Supporting Information

Novel pyrazolylphosphite- and pyrazolylphosphinite-ruthenium(II) complexes as catalysts for hydrogenation of acetophenone

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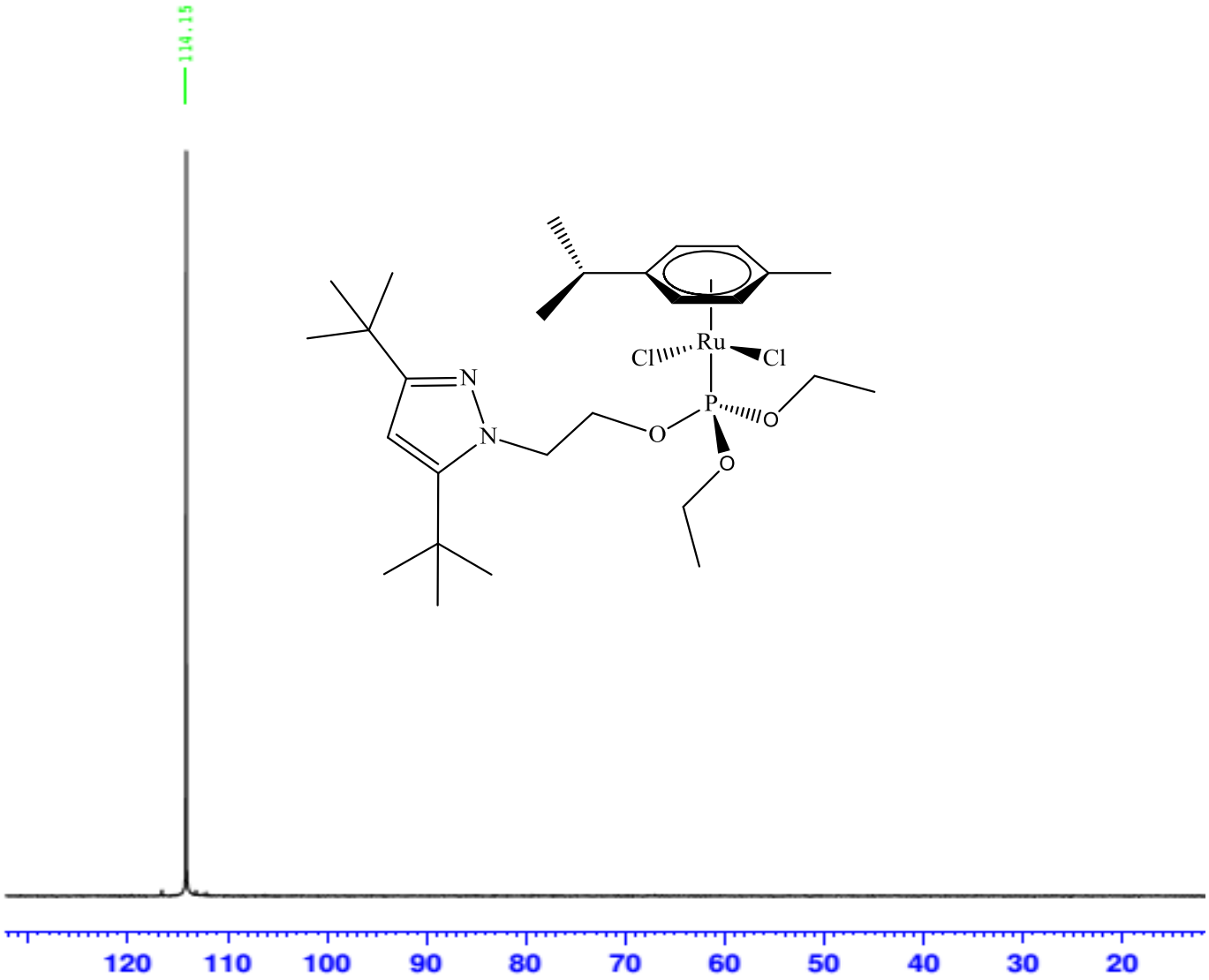


Figure S1: $^{31}P\{^{1}H\}$ NMR spectrum of **3**. Analysis was carried out in $CDCl_3$ at room temperature.

