

Electronic Supplementary Information for:

**Reaction of [2,6-(^tBu₂PO)₂C₆H₃]NiSCH₂Ph with BH₃·THF: borane mediated C–S
bond cleavage**

Jie Zhang,* Ting Liu, Qiang-Qiang Ma, Shujun Li and Xuenian Chen*

*School of Chemistry and Chemical Engineering, Henan Key Laboratory of Boron Chemistry and
Advanced Energy Materials, Henan Normal University, Xinxiang, Henan 453007, China*

E-mails: jie.zhang@htu.edu.cn (J.Z.); xnchen@htu.edu.cn (X.C.)

Fig. S1-S4: ¹ H, ¹³ C{ ¹ H} and ³¹ P{ ¹ H} NMR spectra of complex 5	1-2
Fig. S5-S6: ¹ H NMR spectra of the NMR tube reaction of 1 with 2 equiv. of BH ₃ ·THF.....	3
Fig. S7: ³¹ P{ ¹ H} NMR spectra of the reaction of 1 with 2 equiv. of BH ₃ ·THF.....	4
Fig. S8-S9: ³¹ P{ ¹ H} NMR spectra of the reaction of 1 with 1 equiv. of BH ₃ ·THF.....	4-5
Fig. S10-S12: ¹ H, ¹³ C{ ¹ H} and ¹¹ B NMR spectra of compound 7	5-6
Fig. S13: IR spectra of complex 5	7

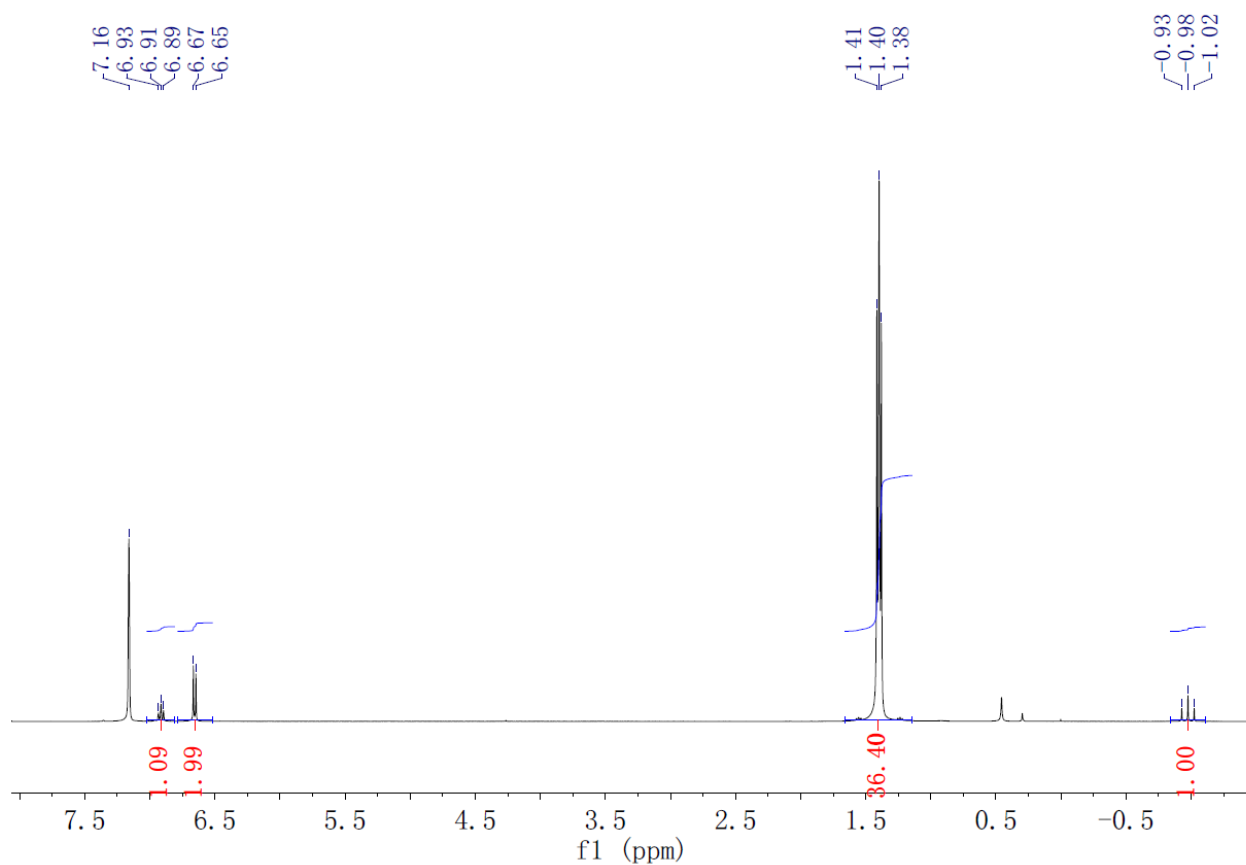


Fig. S1 ¹H NMR spectrum of complex **5** (400 MHz, benzene-*d*₆)

