Electronic Supplementary Information

# Coordination mode and stability of the tetrahydroborate ligand in group 10 metal pincer complexes

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## Contents



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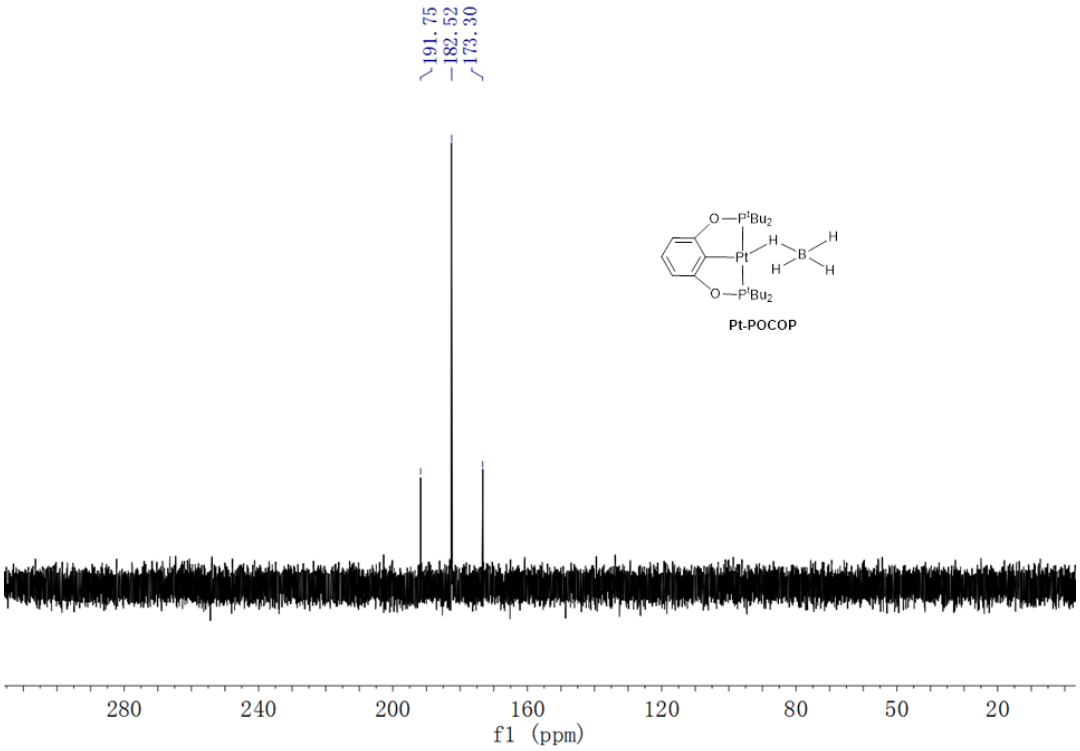