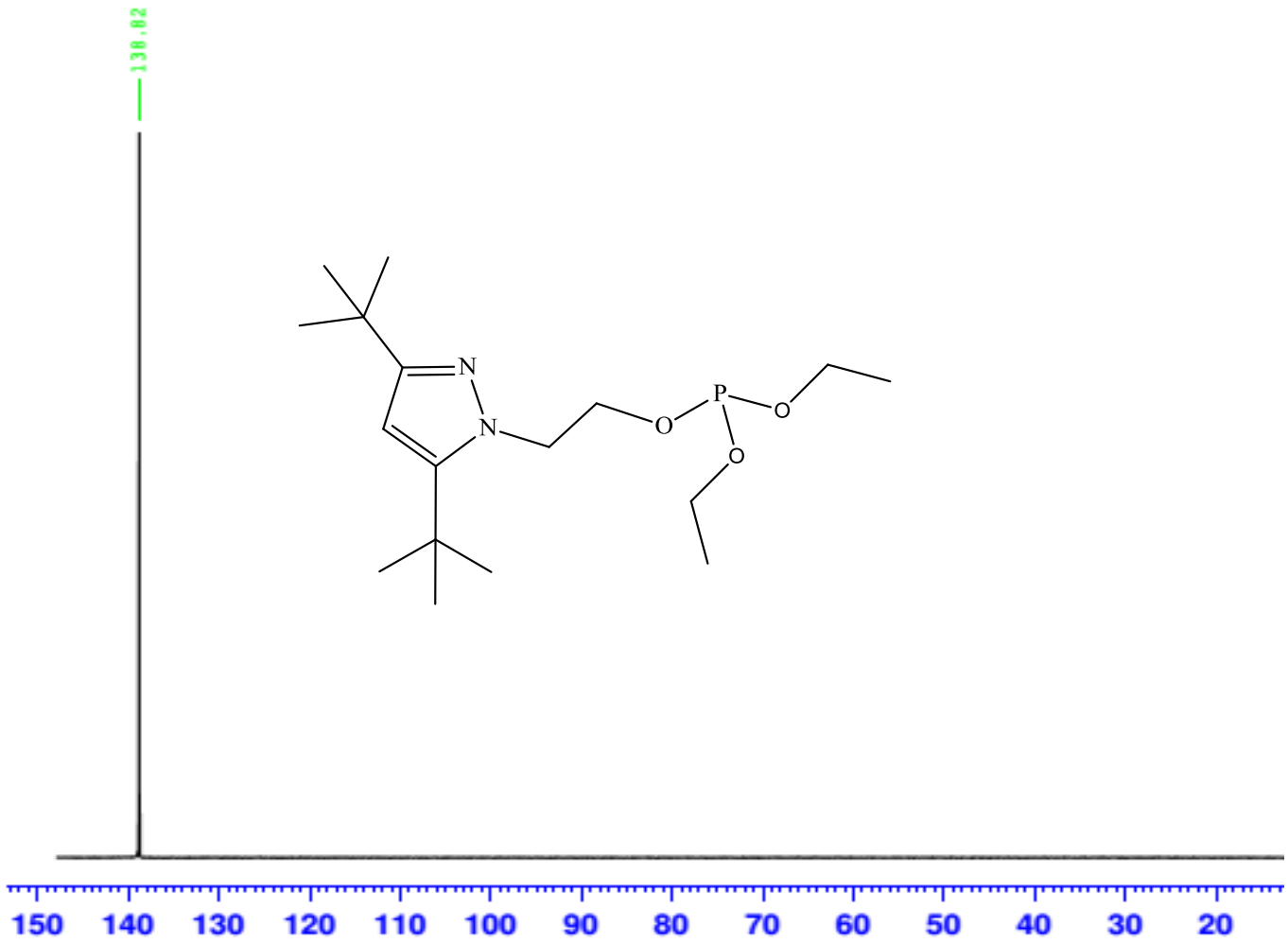


Figure S2: $^{31}P\{^{1}H\}$ NMR spectrum of **L3**. Analysis was carried out in $CDCl_3$ at room temperature.