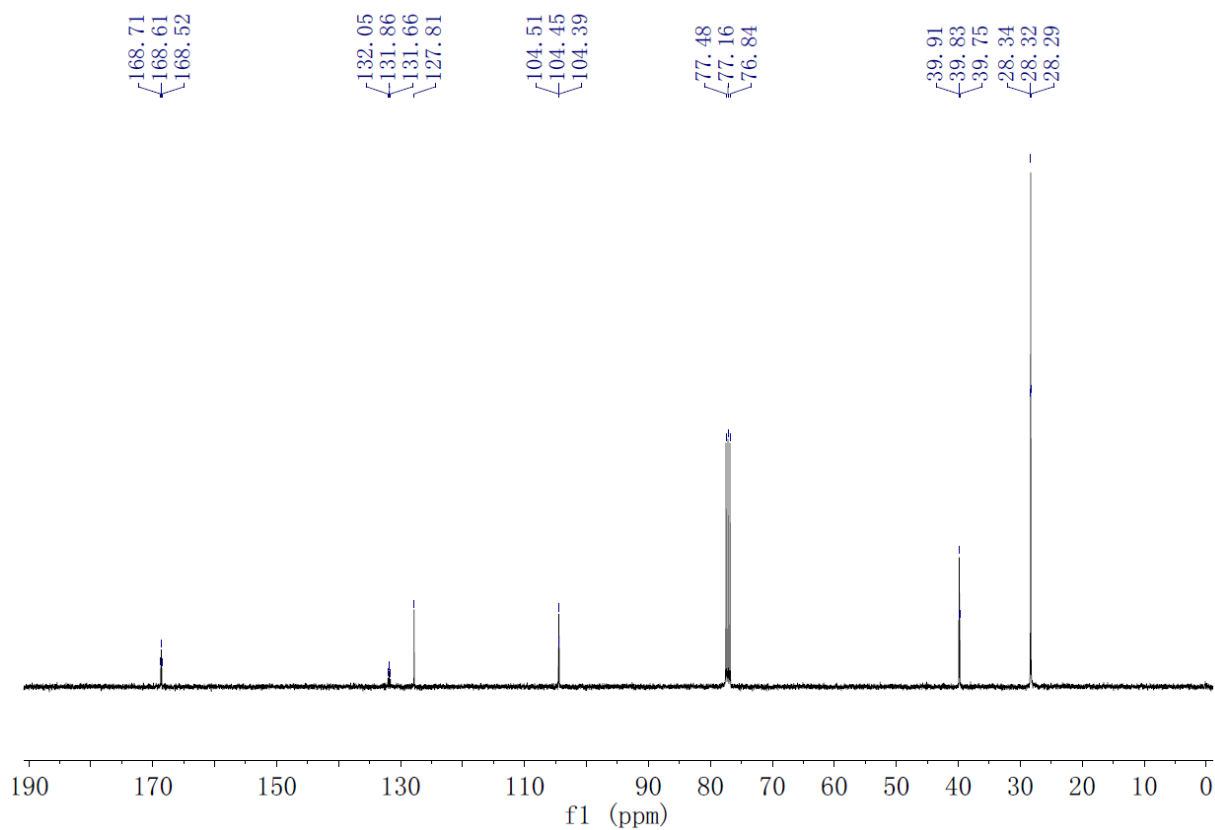


Fig. S2 ¹³C{¹H} NMR spectrum of complex **5** (101 MHz, CDCl₃)

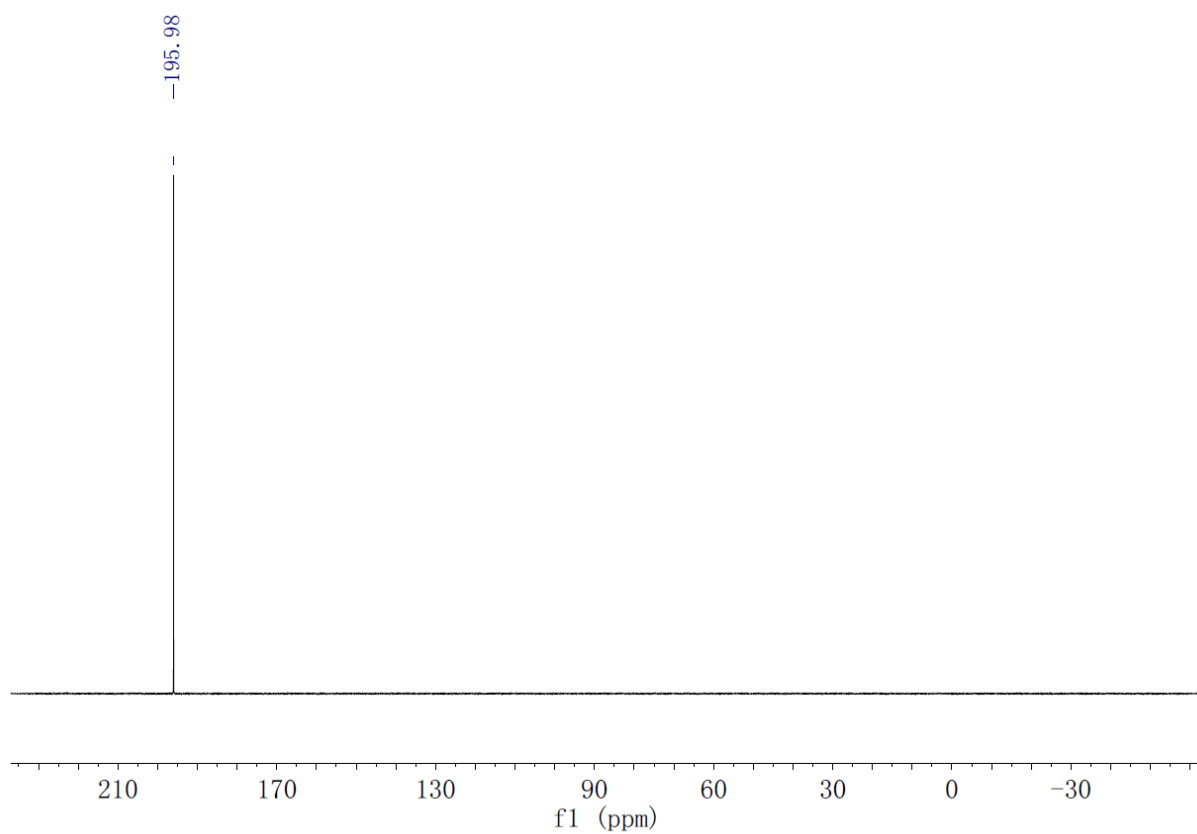


Fig. S3 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex **5** (162 MHz, benzene- d_6)

