NHC-carbene supported half-sandwich hydridosilyl complexes of ruthenium: the impact of supporting ligands on Si…H interligand interactions

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Supporting Information

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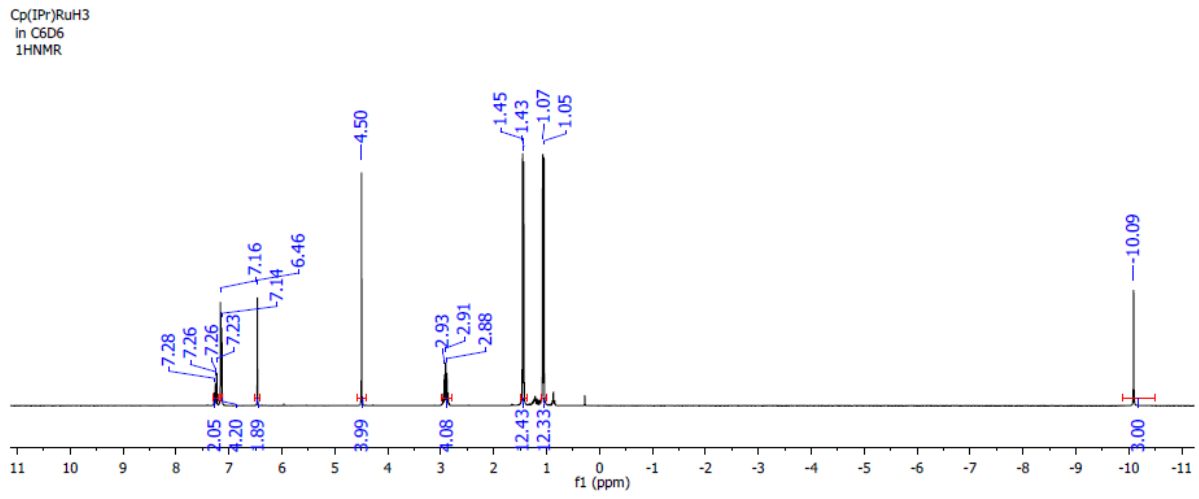
1 General Information

All manipulations were performed using conventional high vacuum or nitrogen-line Schlenk techniques. Solvents were dried by using Grubbs-type purification columns and stored in ampoules equipped with a Teflon valve. Deuterated solvents were dried over sodium, potassium or CaH_2 as appropriate, distilled under reduced pressure and stored in ampoules with a Teflon valve. NMR samples were prepared in New Era tubes equipped with J. Young-type Teflon valves. NMR spectra were obtained with Bruker DPX-400 and Brucker DPX-600 instruments (^{1}H: 400 and 600 MHz; ^{13}C: 100.6 and 151 MHz; ^{29}Si: 119.2 