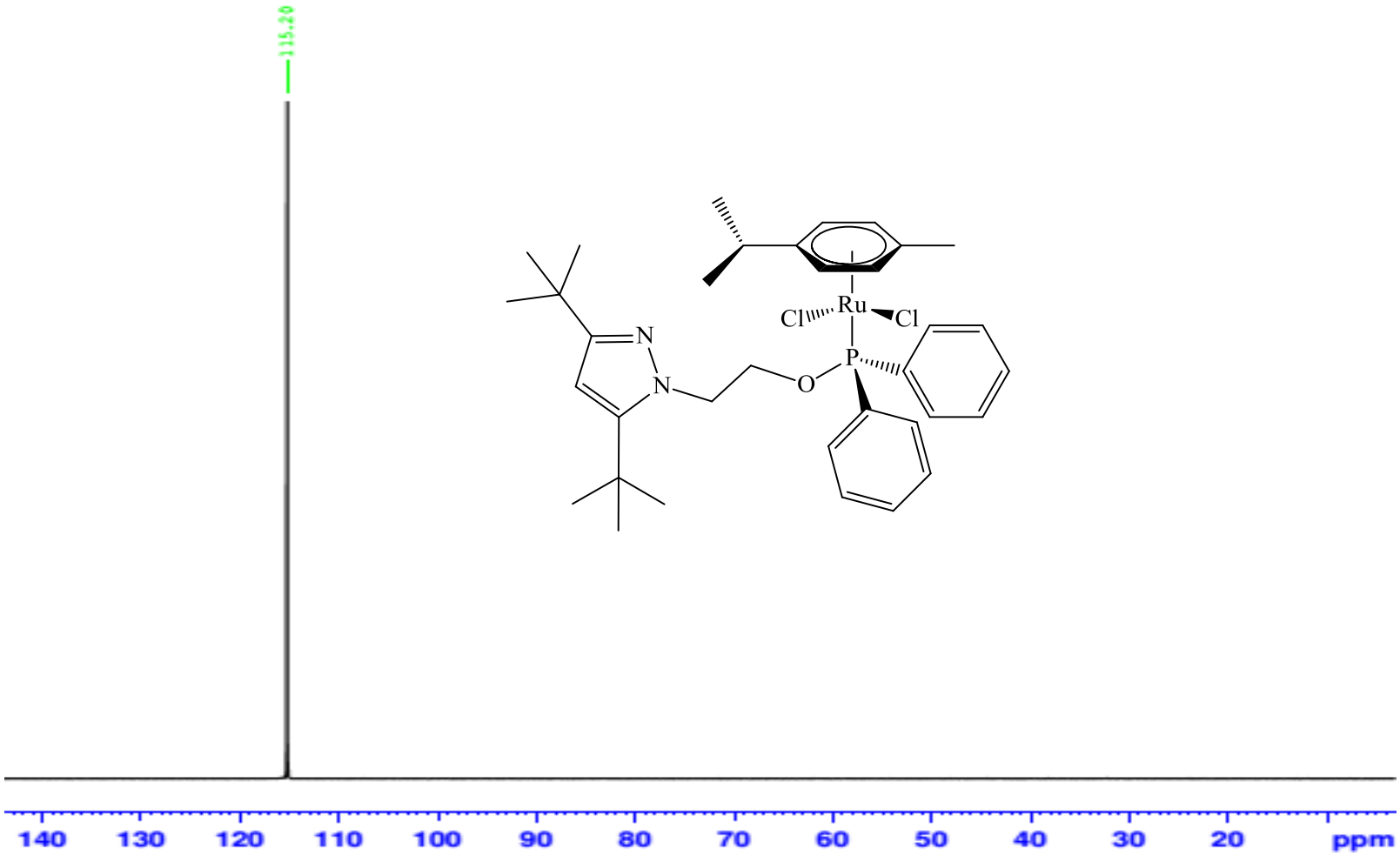


Figure S3: $^{31}P\{^{1}H\}$ NMR spectrum of **1**. Analysis was carried out in $CDCl_3$ at room temperature.