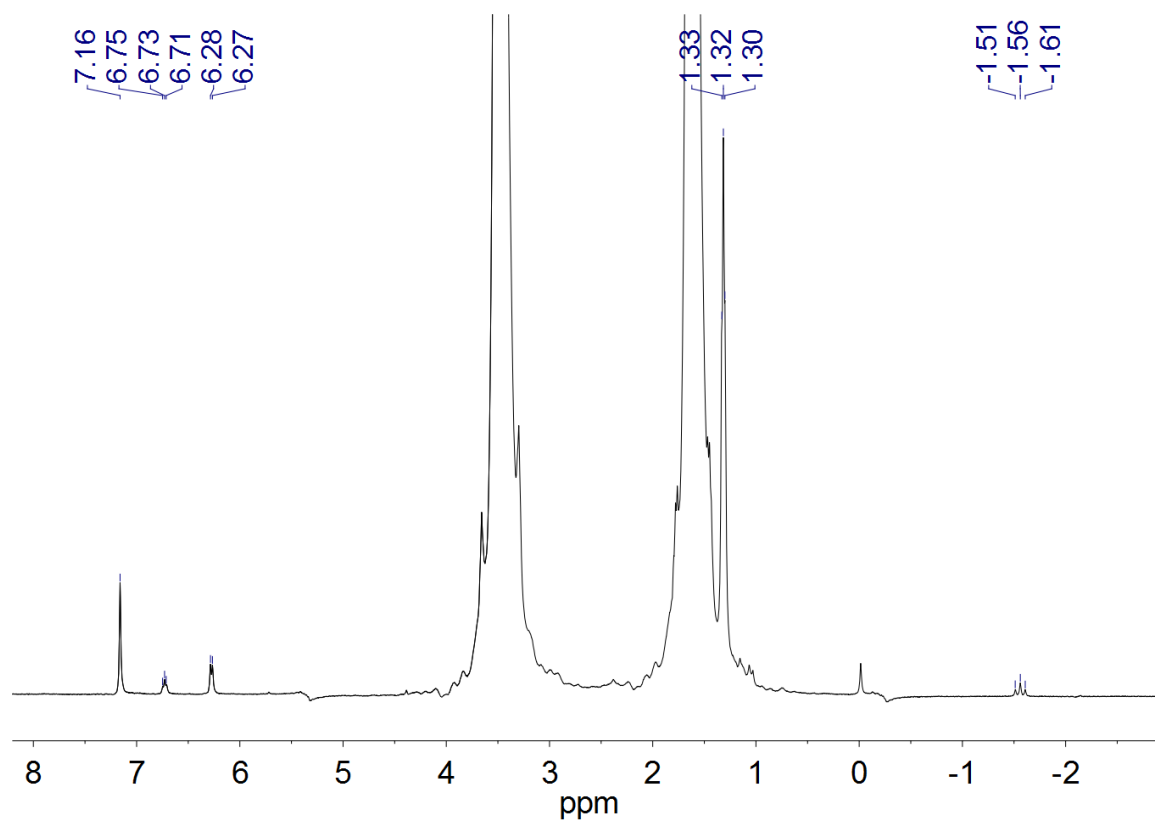


Fig. S4 ^1H NMR spectrum of complex **5** (400 MHz, THF/benzene- d_6 (1:1))