MHz; ^{31}P: 162.0 and 243 MHz) spectrometers at 298 K. ^{1}H and ^{13}C NMR spectra were referenced internally to residual protiosolvent (^{1}H) or solvent (^{13}C) resonances and are reported relative to tetramethylsilane (δ=0 ppm). Chemical shifts are quoted in δ[ppm], and coupling constants in Hertz. IR spectra were recorded by using a PerkinElmer 1600 FTIR spectrometer as Nujol mulls between NaCl windows. All chemicals were purchased from Sigma– Aldrich and Alfa Aesar were used without further purification. CD_3CN, CD_2Cl_2, C_6D_6 were purchased from Cambridge Isotope Laboratories. These NMR solvents were dried over CaH_2 before use. CH_3CN, Et_2O and hexane were dried by using a Grubbs-type solvent purification system supplied by Innovative Technology.

2 NMR Spectra

Cp(IPr)RuH$_3$ (5)



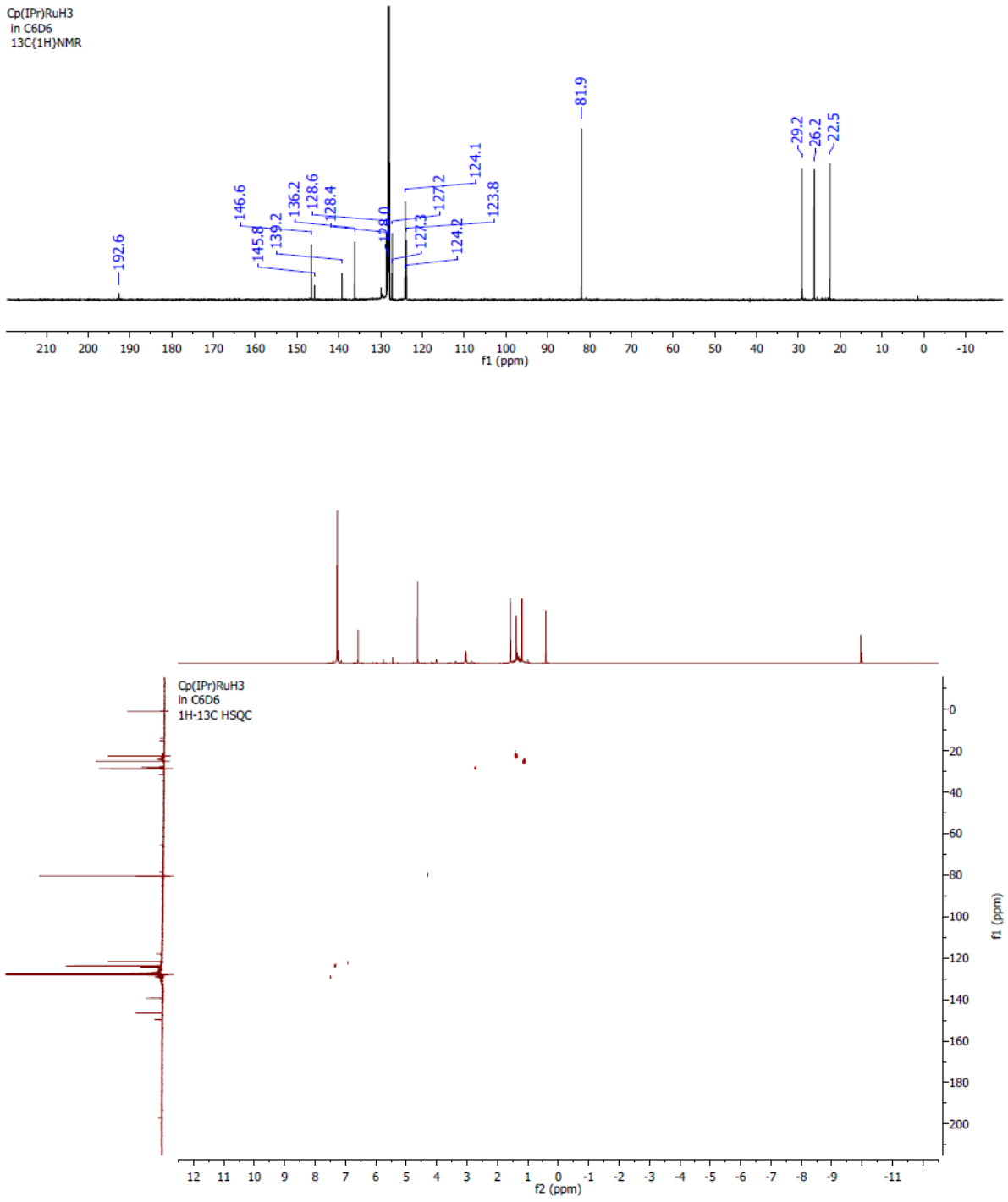
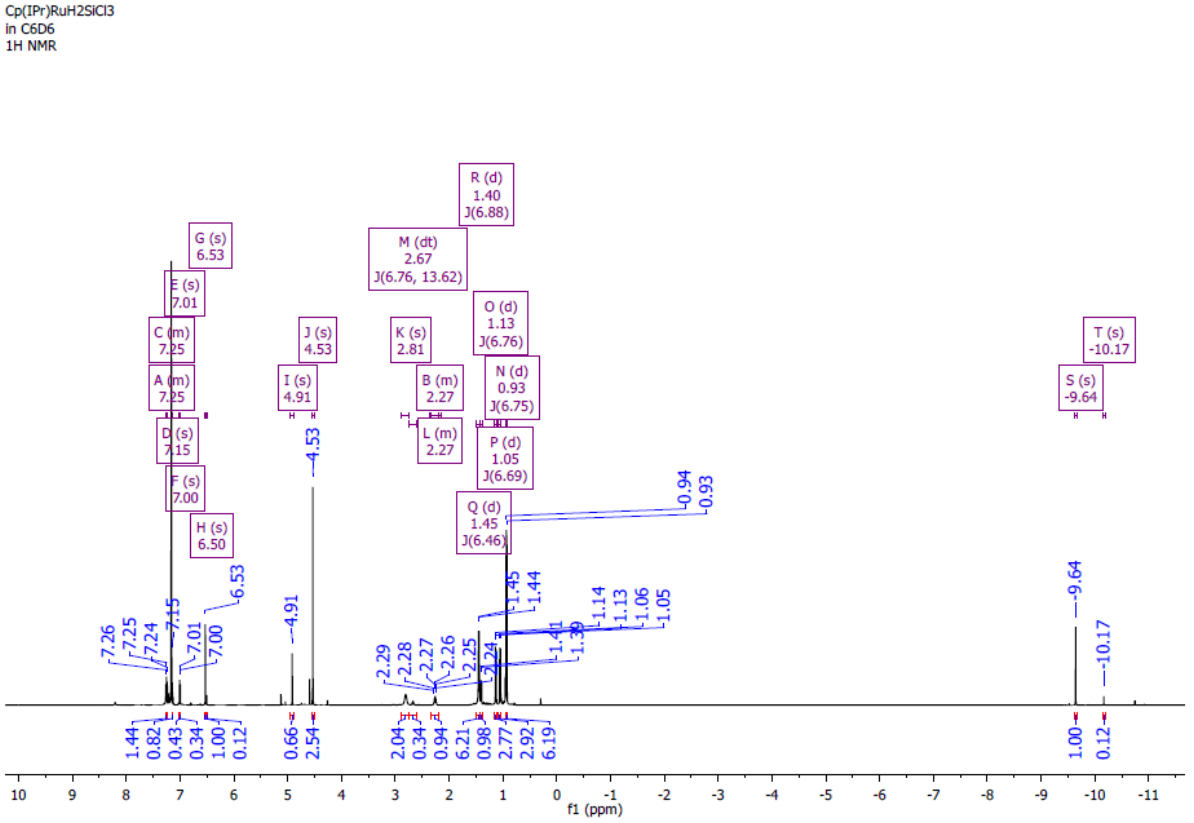
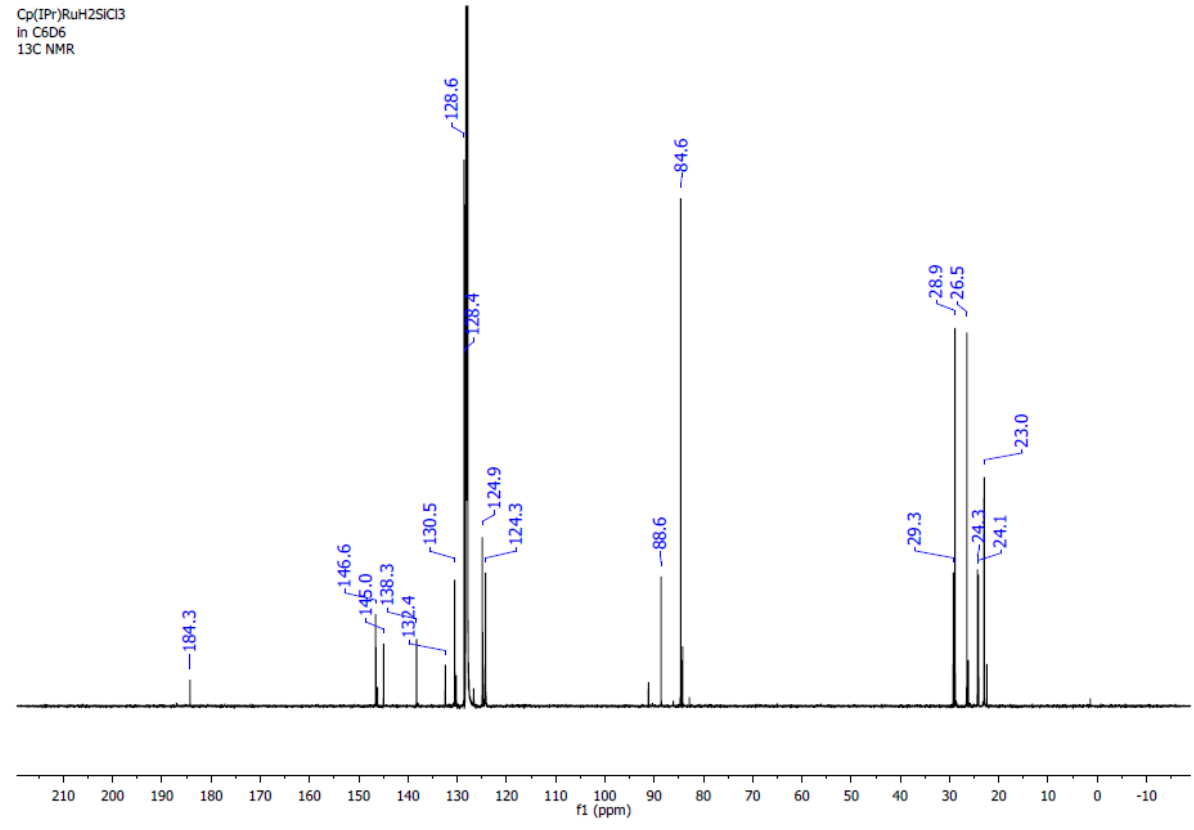