**Fig. S1** $^{31}P\{^{1}H\}$ NMR spectrum of **Pt-POCOP** (162 Hz, THF with THF-$d_8$)

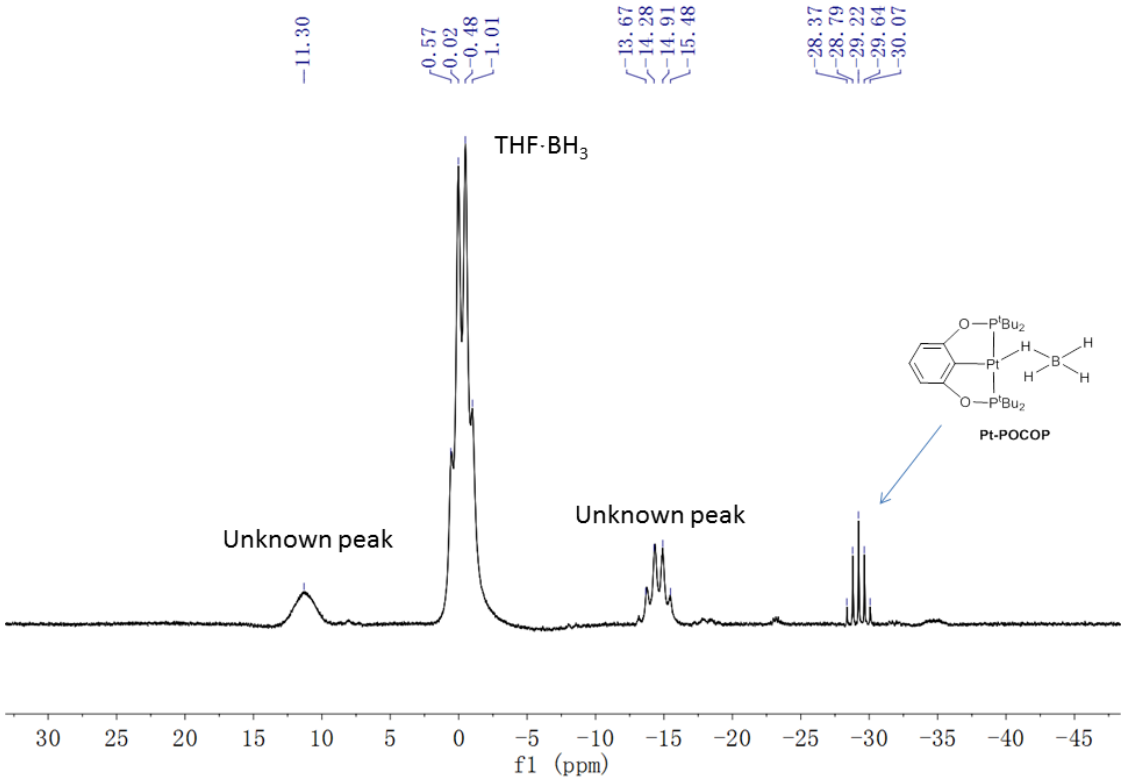


**Fig. S2** $^{11}B$ NMR spectrum of **Pt-POCOP** (193 Hz, THF)

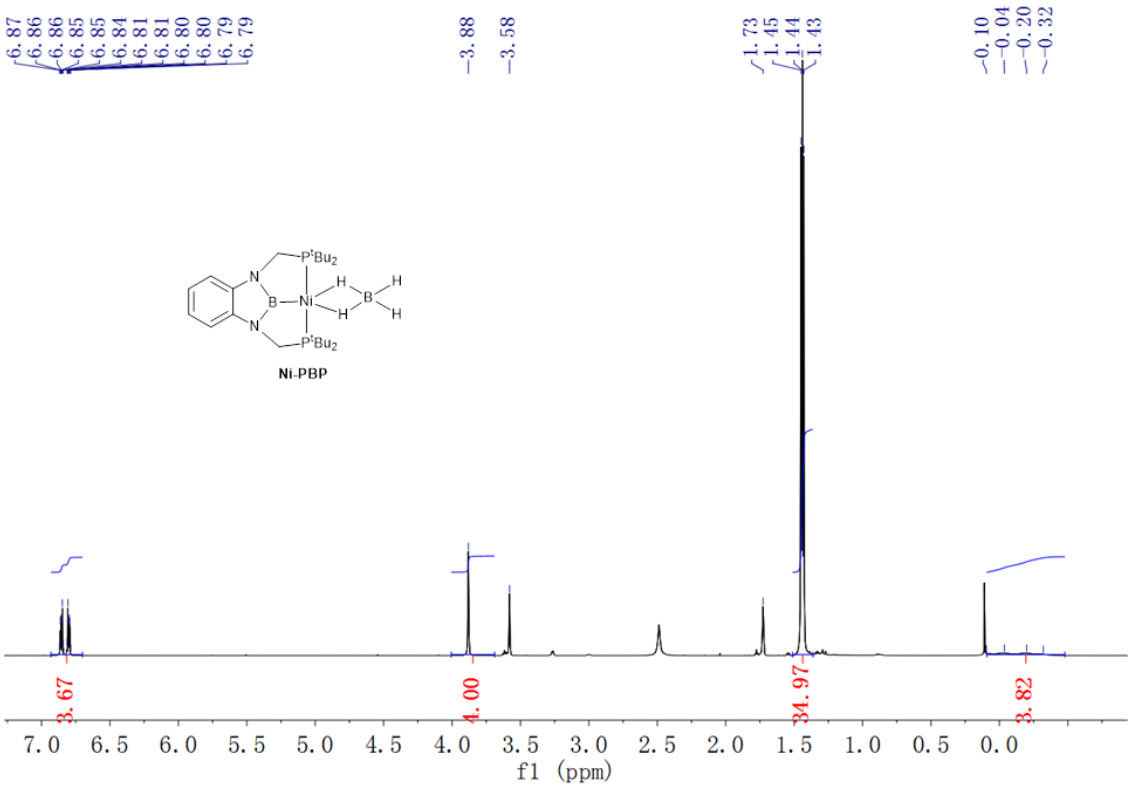


**Fig. S3** $^{1}$H NMR spectrum of **Ni-PBP** (600 Hz, THF-$d_8$)

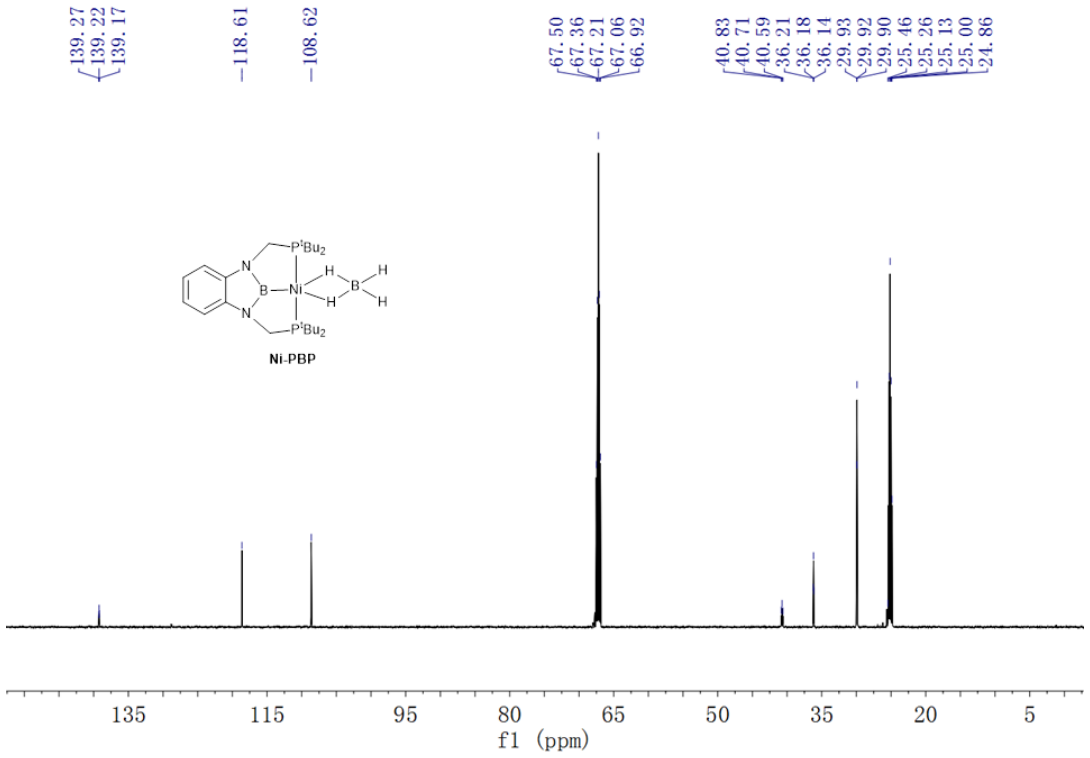


