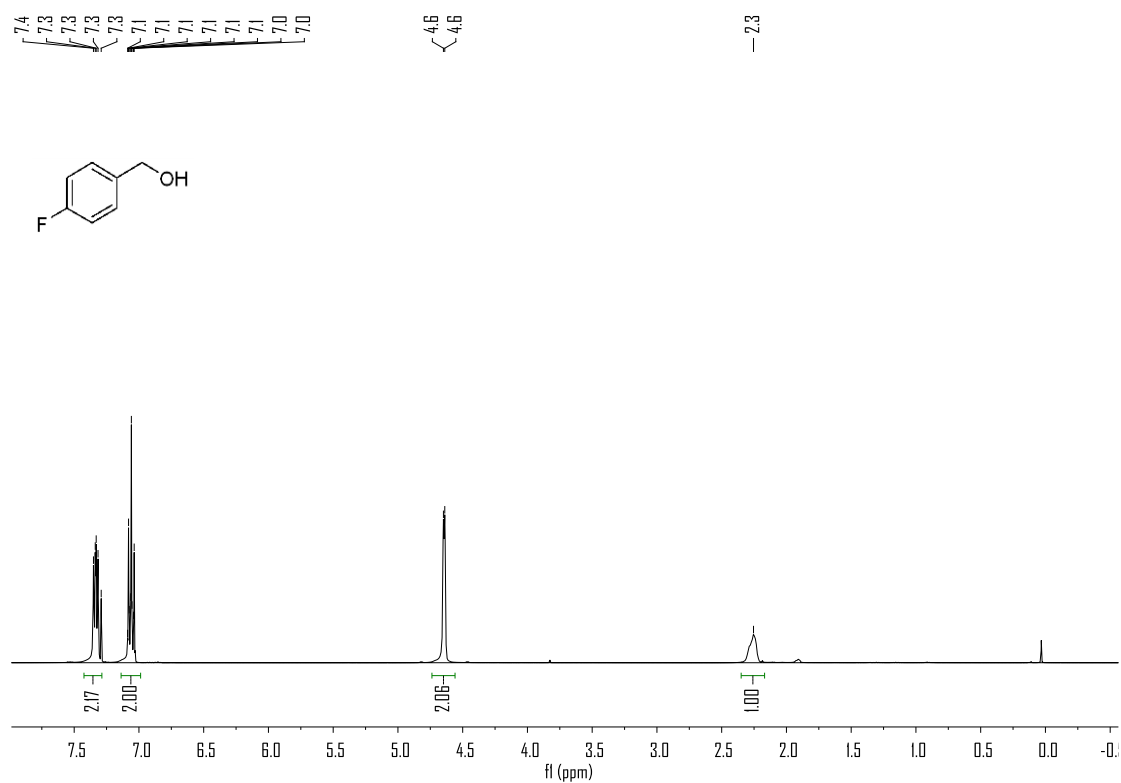


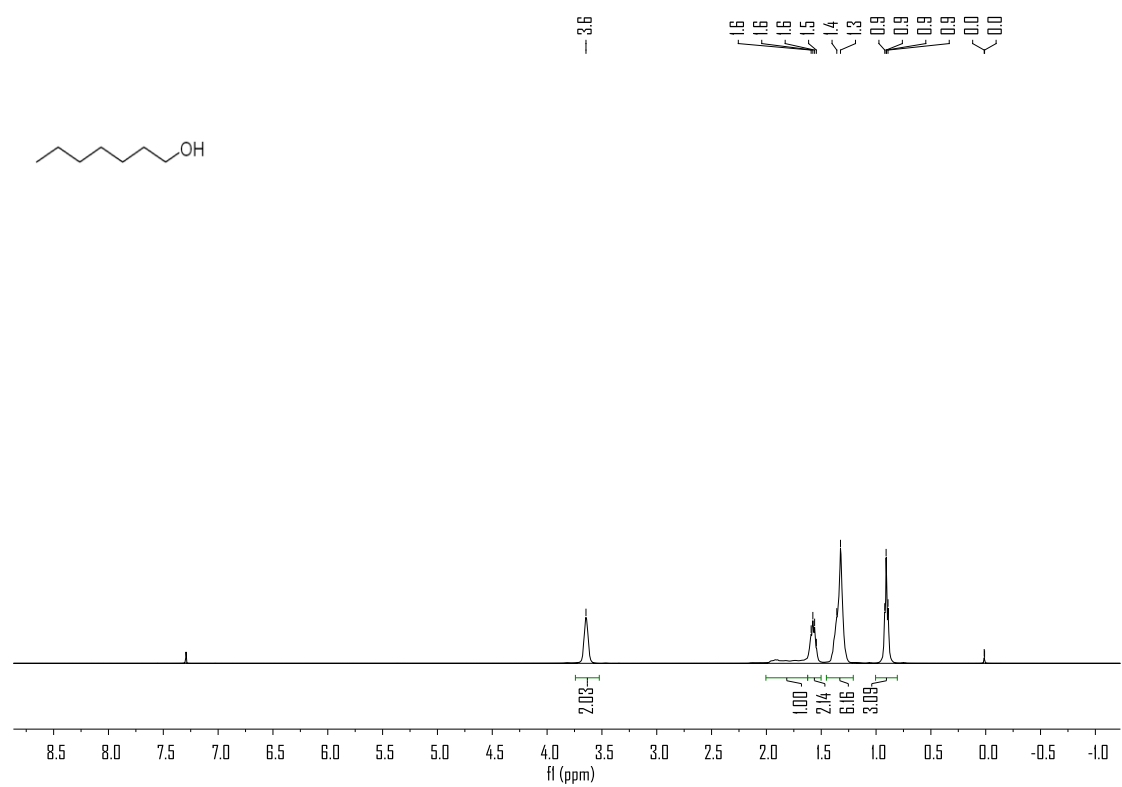
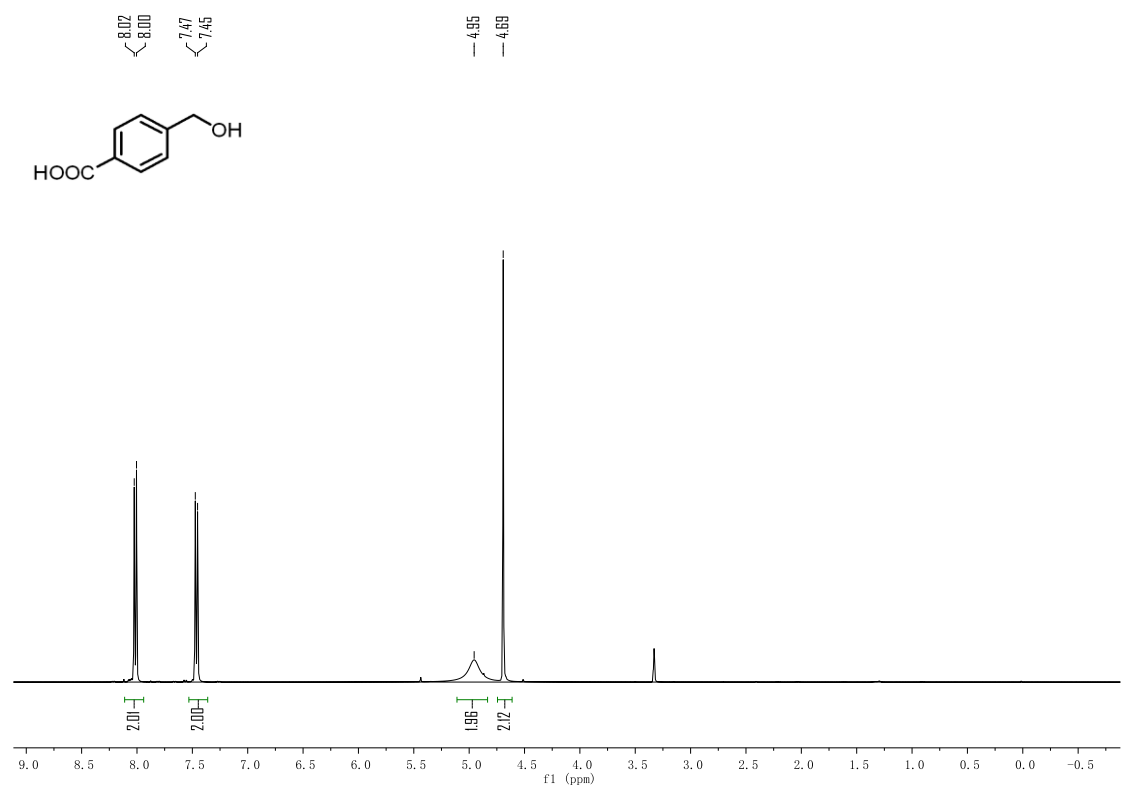












Cartesian Coordinates of M06-L Optimized Structures

Acetaldehyde

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H	-1.712083	0.219287	-0.877484
H	-1.158180	-1.241438	0.000331
H	-1.712399	0.219918	0.877004
C	0.230597	0.395666	0.000000
O	1.236729	-0.274284	0.000001
H	0.292323	1.513846	-0.000009

H₂

H	0.000000	0.000000	0.371963
H	0.000000	0.000000	-0.371963

Alcohol

C	1.162868	-0.406777	0.000000
H	1.128228	-1.051025	0.885300
H	1.128228	-1.051025	-0.885300
H	2.117405	0.131166	0.000000
O	-1.189912	-0.215593	0.000000
H	-1.933040	0.401391	0.000000
C	0.000000	0.552429	0.000000
H	0.050637	1.210160	0.886987
H	0.050637	1.210160	-0.886987