Figure SI1. NMR spectra for $Cp(IPr)RuH_3$ (**5**)

Cp(IPr)RuH$_2$(SiCl$_3$) (6a)





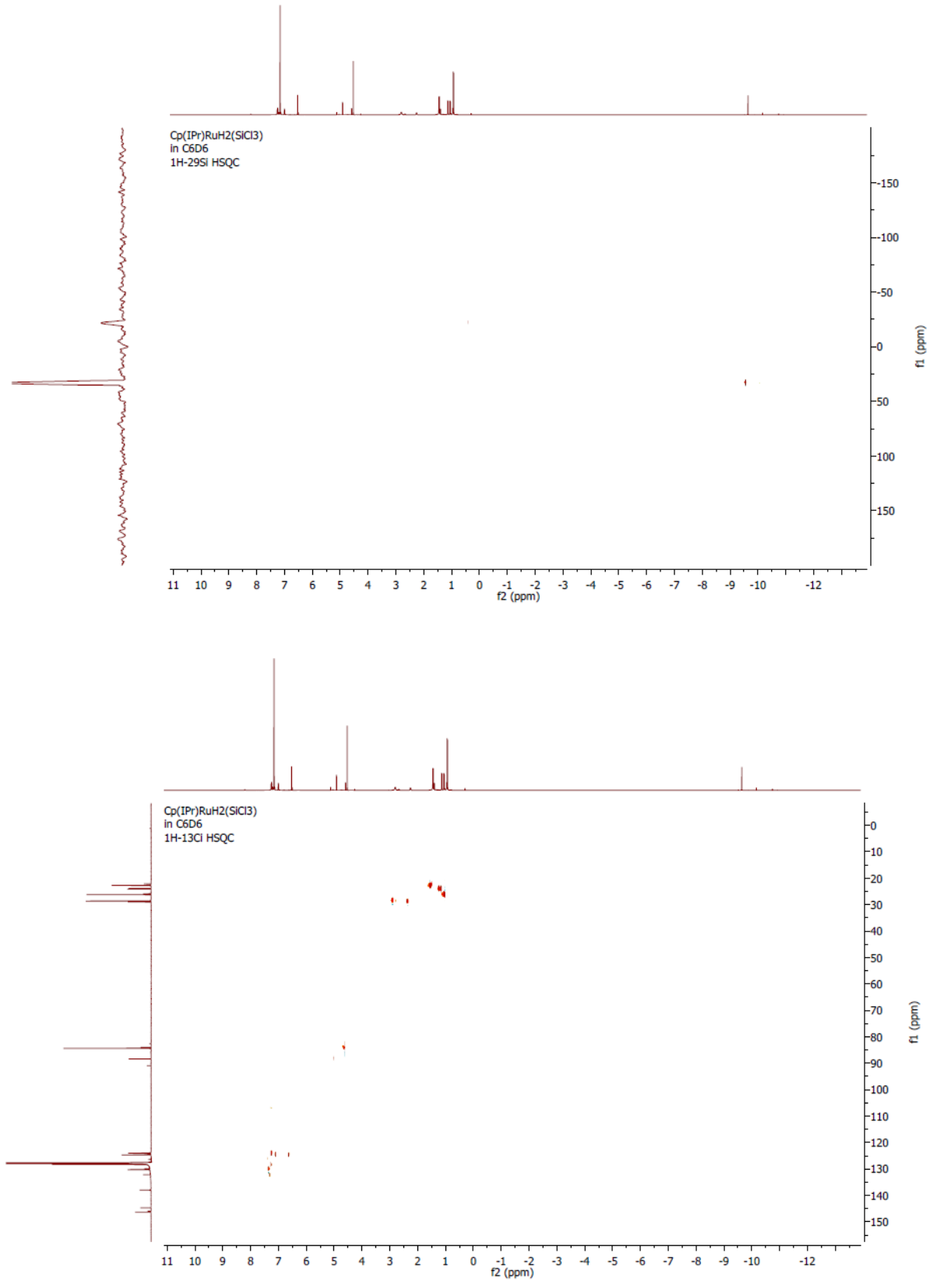
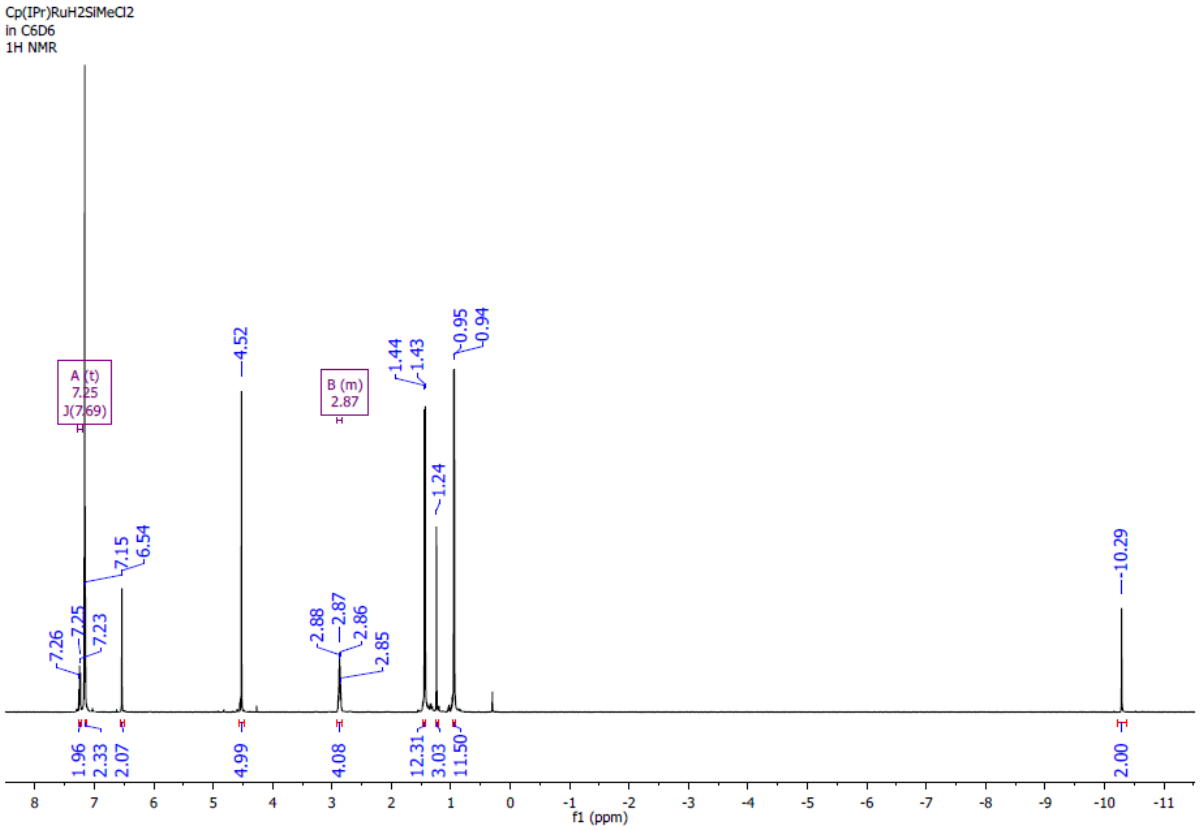
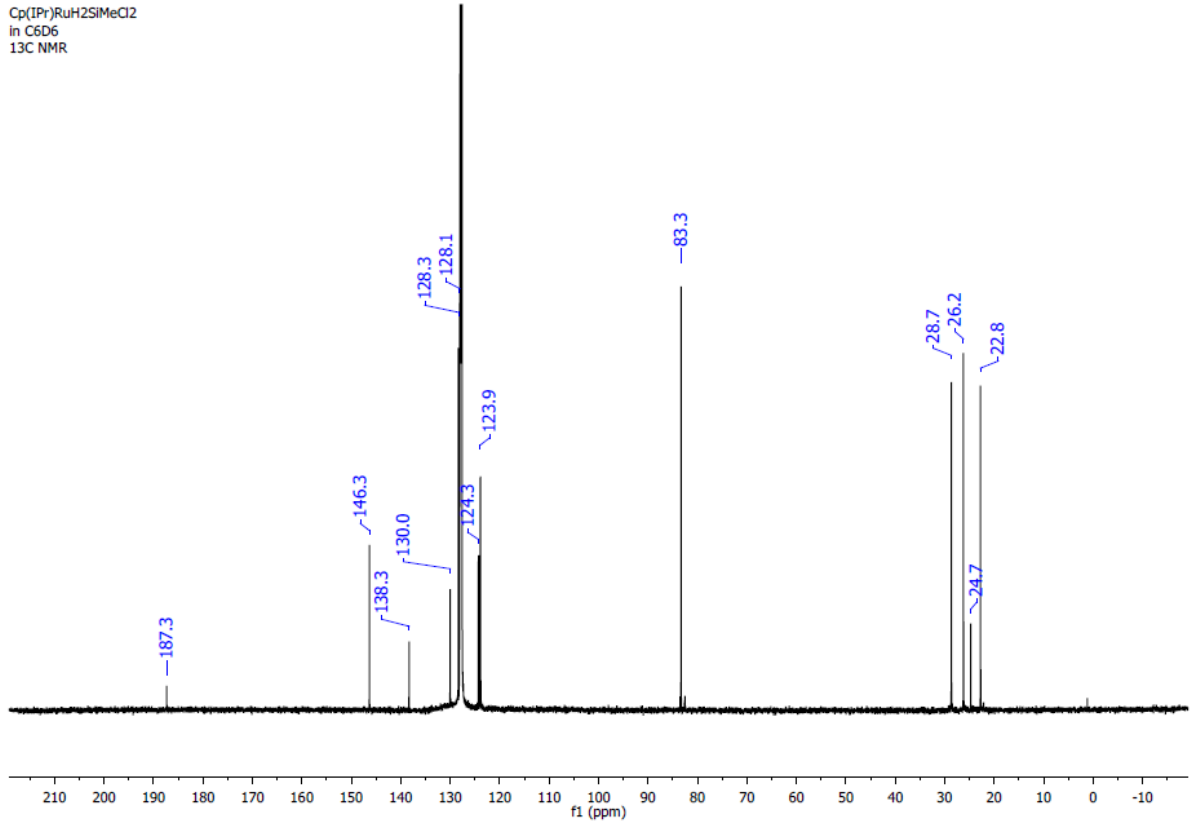


Figure SI2. NMR spectra for Cp(IPr)$RuH_2(SiCl_3)$ (**6a**)

Cp(IPr)RuH$_2$(SiCl$_2$Me) (6b)