**Fig. S4** $^{13}$C{$^{1}$H} NMR spectrum of **Ni-PBP** (151 Hz, THF-$d_8$)

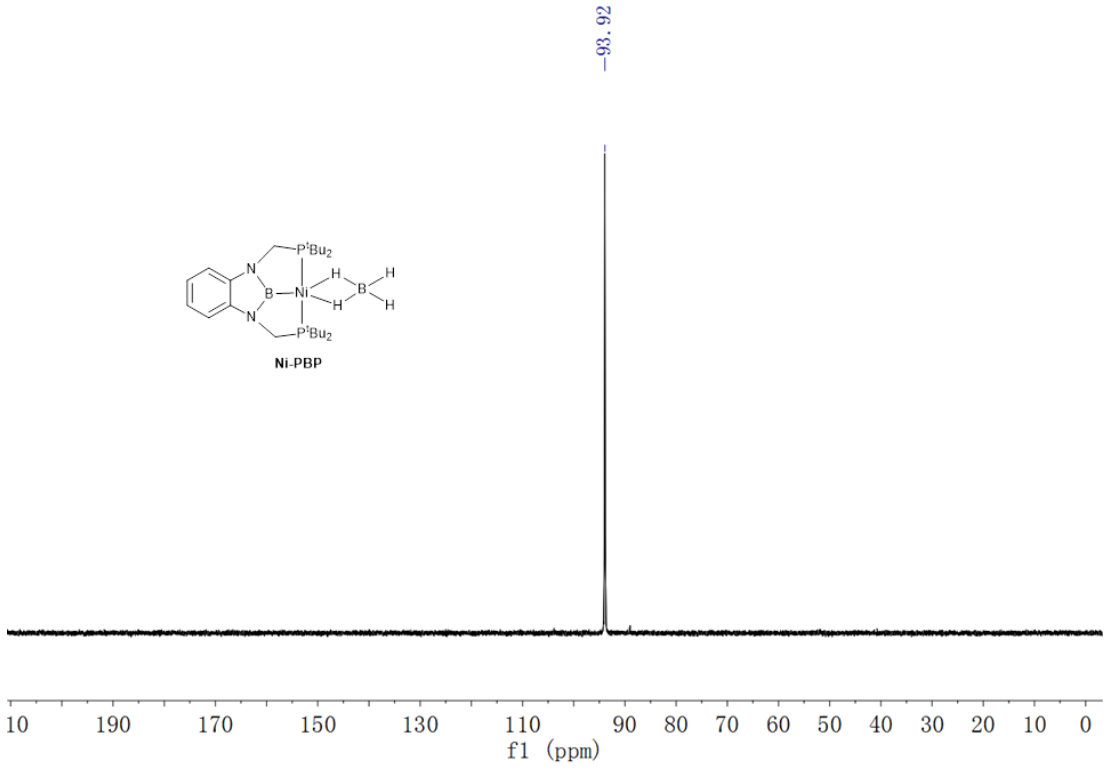


**Fig. S5** $^{31}P\{^{1}H\}$ NMR spectrum of **Ni-PBP** (243 MHz, THF-$d_8$)

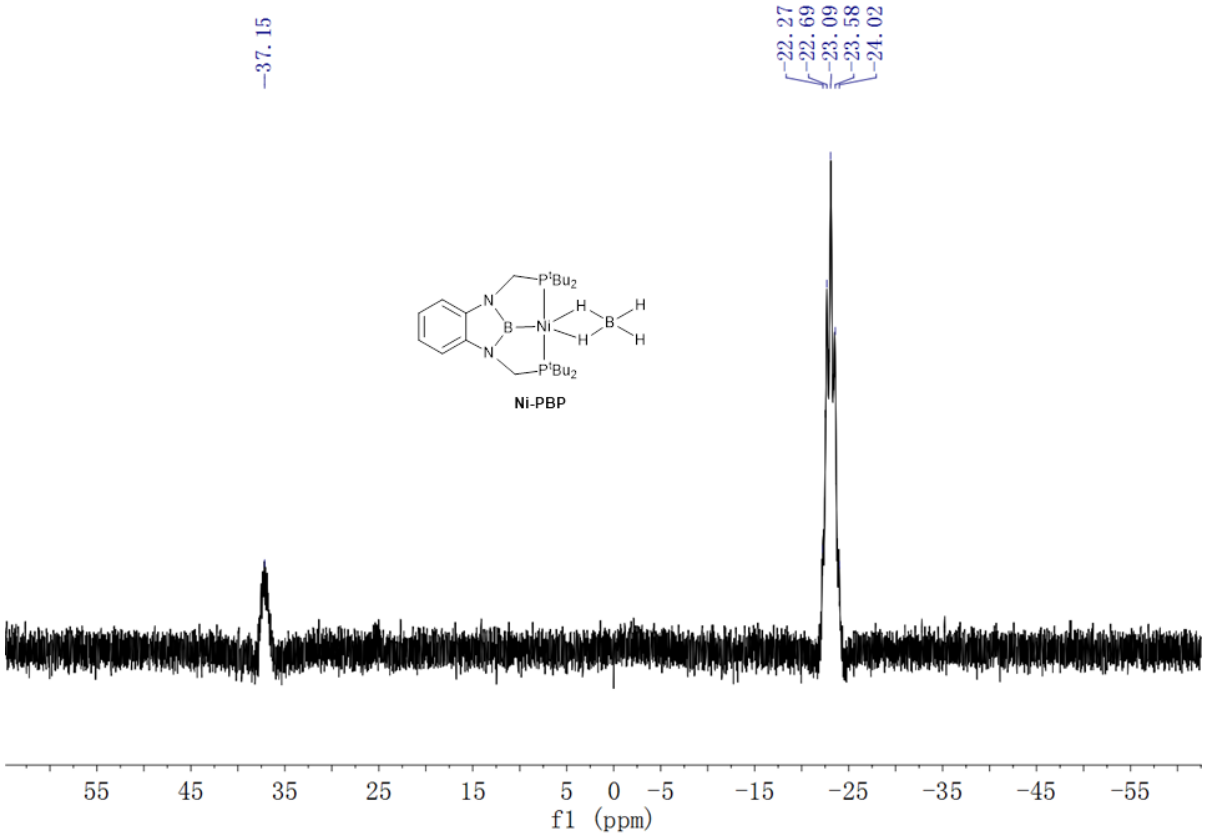


**Fig. S6** $^{11}B$ NMR spectrum of **Ni-PBP** (193 MHz, $C_6D_6$)

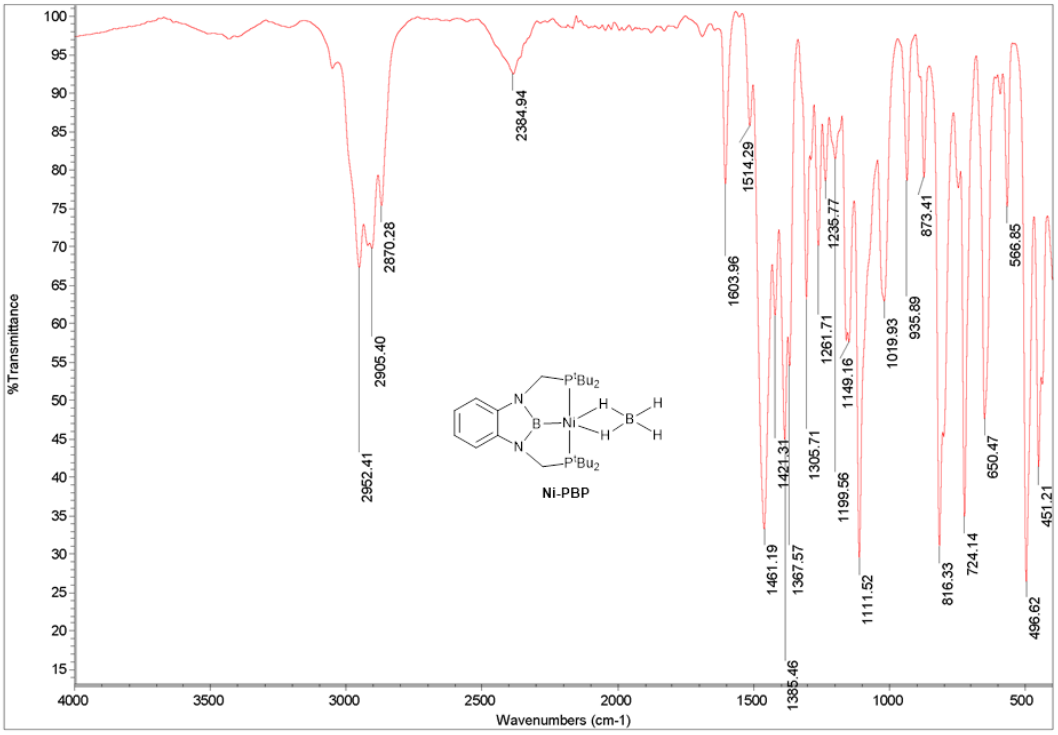