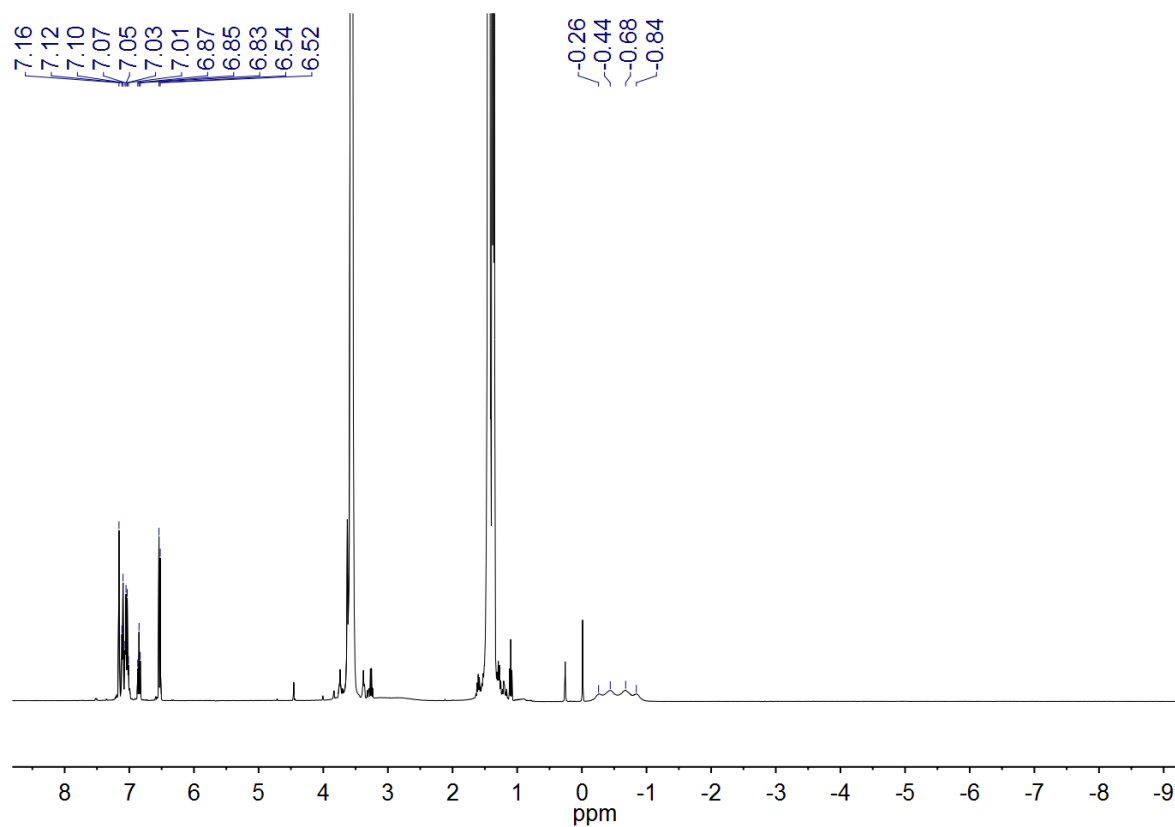


Fig. S5 ^1H NMR spectrum of the NMR tube reaction of **1** with 2 equiv. of $\text{BH}_3 \cdot \text{THF}$ recorded 1 h after mixing the two reactants (400 MHz, $\text{THF}/\text{benzene-}d_6$ (1:1))

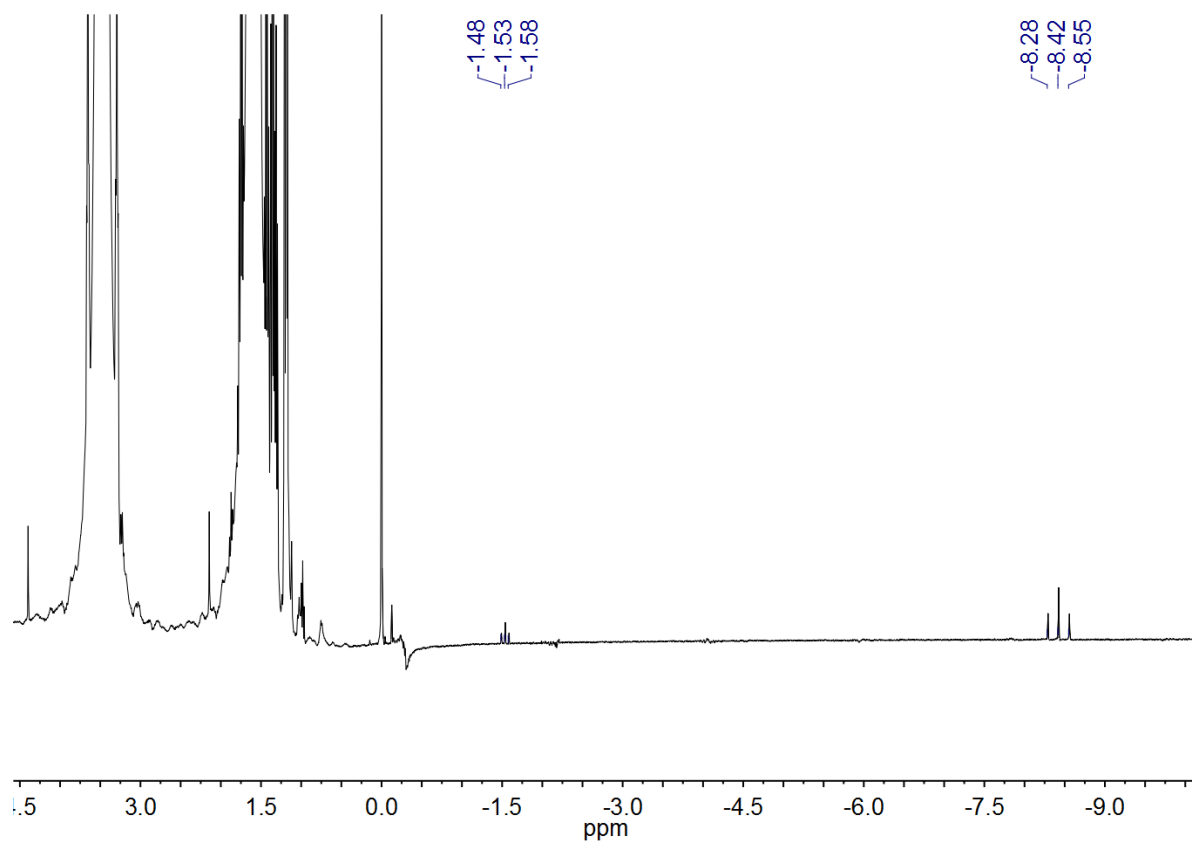


Fig. S6 ^1H NMR spectrum of the NMR tube reaction of **1** with 2 equiv. of $\text{BH}_3 \cdot \text{THF}$ recorded 72 h after mixing the two reactants (400 MHz, $\text{THF}/\text{benzene-}d_6$ (1:1))