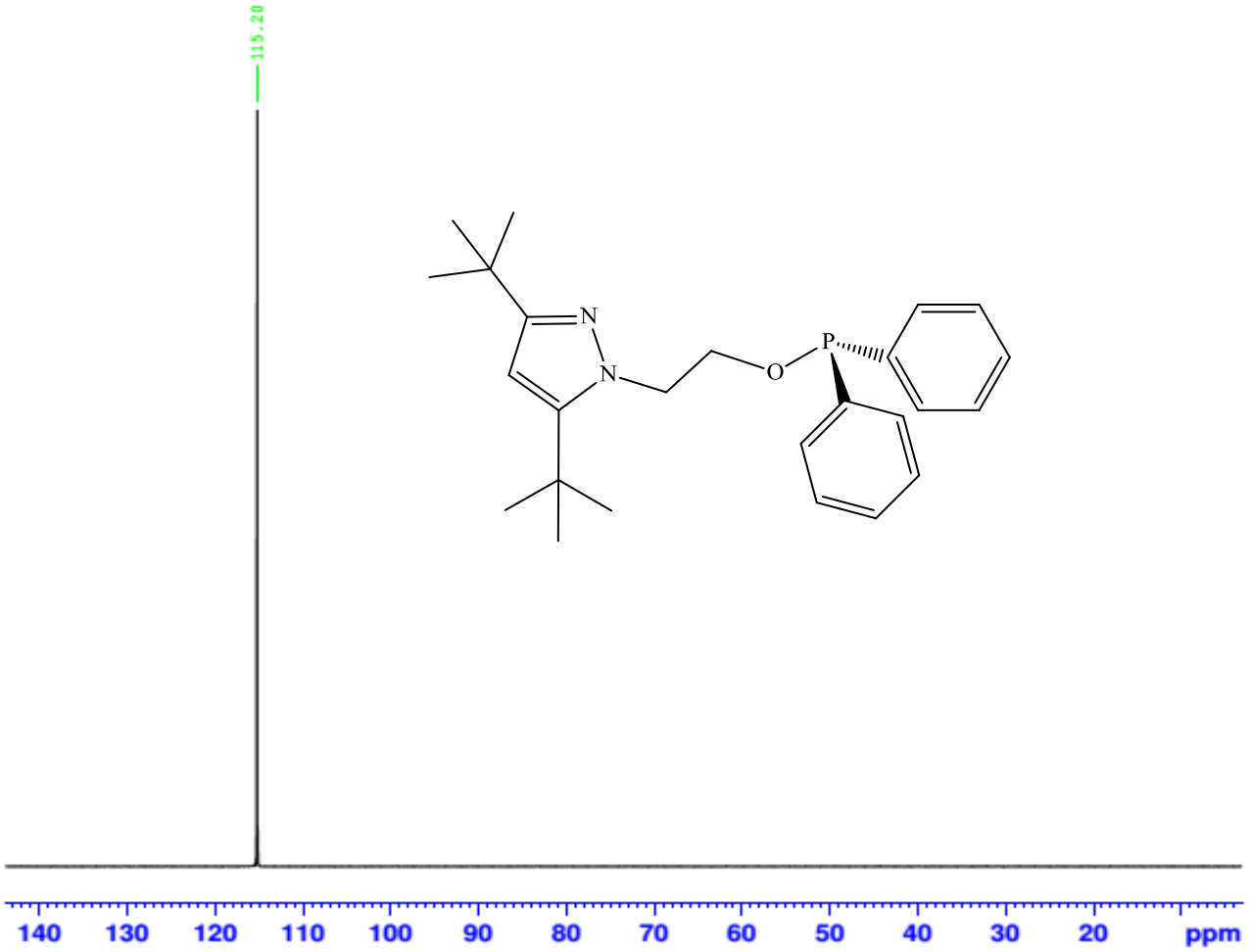


Figure S4: $^{31}P\{^{1}H\}$ NMR spectrum of **L1**. Analysis was carried out in $CDCl_3$ at room temperature.