**Fig. S7** FTIR spectrum of **Ni-PBP** (KBr disc)

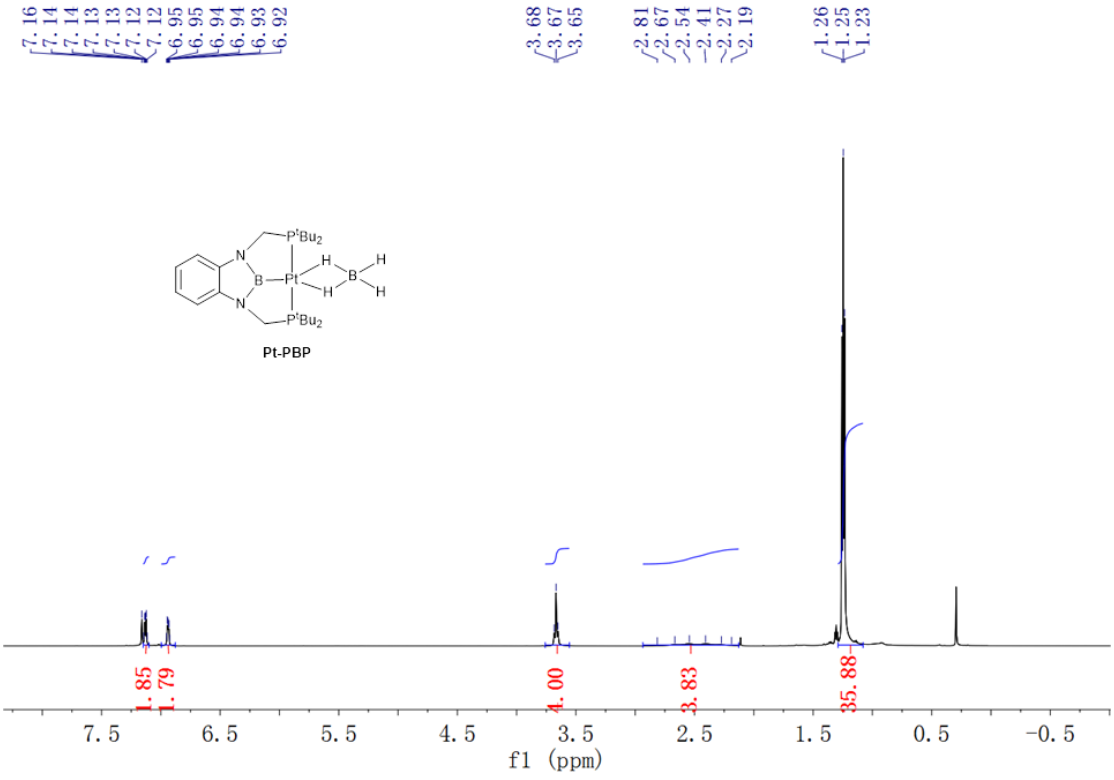


**Fig. S8** $^{1}$H NMR spectrum of **Pt-PBP** (600 MHz, $C_6D_6$)

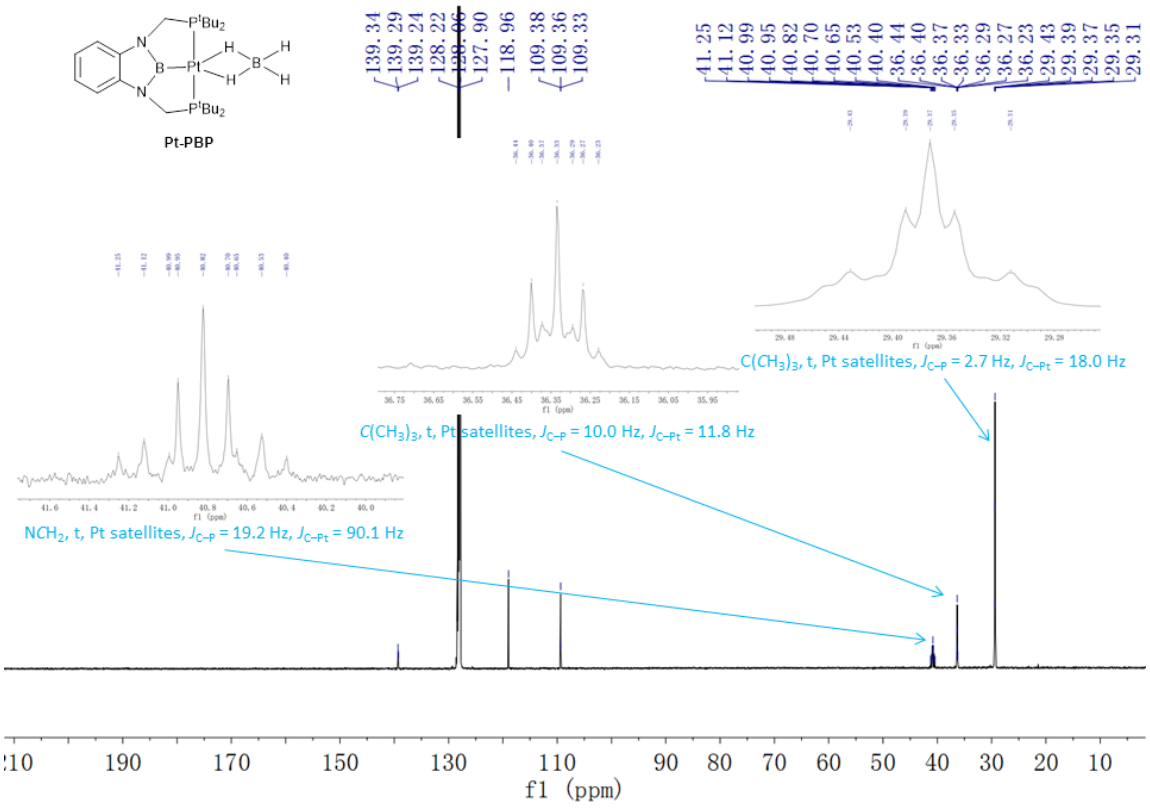


**Fig. S9** $^{13}C\{^{1}H\}$ NMR spectrum of **Pt-PBP** (151 Hz, $C_6D_6$)

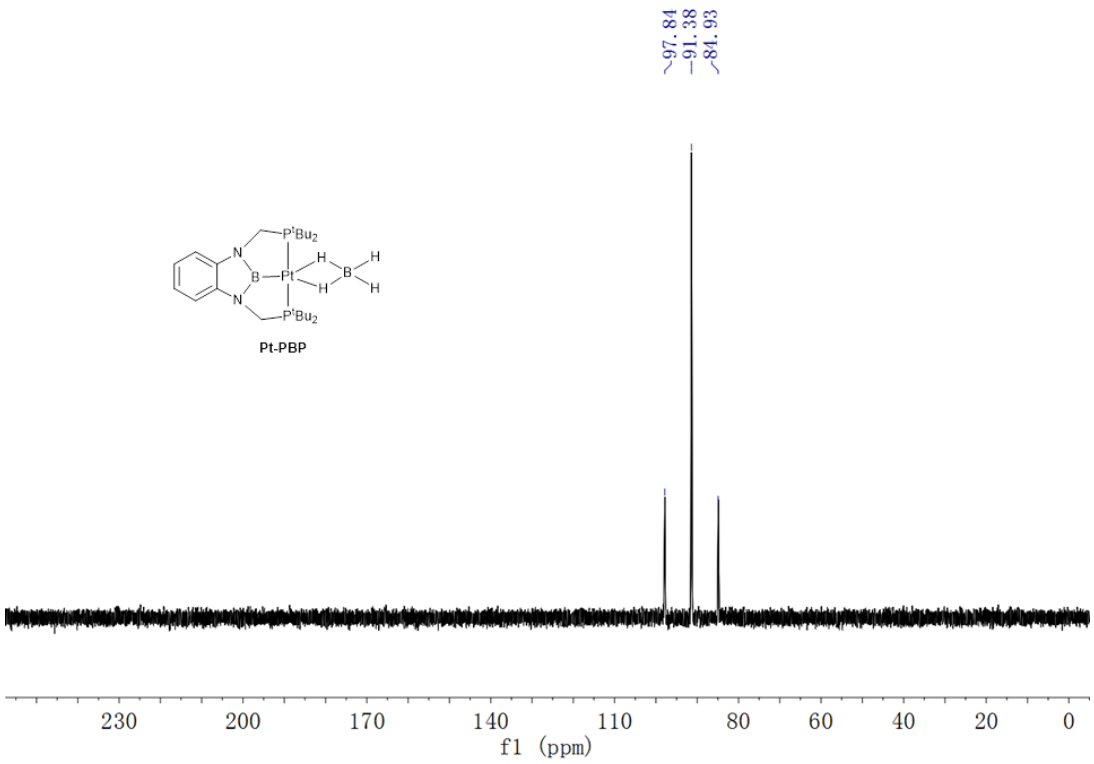