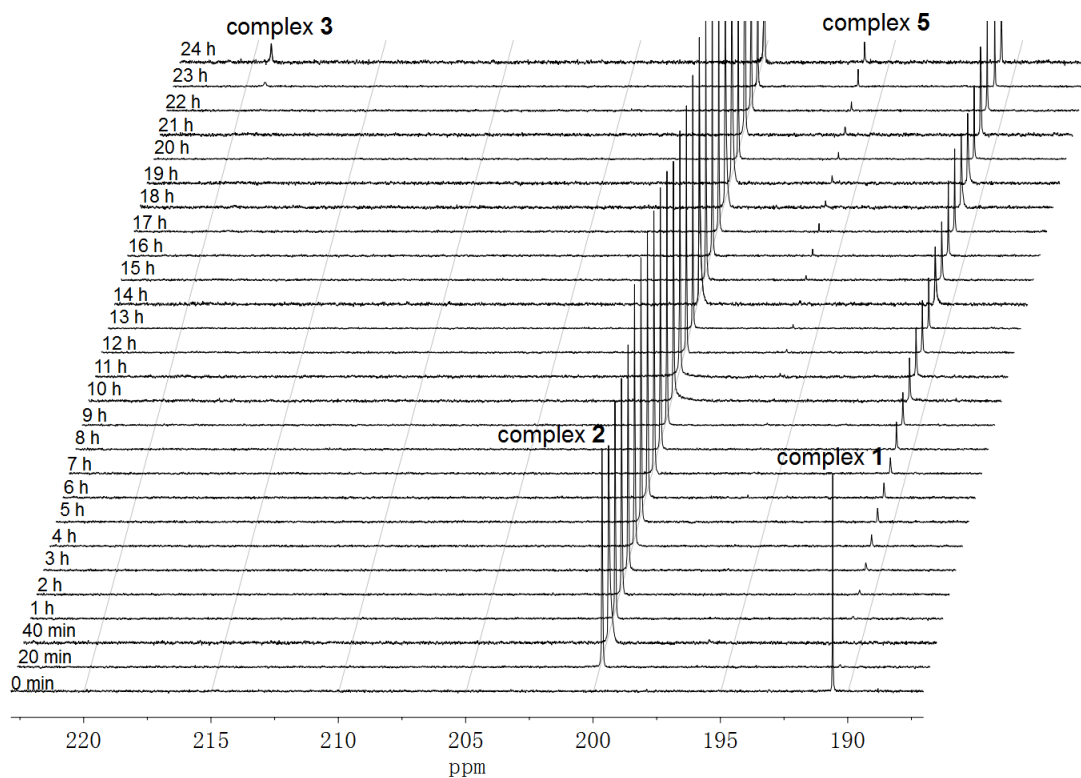


Fig. S7 $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of the reaction of **1** with 2 equiv. of $\text{BH}_3 \cdot \text{THF}$ in $\text{THF}/\text{benzene-}d_6$ (1:1) at room temperature.

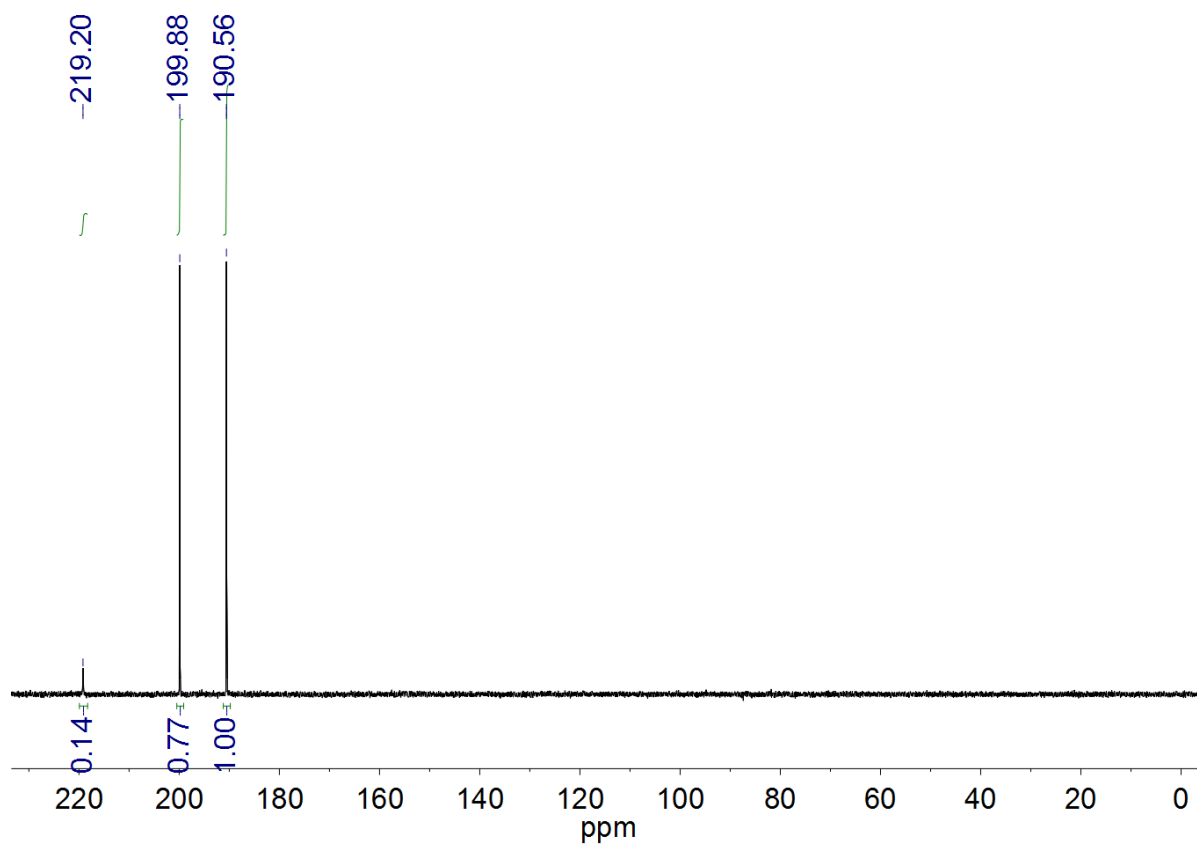


Fig. S8 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of the reaction of **1** with 1 equiv. of $\text{BH}_3 \cdot \text{THF}$ recorded 10 min after mixing the two reactants (room temperature, $\text{THF}/\text{benzene-}d_6$ (1:1)).