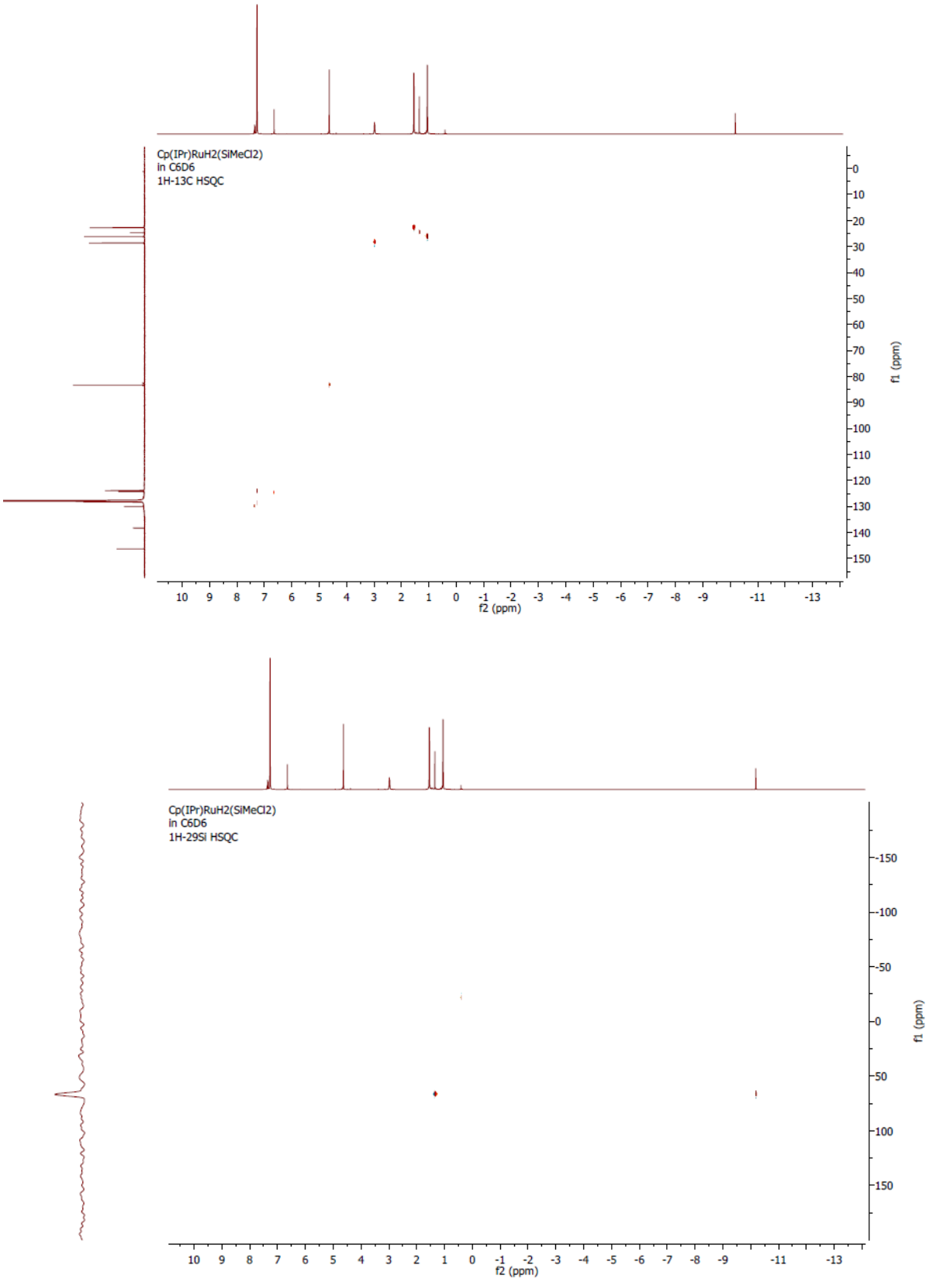
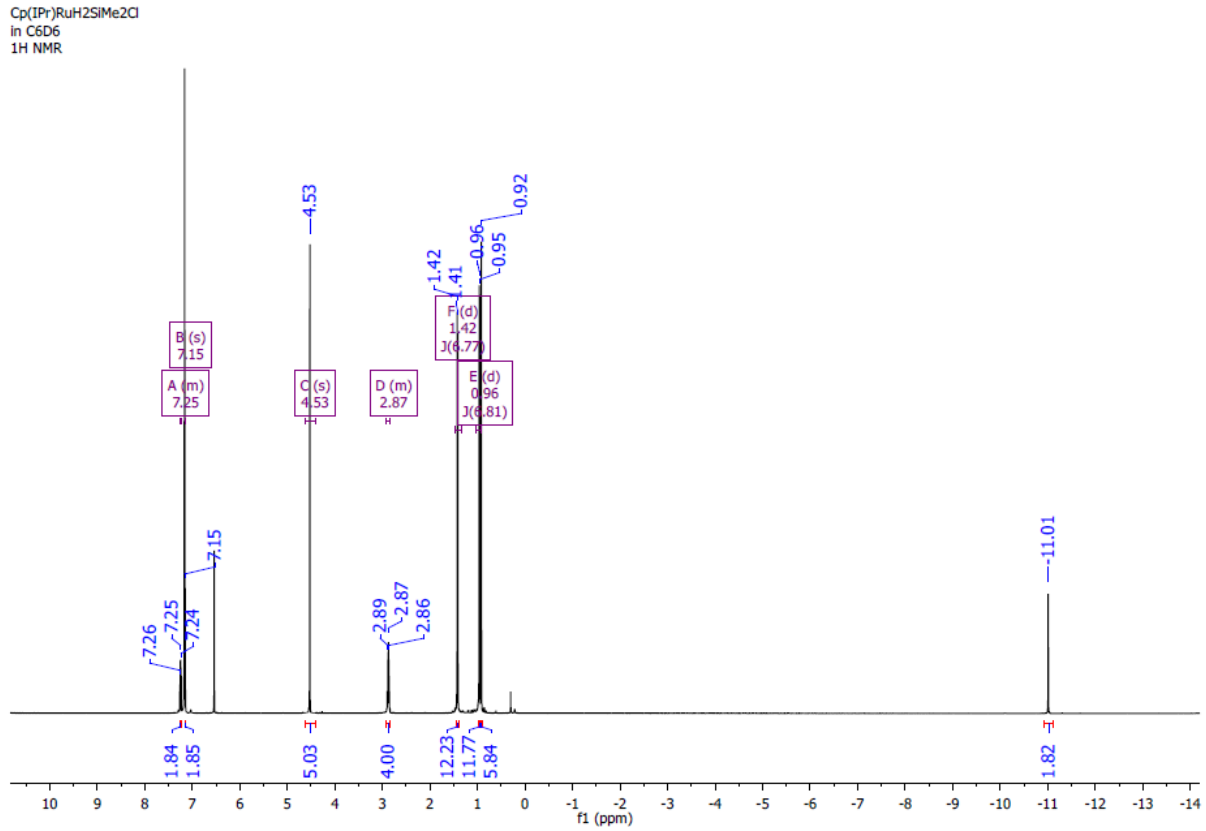
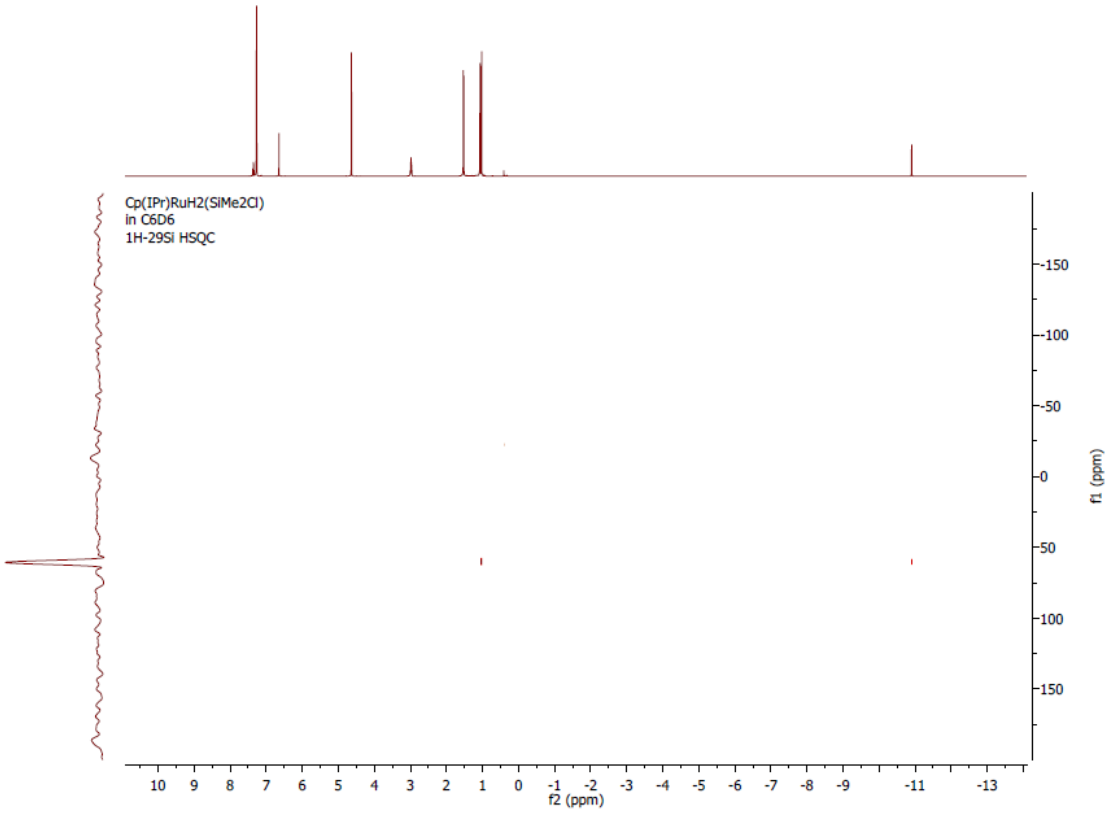
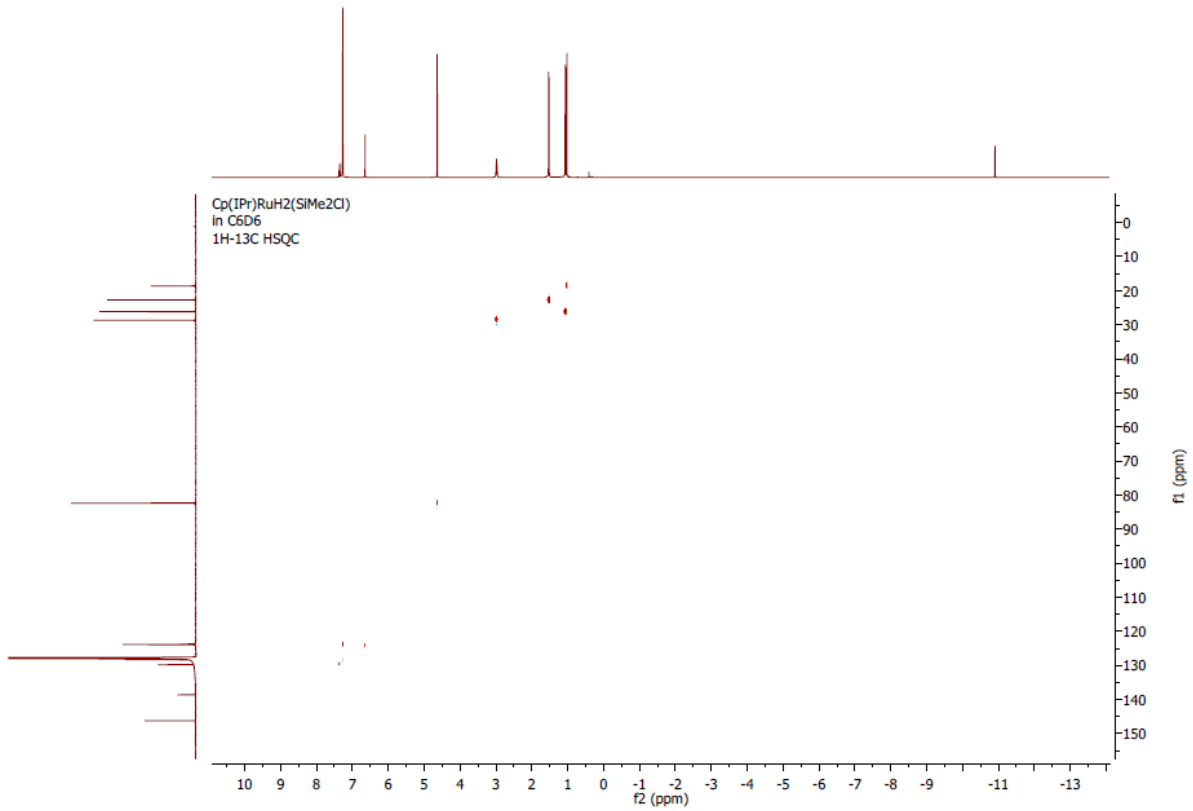