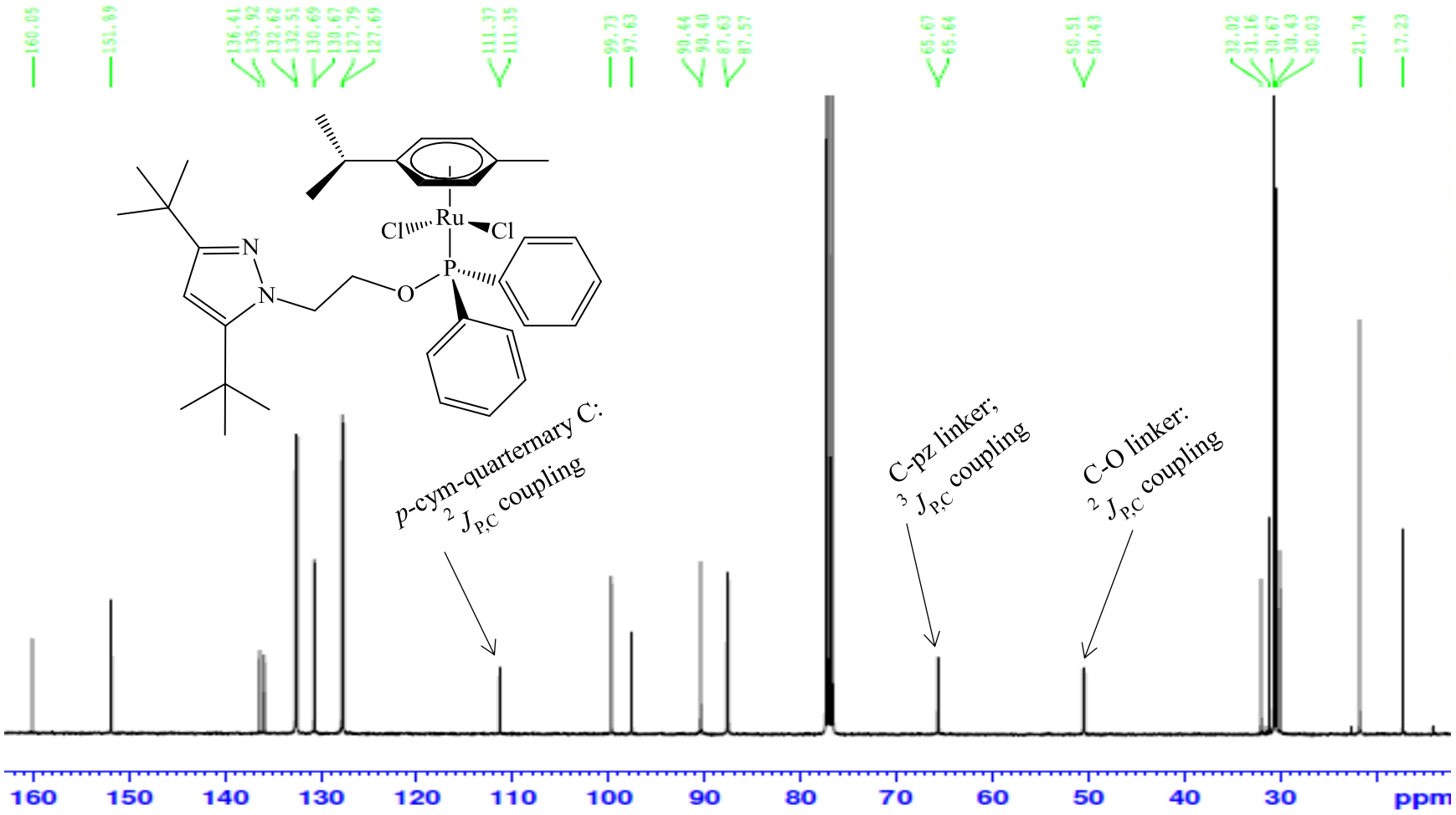


Figure S5: $^{13}C\{^{1}H\}$ NMR spectrum of **1**. Analysis was carried out in $CDCl_3$ at room temperature.