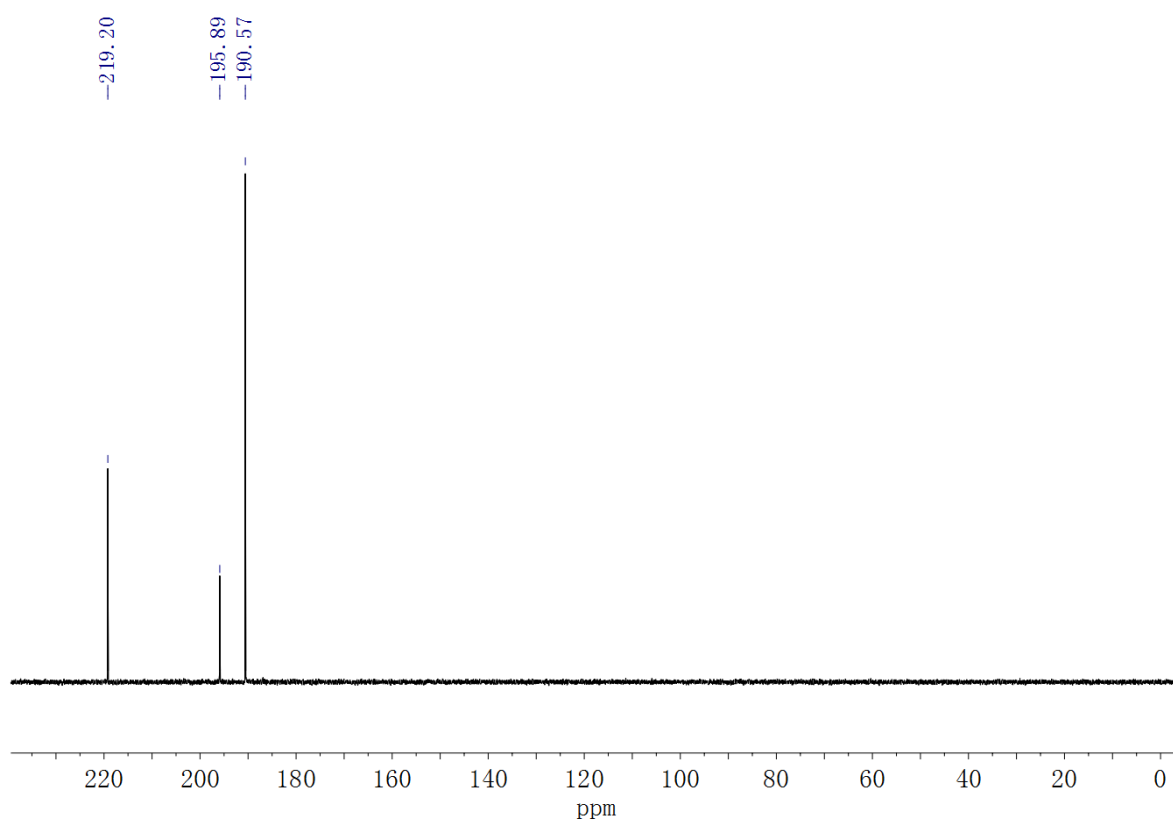


Fig. S9 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of the reaction of **1** with 1 equiv. of $\text{BH}_3 \cdot \text{THF}$ recorded 76 h after mixing the two reactants (room temperature, $\text{THF}/\text{benzene-}d_6$ (1:1)).