**Fig. S10** $^{31}P\{^{1}H\}$ NMR spectrum of **Pt-PBP** (243 MHz, $C_6D_6$)

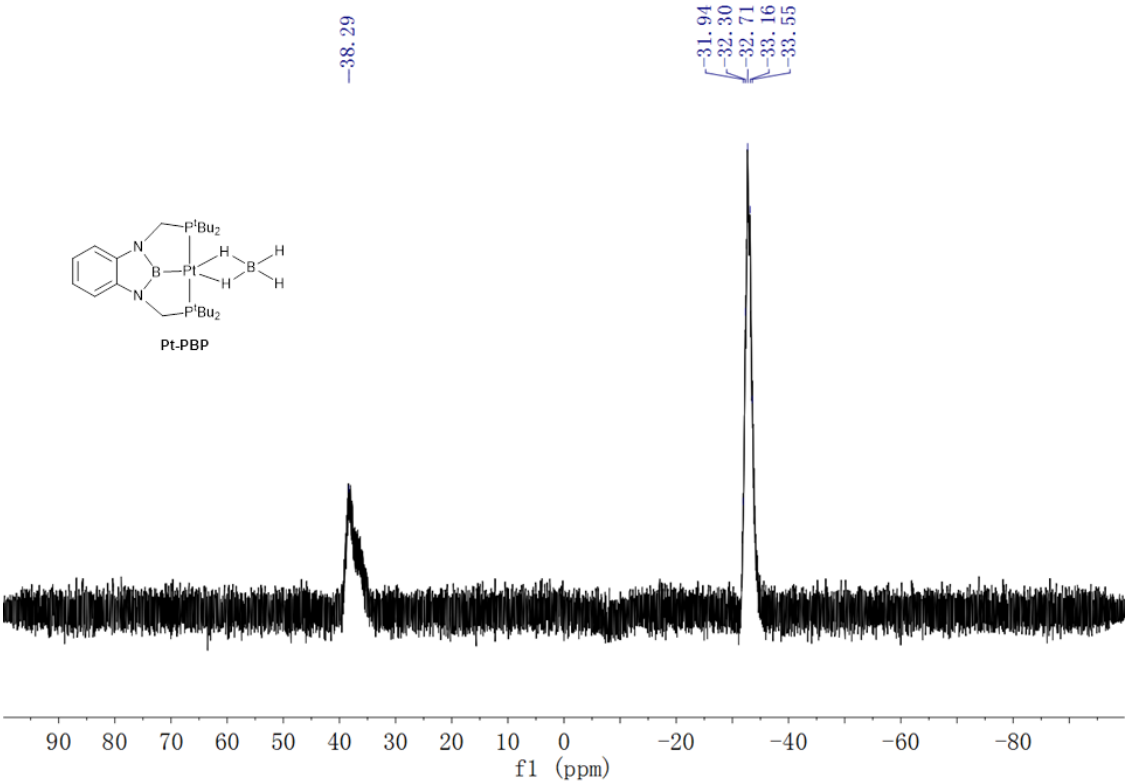


**Fig. S11** $^{11}$B NMR spectrum of **Pt-PBP** (193 MHz, $CDCl_3$)

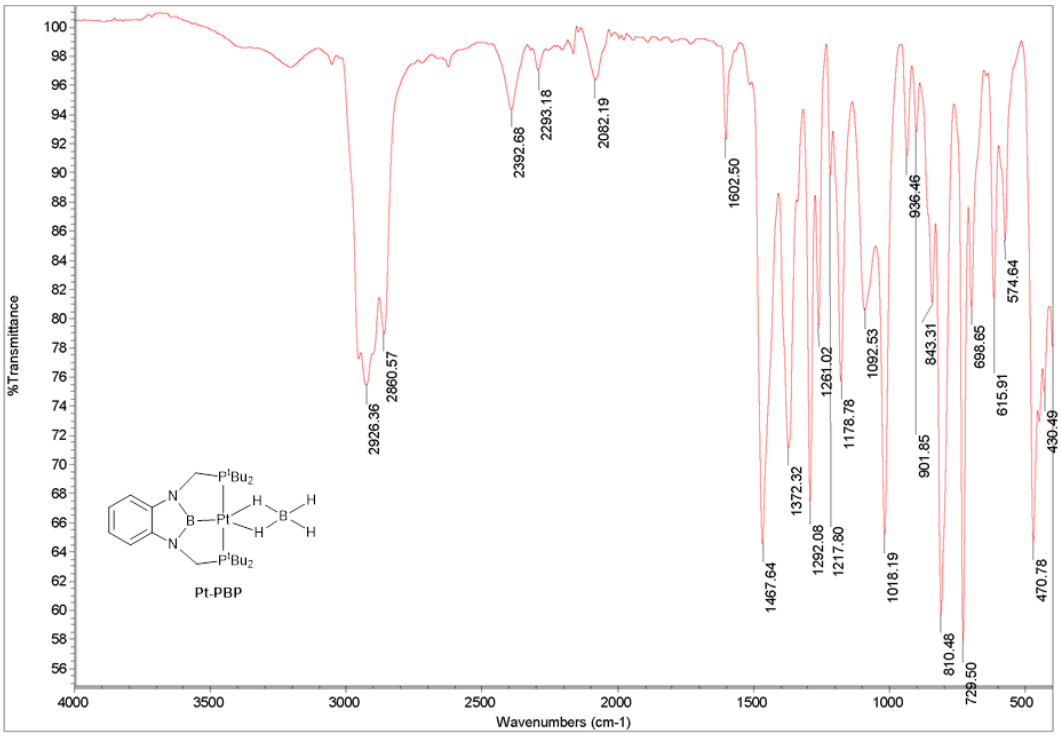


**Fig. S12** FTIR spectrum of **Pt-PBP** (KBr disc)

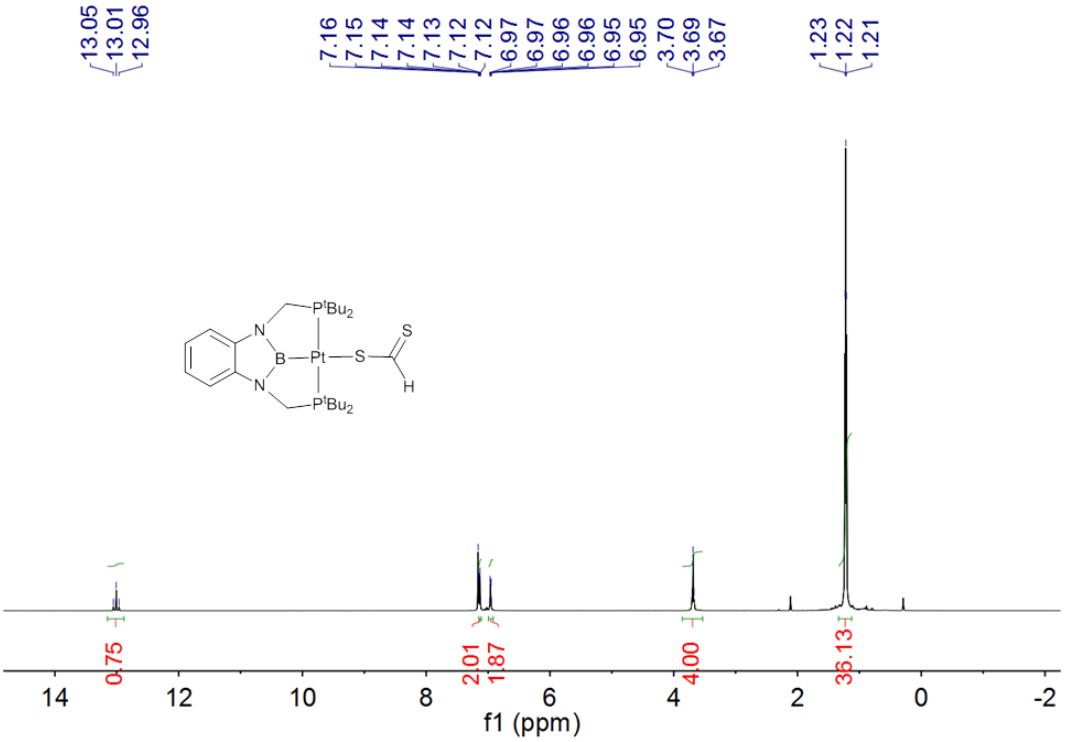


**Fig. S13** $^{1}$H NMR spectrum of **Pt-PBP'** (600 MHz, $C_6D_6$)

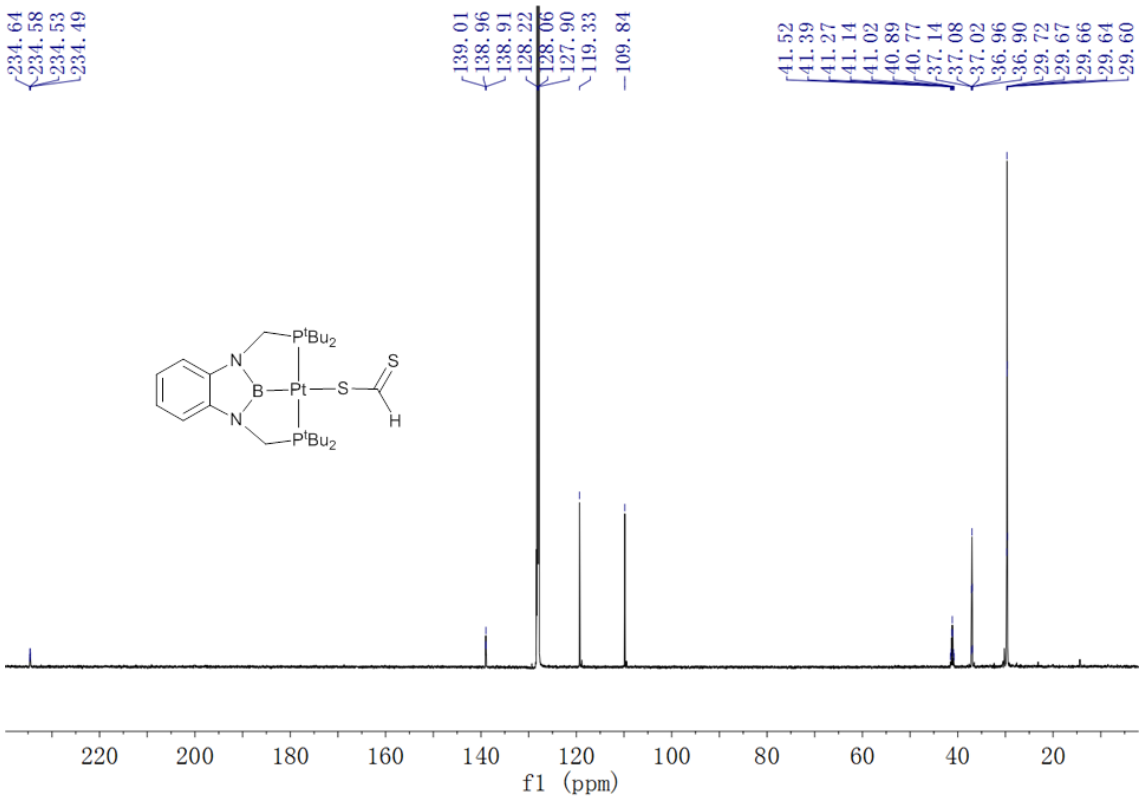