Figure SI3. NMR spectra for $Cp(IPr)RuH_2(SiCl_2Me)$ (**6b**)

Cp(IPr)RuH$_2$(SiClMe$_2$) (6c)







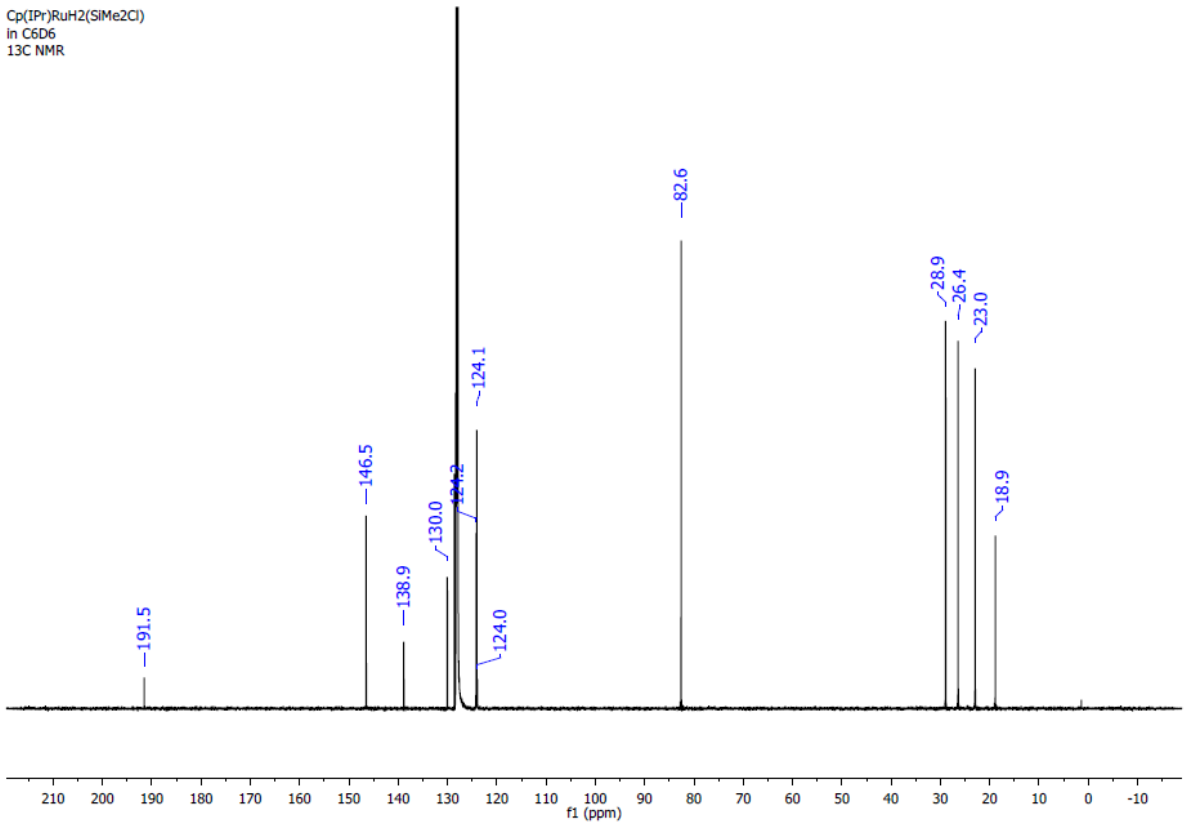
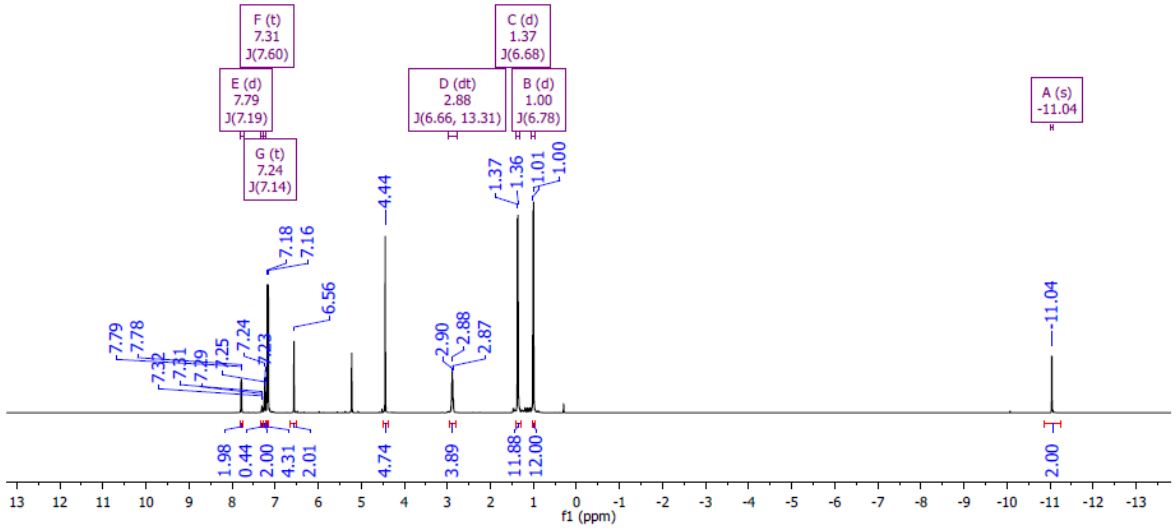