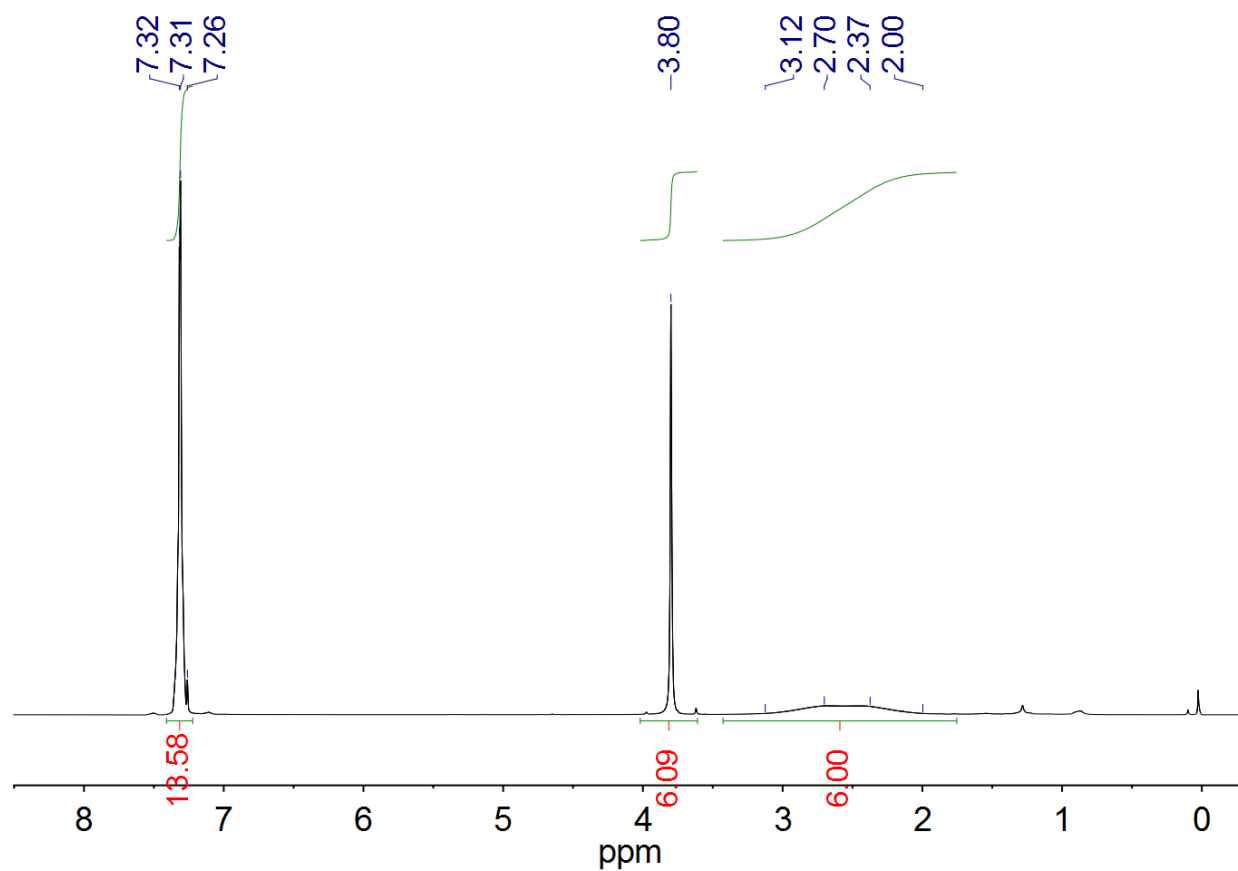


Fig. S10 ^1H NMR spectrum of compound **7** (400 MHz, CDCl_3)

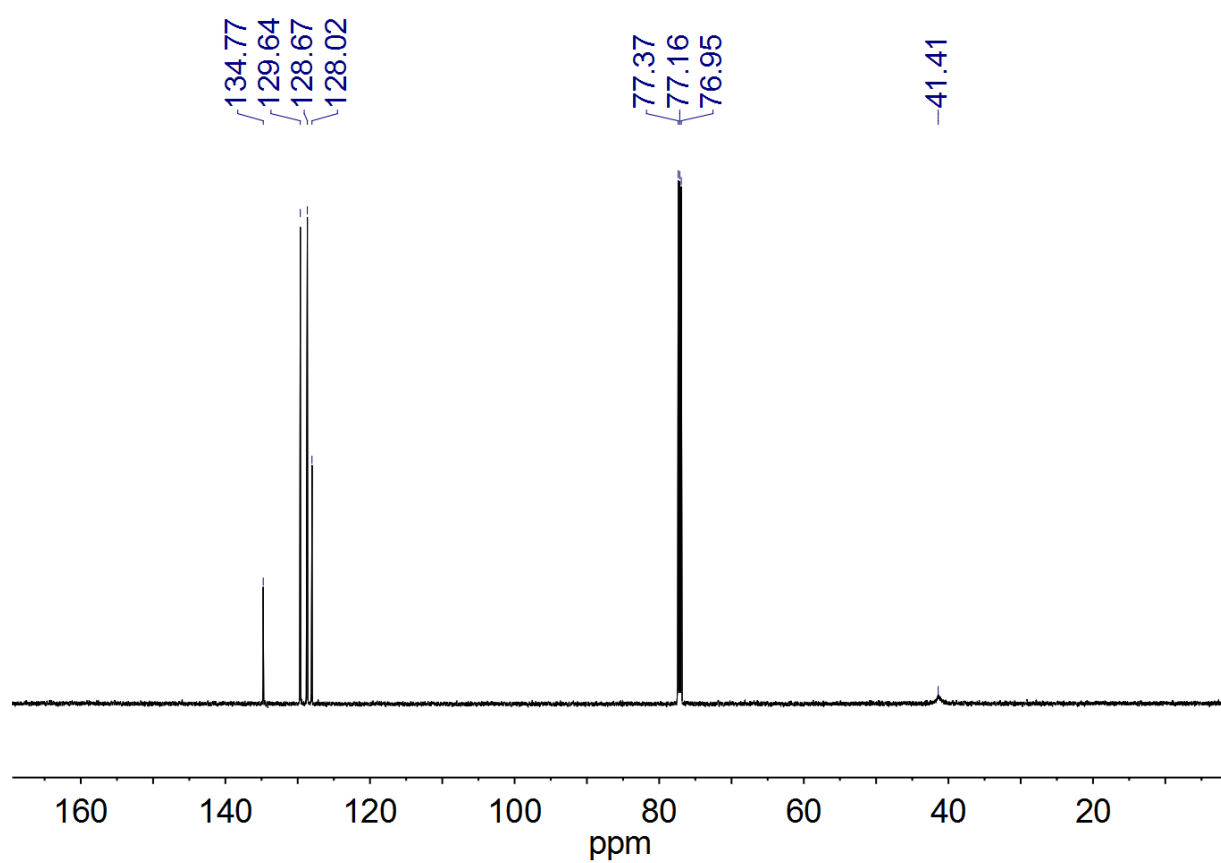


Fig. S11 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **7** (101 MHz, CDCl_3)