**Fig. S14** $^{13}$C{$^{1}$H} NMR spectrum of **Pt-PBP'** (151 Hz, $C_6D_6$)

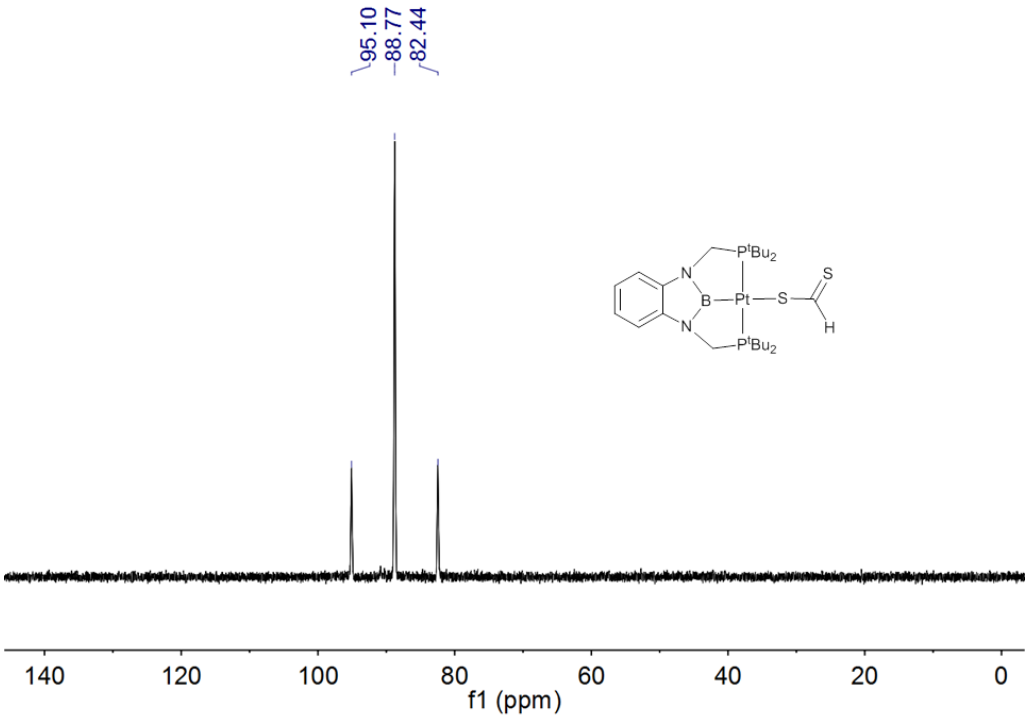


**Fig. S15** $^{31}P\{^1H\}$ NMR spectrum of **Pt-PBP'** (243 MHz, $C_6D_6$)

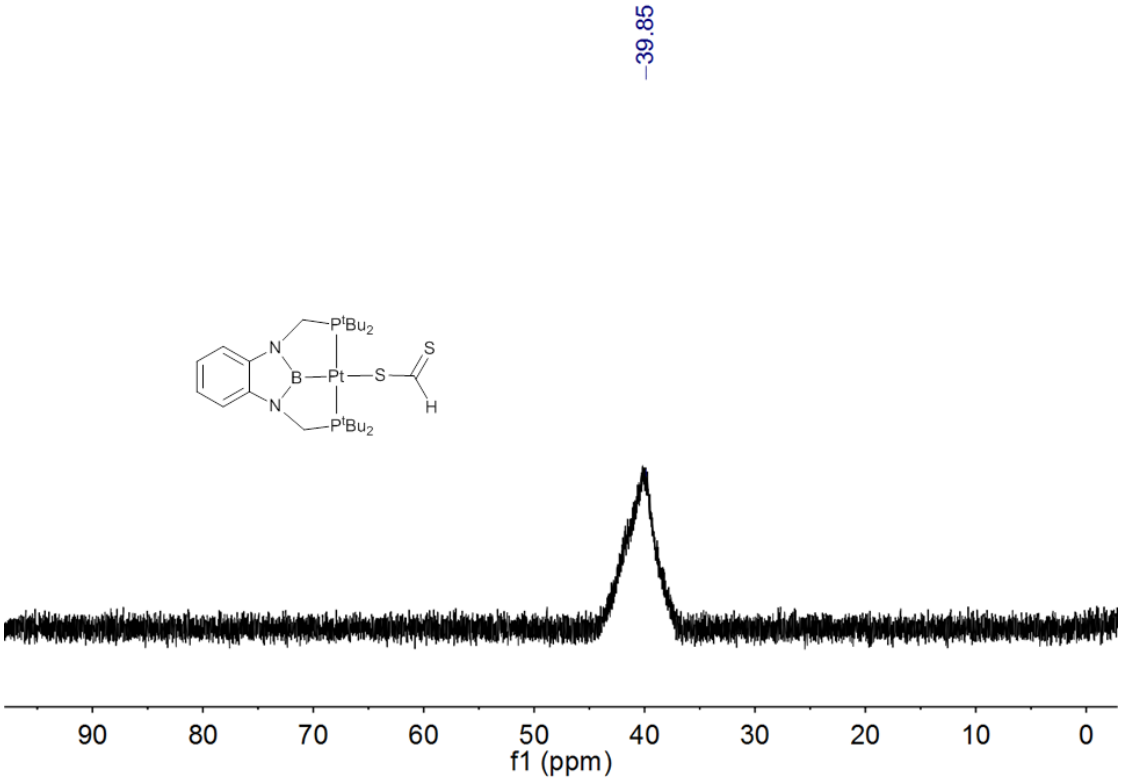


**Fig. S16** $^{11}B$ NMR spectrum of **Pt-PBP'** (193 MHz, $C_6D_6$)

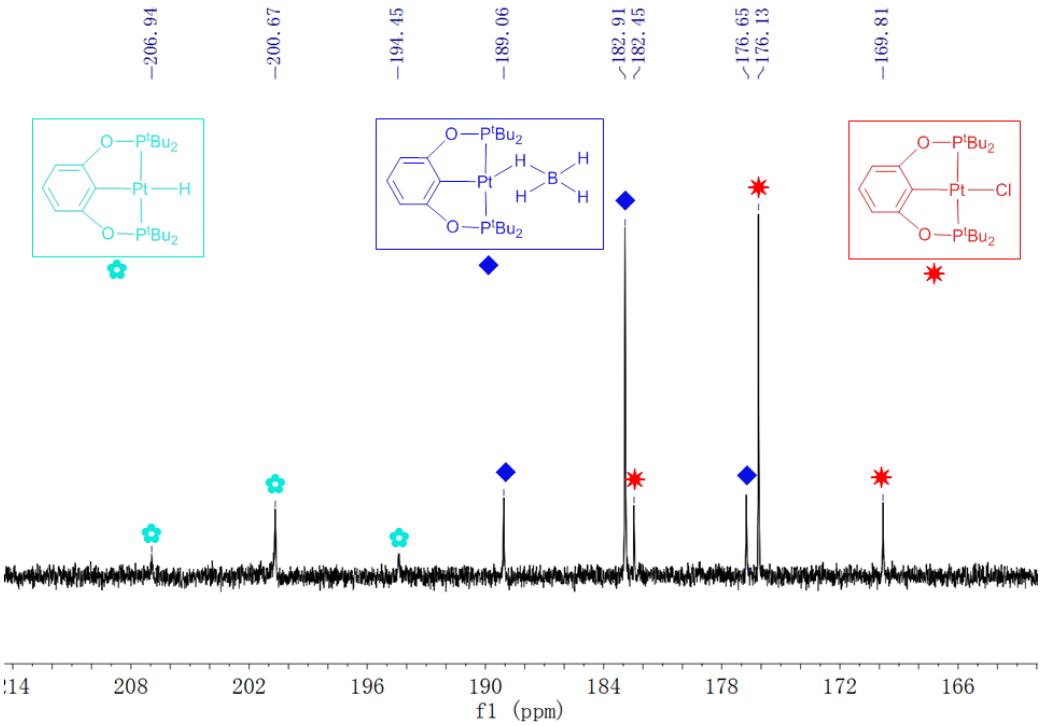