PPh₃

P	-0.001128	0.007322	-1.271335
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C	3.171484	2.487120	-0.506711
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H	4.434762	2.632684	1.233173

Benzaldehyde

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O 0.0583650125 3.9615974825 -1.1939878415
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C 0.051684478 2.0512074314 0.4450979294
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C 4.038980914 -2.801380847 -2.1516223204
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H -0.3165661908 -3.2474812531 -0.8095597645
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H -0.500129006 -1.0340965789 -4.2202116522
H -1.9379112764 -1.88428757 -3.6007083659
H -0.623329942 -2.8053477468 -4.356755606
C -0.1857377472 -2.1086543145 -2.3739324261
O -0.6898088064 -3.2232846067 -1.7283694564
H 0.9140829174 -2.1258207286 -2.4733041631

VI

Ru 0.0264705479 0.7479884966 -0.2587611535
P 2.2802079173 1.184242137 0.146077639
P -2.2710595985 0.9155587026 0.1029557564
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C -2.6482177973 2.5742695259 0.795146686
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C -1.6604632317 3.5633317746 0.699473546
C 3.3151706174 -0.0843516249 0.9574118848
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H 3.0084070035 -2.5345106277 3.3027514032
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C 3.414634855 2.8289122298 2.1712994005
H 4.272440764 2.1556523064 2.1638679224
C 4.2656026173 1.1773859464 -3.4300575333
H 4.5634989285 0.4311617831 -4.1648252528
C -3.6482899807 -2.2109771681 3.2159800659
H -3.9374008339 -2.9630842424 3.9480342929
C 4.1046038353 3.4798338945 -2.732445974
H 4.2664206238 4.5391031037 -2.9236598868
C -3.5322102849 -2.5537491601 1.8702612898
H -3.7277751194 -3.5740552405 1.5456362915
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H 4.2134589576 4.0791880811 3.7309804295
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H 5.1723719718 0.4867471562 0.0122013422
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H -3.6812972235 1.7474519484 -4.5403919422
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H 3.4547053535 -0.2821326489 -2.0716047339

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C -5.6654485669 0.3091794398 -2.1812449504
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H 6.5291679844 -1.1768645188 1.2399913537
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H 0.4988594584 0.7500616491 -2.0458599352
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C 0.7151889473 2.6895210163 -4.1043401153
H 1.2110335893 3.5688182168 -4.5558890191
H 1.4174006013 2.3043110905 -3.3419049128
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TSIII

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P 2.3015237414 1.2066597455 0.1831478917
P -2.2156359728 0.9221625548 0.0721839033
P -0.0173169908 3.1315349628 0.036098533
O 0.1985175769 -2.2679500256 -0.3609643913
C -2.6362683243 2.5729854597 0.7799301101
C 1.253543719 3.5132925871 1.3143975133
C 0.1480142894 -1.1040080602 -0.3250095864
C -1.6574281041 3.5765740715 0.7225018724
C 3.3006377207 -0.0596598933 1.0492459453
C 3.3548314592 1.6827680242 -1.2337421122
C 2.6691540204 -0.8995671059 1.9747116674
H 1.5939248992 -0.8073783017 2.129658402
C -2.916306918 -0.2772287713 1.2611696539
C -3.0552144575 0.0246995035 2.6196082686
H -2.8202959277 1.027069119 2.9768269216
C -3.4047038327 0.8128701958 -1.3303417093
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H -1.2699857082 5.6859538006 0.9335945156

C 2.3681761711 2.6544537544 1.3141074662
C 3.9002090896 2.9602610768 -1.3842208266
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H 5.321968555 2.6121589829 -4.4546648397
C 1.2473983251 4.6105128894 2.1776548518
H 0.3894912934 5.2804484708 2.2016714253
C 3.4043556162 -1.843819949 2.6834254102
H 2.9011434949 -2.4932327068 3.3978217721
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H -3.5937888338 -0.6988767756 4.5717567737
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O 0.2519175806 4.1332104614 -1.1365355702
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TSIIIa

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C -0.0202284204 0.5019889802 1.994040098
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C 2.4187472082 2.6895954728 1.3551722711
C 3.6295378521 2.9589157325 -1.5026548467
H 3.4880632036 3.737969848 -0.7541421426

C -3.2124058174 -1.588409169 0.9137800341
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H 4.8590277494 2.5323550841 -4.6457154208
C 1.3337691112 4.6874258822 2.1850324676
H 0.4754369988 5.3559381546 2.2169261781
C 3.8492087778 -2.0226685852 2.3281175257
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VII

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H 4.2760997341 2.3405201605 1.9162156102
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H 4.1452402708 0.2713149452 -4.3320689855
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C 4.6394884104 3.1781801139 -2.6417982353
H 5.1452630341 4.1379785317 -2.7353999115
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II_{in}

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O 0.4510195054 -3.208048199 0.421417496
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C 1.5651739345 -1.2848373558 1.9961285709
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