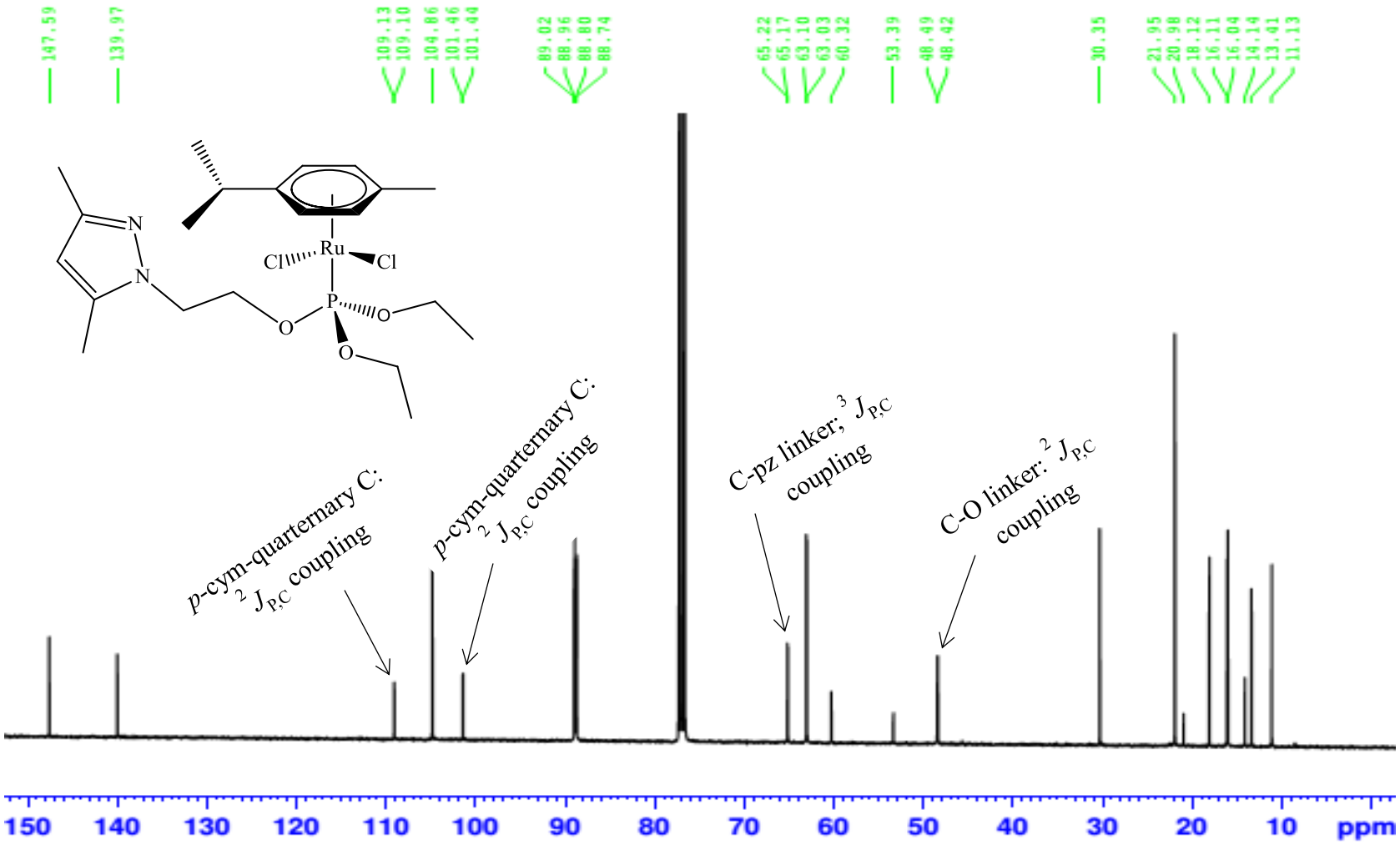
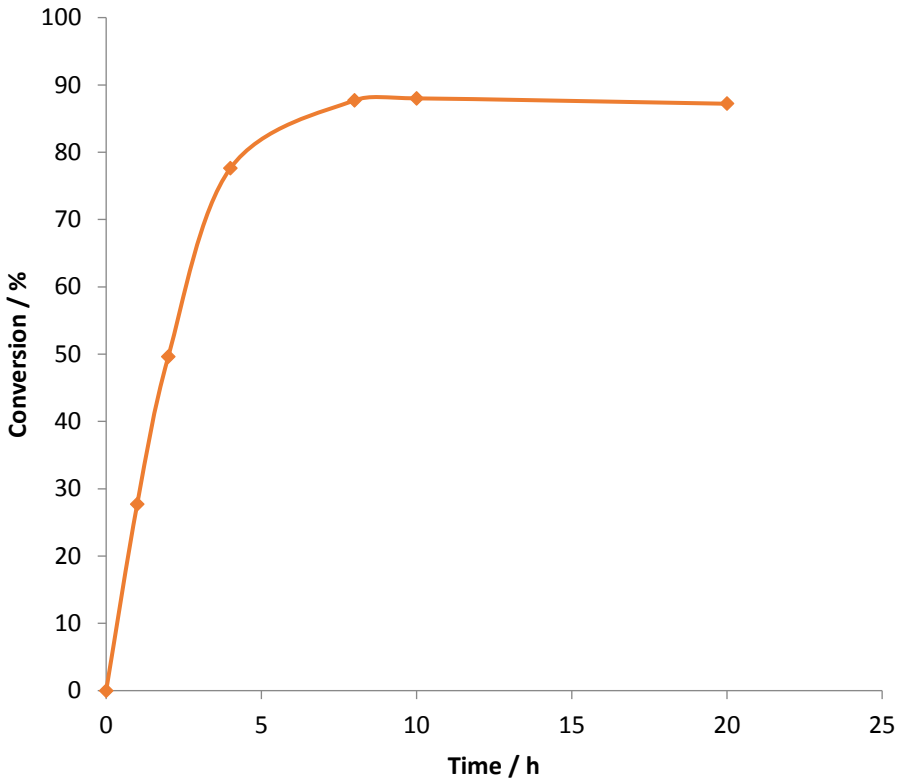