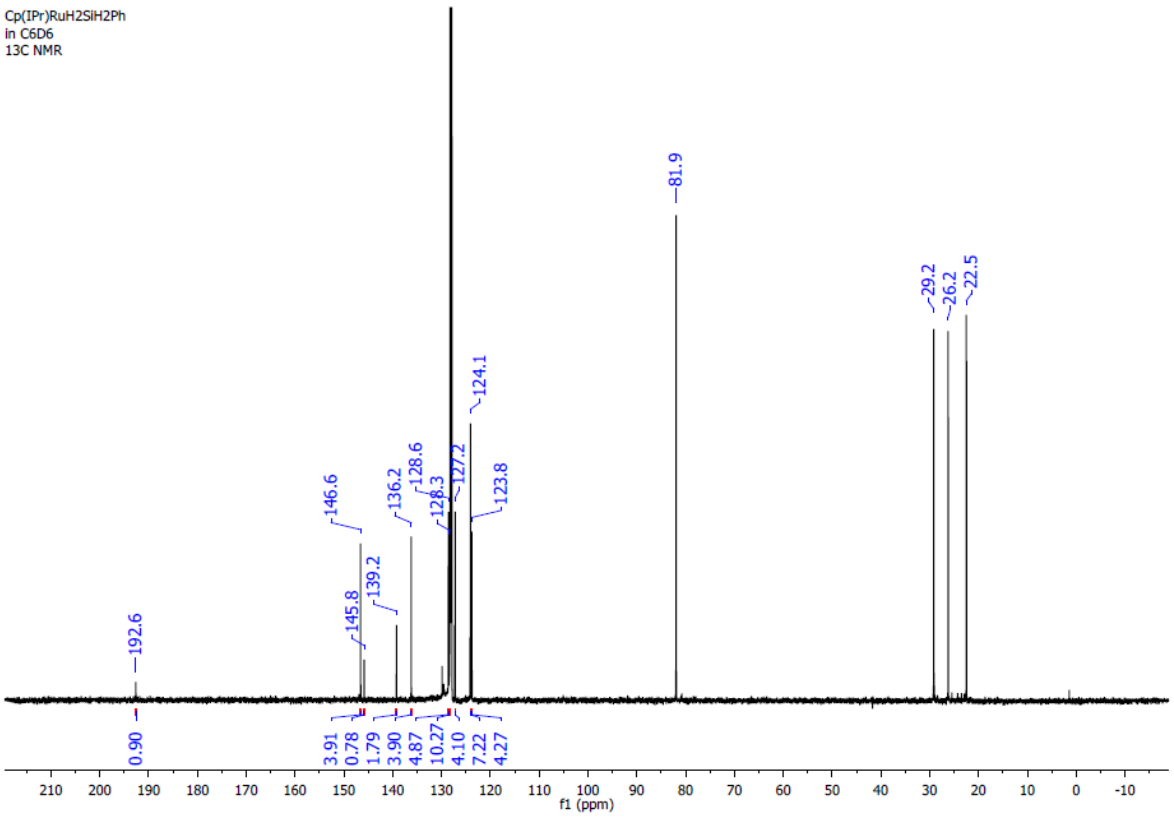
Figure SI4. NMR spectra for Cp(IPr)$RuH_2(SiClMe_2)$ (**6c**).

Cp(IPr)RuH$_2$(SiH$_2$Ph) (6d)

Cp(IPr)RuH2SiH2Ph
in C6D6
1H NMR



Cp(IPr)RuH2SiH2Ph
in C6D6
13C NMR



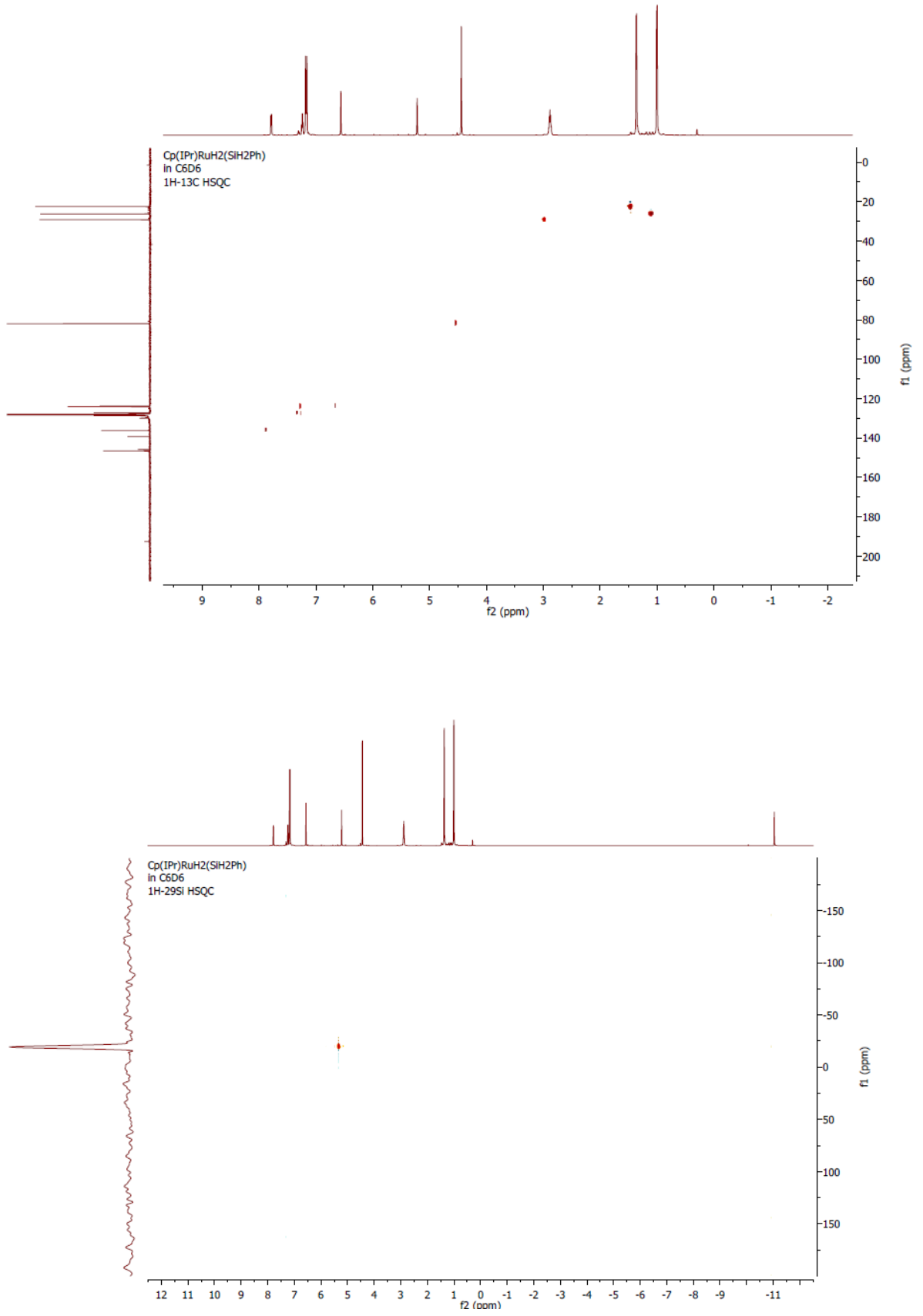
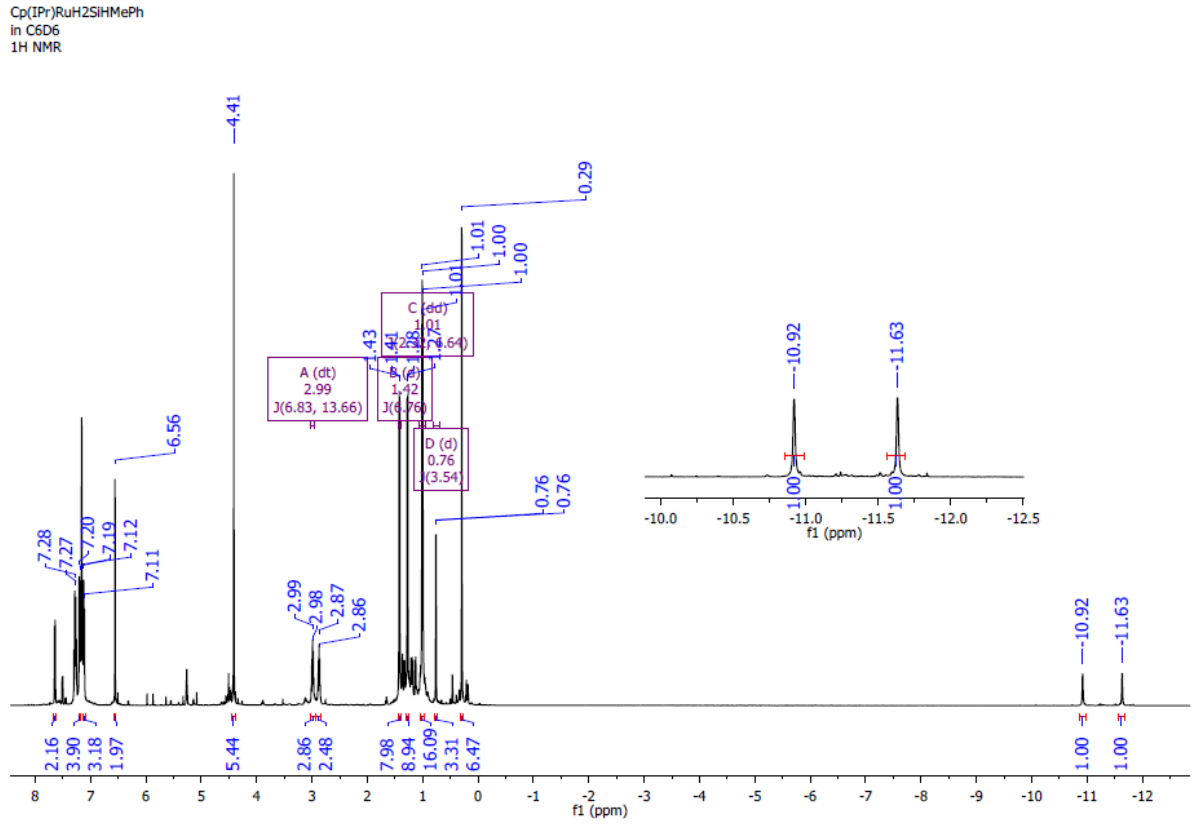
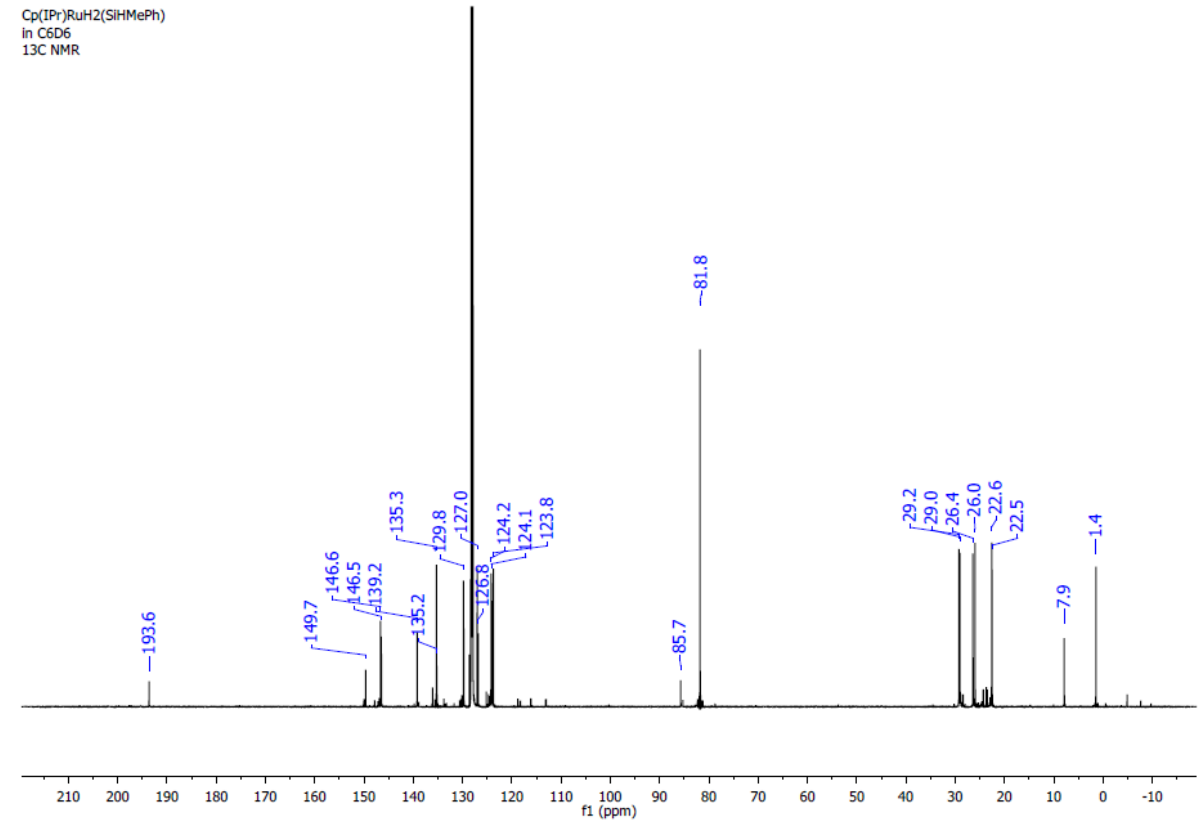