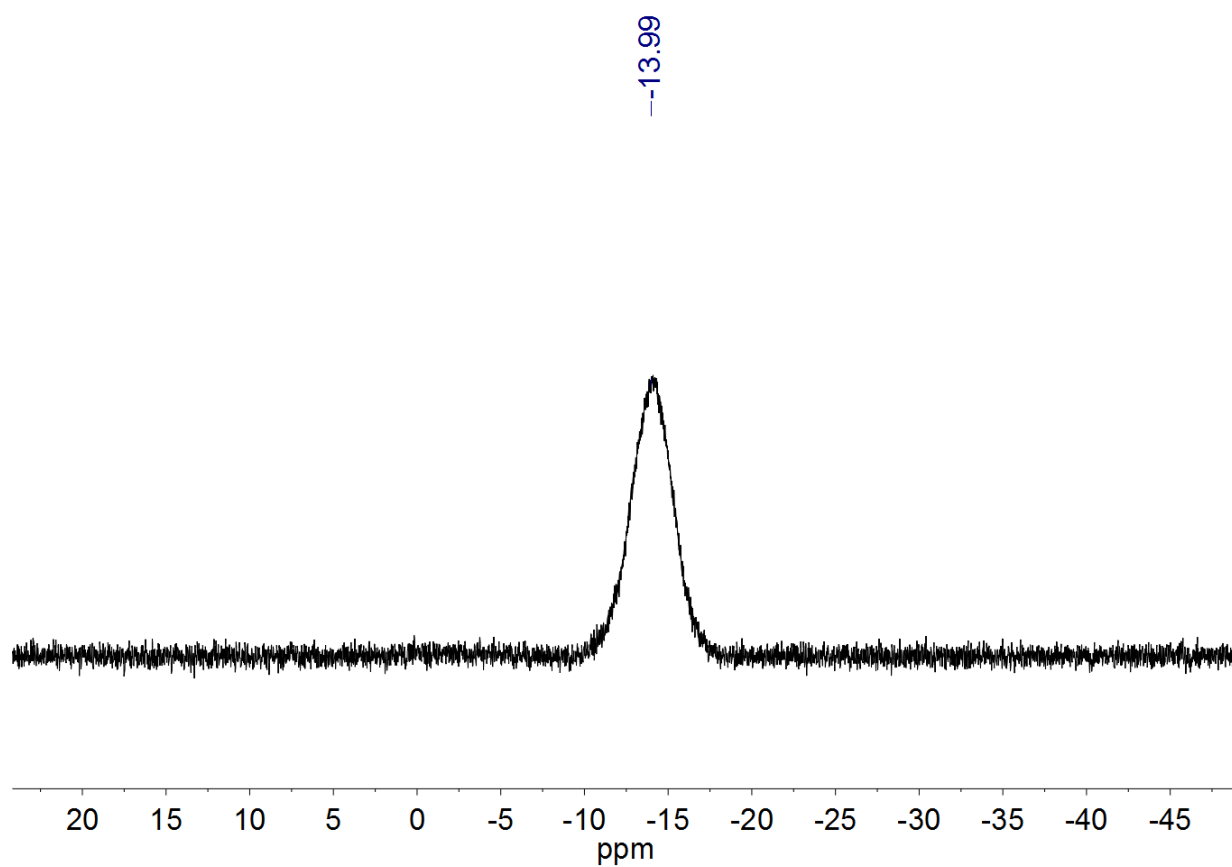


Fig. S12 ^{11}B NMR spectrum of compound **7** (128 MHz, CDCl_3)

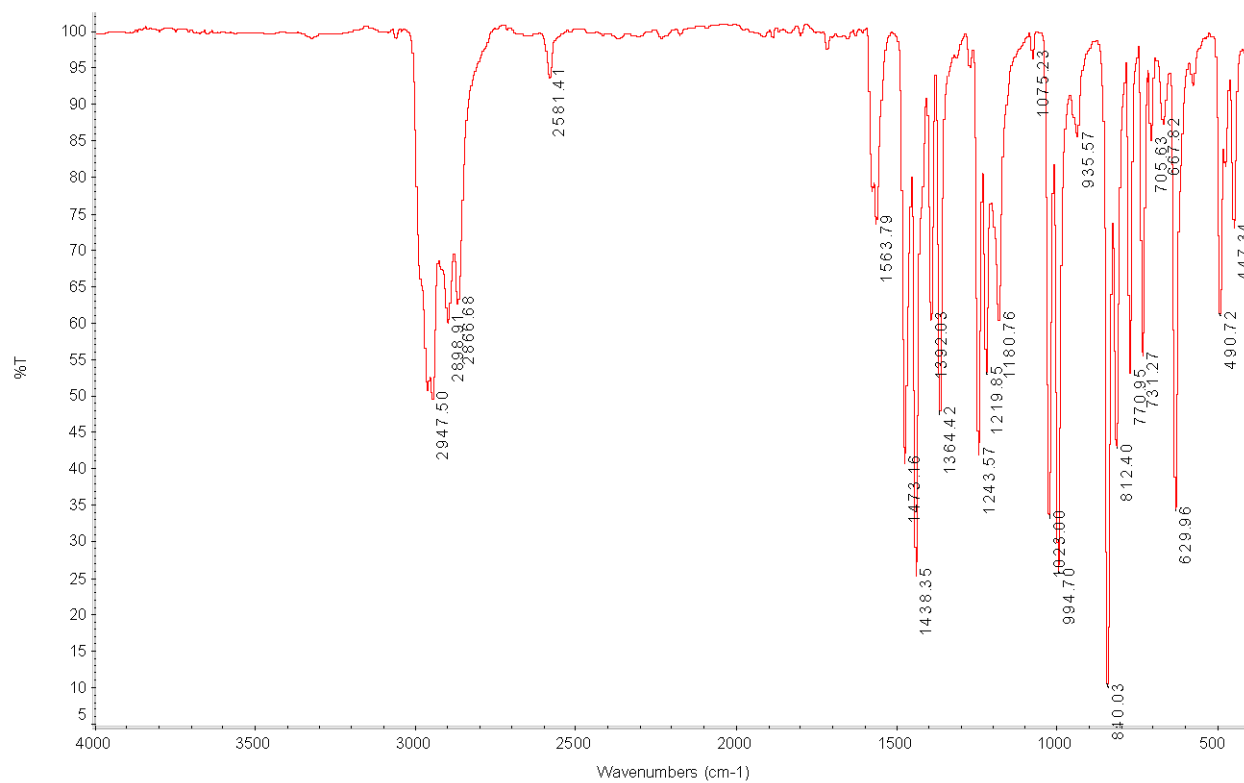


Fig. S13 FTIR spectra of complex **5** (KBr disc)