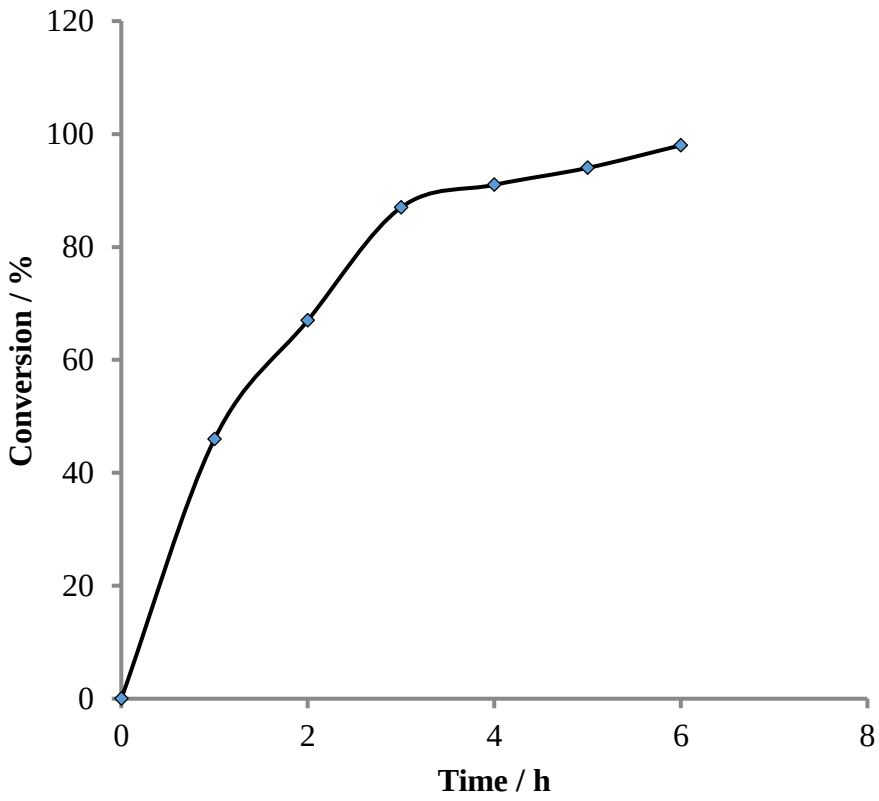