Figure SI5. NMR spectra for Cp(IPr)$RuH_2(SiH_2Ph)$ (**6d**)

Cp(IPr)RuH$_2$(SiHMePh) (6e)





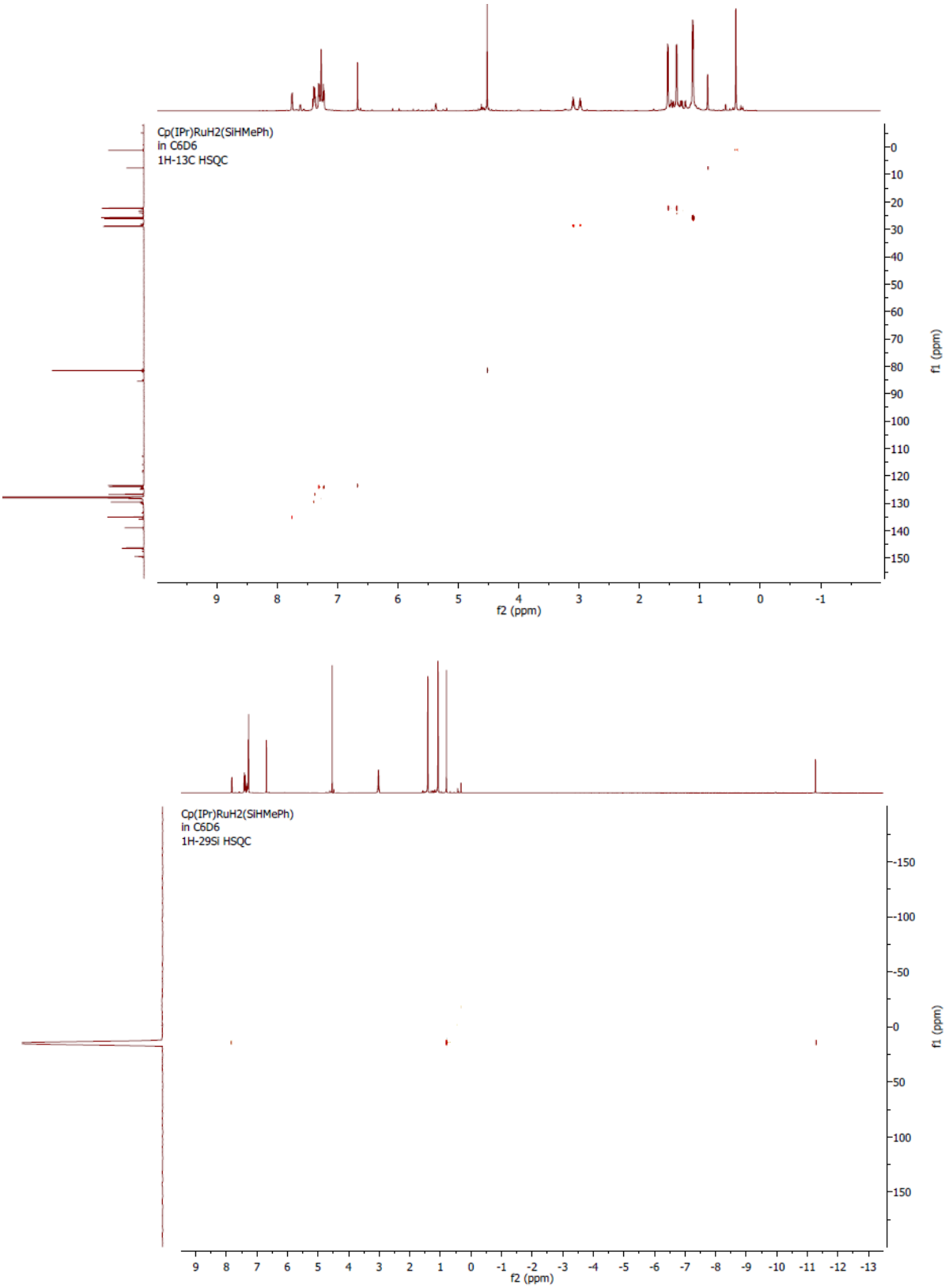
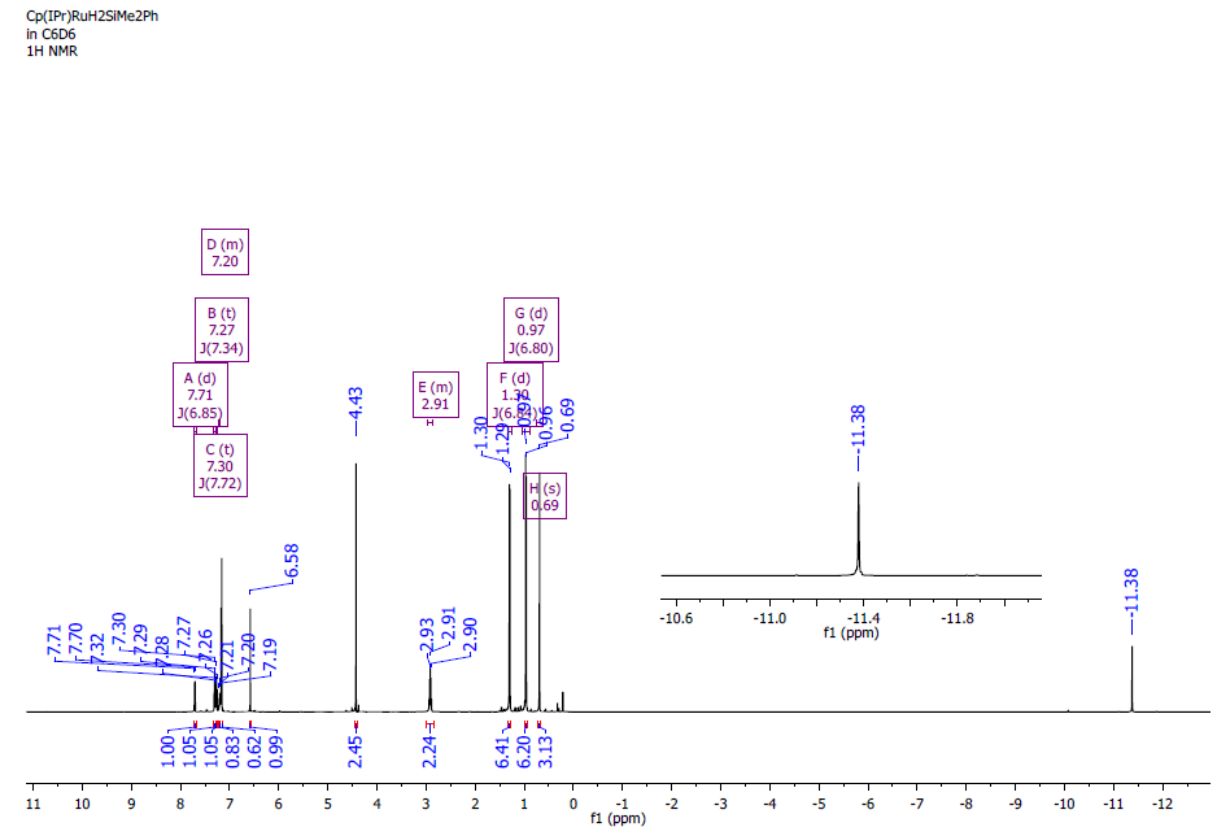
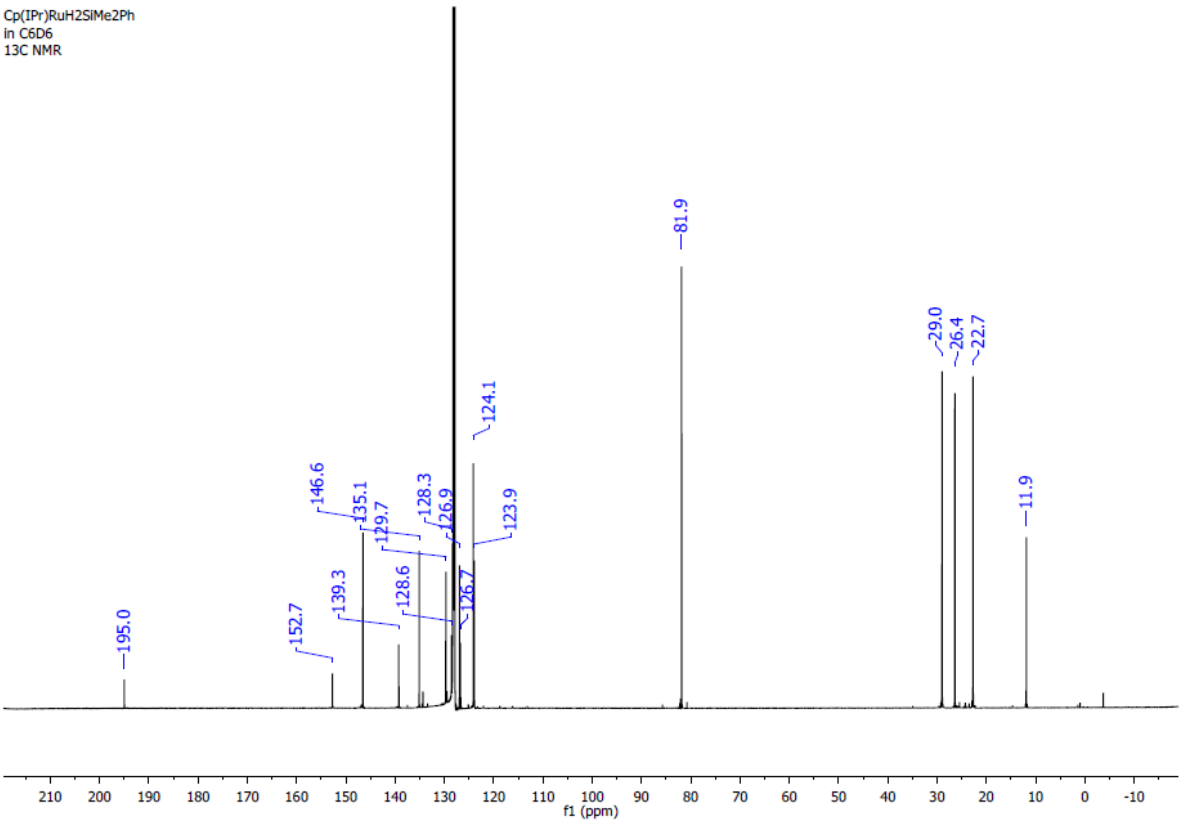