**Fig. S17** $^{31}P\{^{1}H\}$ NMR spectrum of the reaction of [2,6-($^{t}Bu_2PO)_2C_6H_3$]PtCl with $BH_3$·THF (243 MHz, THF with THF-$d_8$). Spectrum recorded 5 min after adding $BH_3$·THF to the solution of the chloride complex at room temperature.

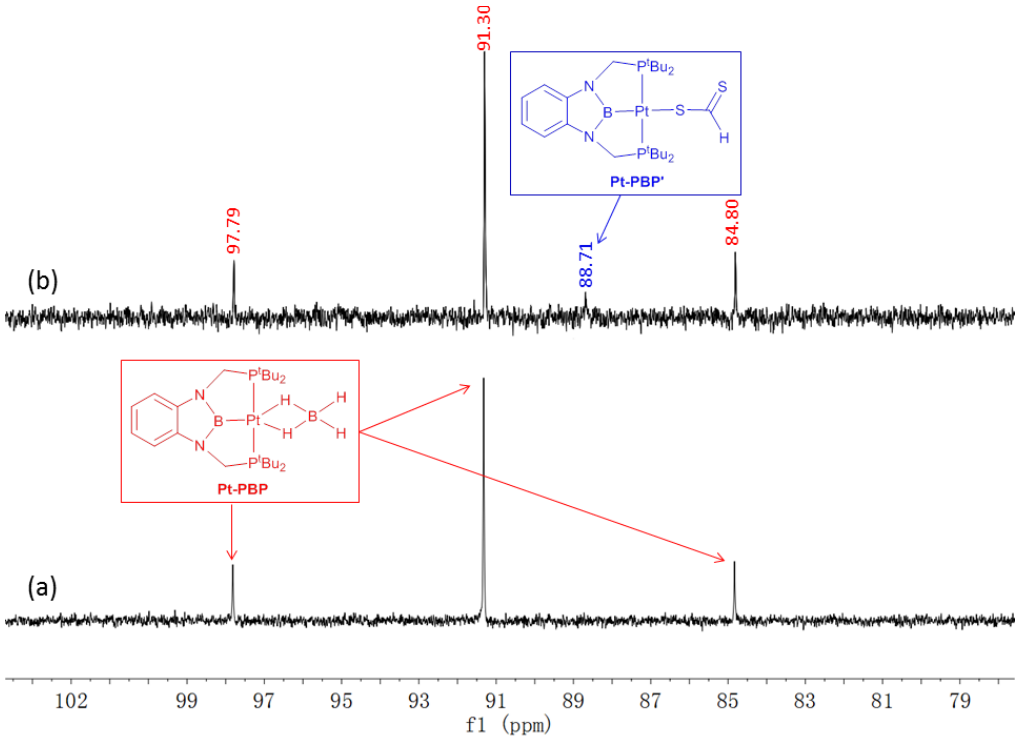


**Fig. S18** $^{31}P\{^{1}H\}$ NMR spectrum of the interaction of **Pt-PBP** with $CS_2$ (243 MHz, THF-$d_8$).
(a) Spectrum recorded immediately after **Pt-PBP** was mixed with 10 equiv. of $CS_2$ in THF-$d_8$.
(b) Spectrum recorded after the NMR tube was heated at 50˚C for 12 h.

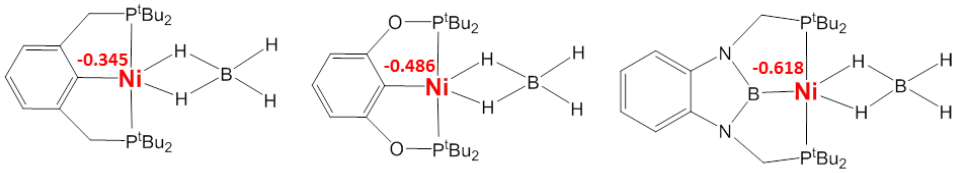


**Fig. S19** NPA charges of the nickel centers in different nickel complexes