Figure S6: $^{13}C\{^{1}H\}$ NMR spectrum of **2**. Analysis was carried out in $CDCl_3$ at room temperature.



Conditions: acetophenone = 2 mmol, ruthenium(II) catalyst = 0.02 mmol, (1 mol%) KOH = 1 mmol, 2-propanol (10 mL), 80 °C. Conversions were determined by GC.

Figure S7: %Conversion vs time for transfer hydrogenation of acetophenone to 1-phenylethanol using complex **6** as catalyst.



Conditions: acetophenone = 2 mmol, catalyst = 0.02 mmol (1 mol%), H_2 = 20 bar, KOH = 1 mmol, 70 °C, 6 h, ethanol = 5 mL

Figure S8: Time study of molecular hydrogenation of acetophenone to 1-phenylethanol using complex **3**.

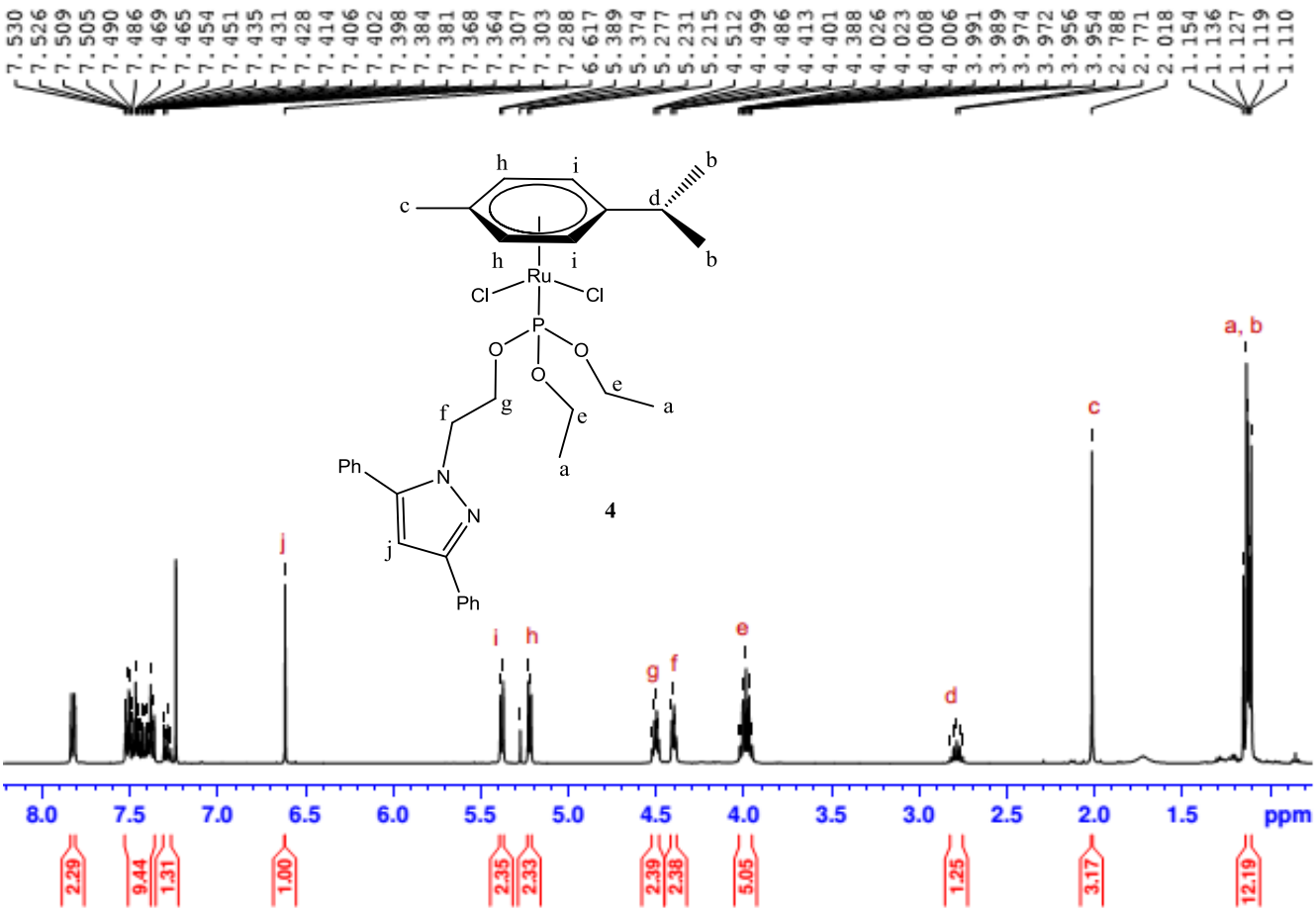


Figure S9a: ^{1}H NMR spectrum of **4**. Analysis was carried out in $CDCl_3$ at room temperature.

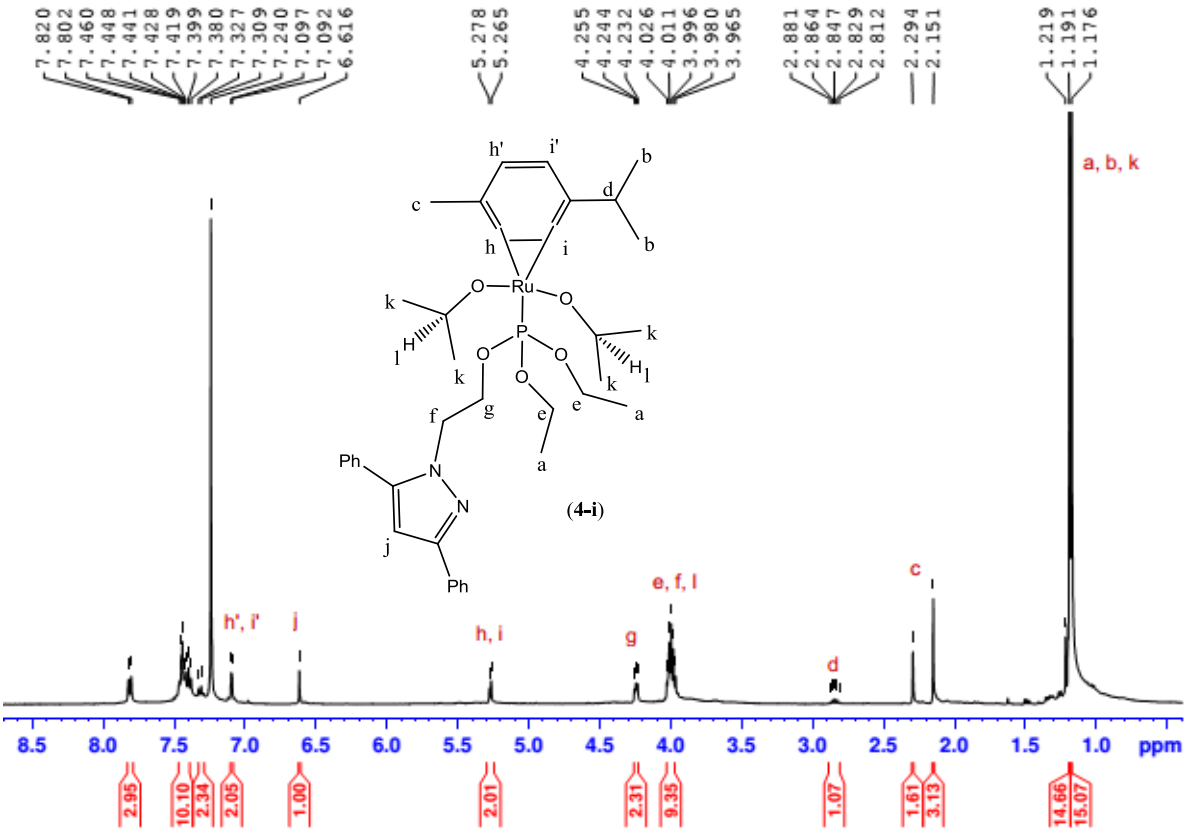


Figure S9b: ^{1}H NMR spectrum of (**4-i**). Analysis was carried out in $CDCl_3$ at room temperature. (**4-i**) was isolated from a reaction mixture of 2-propanol, **4** and KOH.