Figure SI6. NMR spectra for Cp(IPr)RuH_2(SiHMePh) (**6e**)

Cp(IPr)RuH$_2$(SiMe$_2$Ph) (6f)





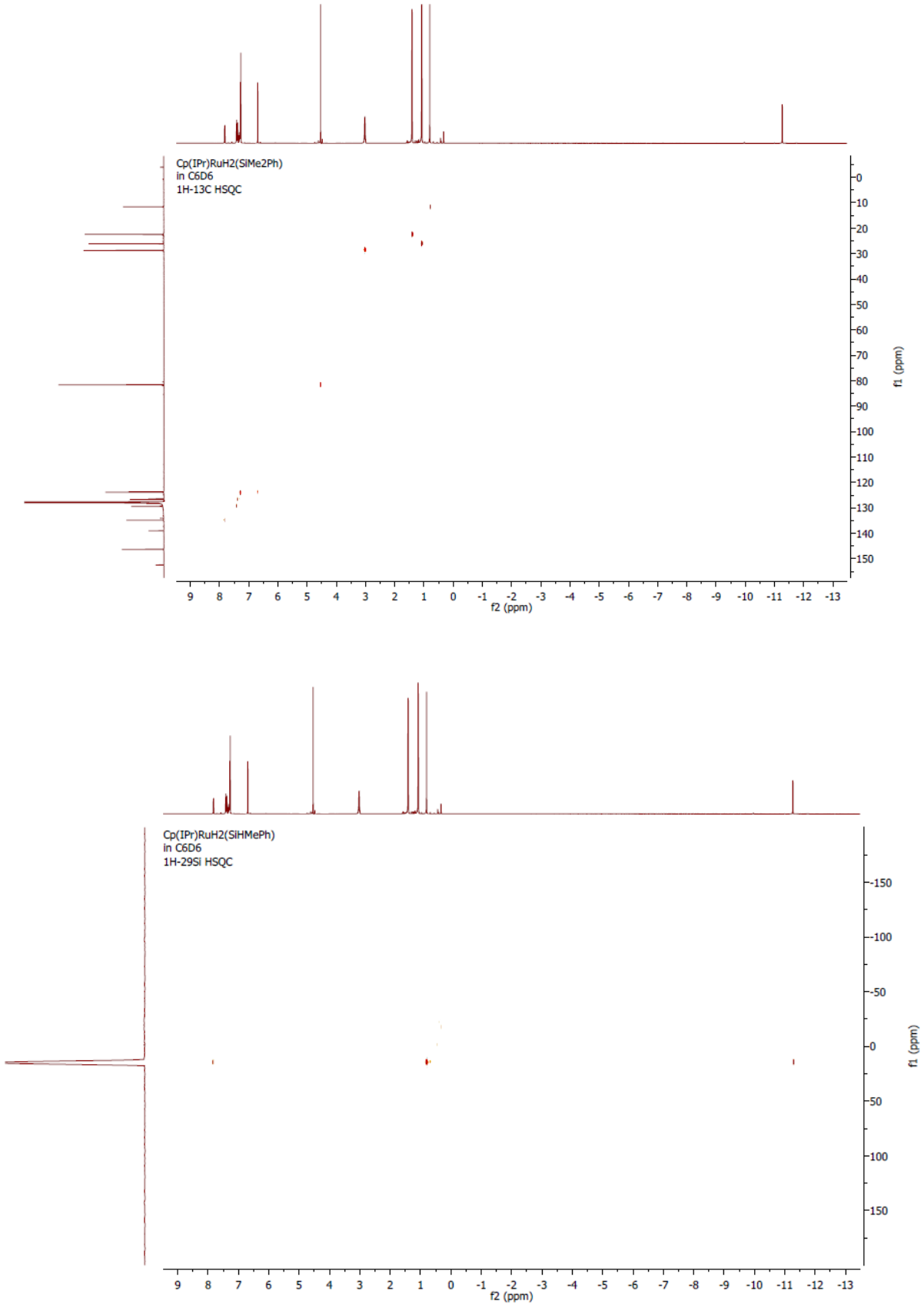


Figure SI7. NMR spectra for Cp(IPr)$RuH_2(SiMe_2Ph)$ (**6f**)