

Supporting Information for:

**Synthesis, Structures and Ethylene Dimerization Reactivity of Palladium Alkyl
Complexes that Contain a Chelating Phosphine-Trifluoroborate Ligand**

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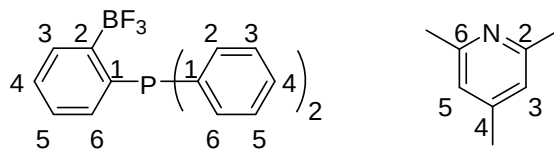


Figure S1. Numbering scheme used for NMR labeling.

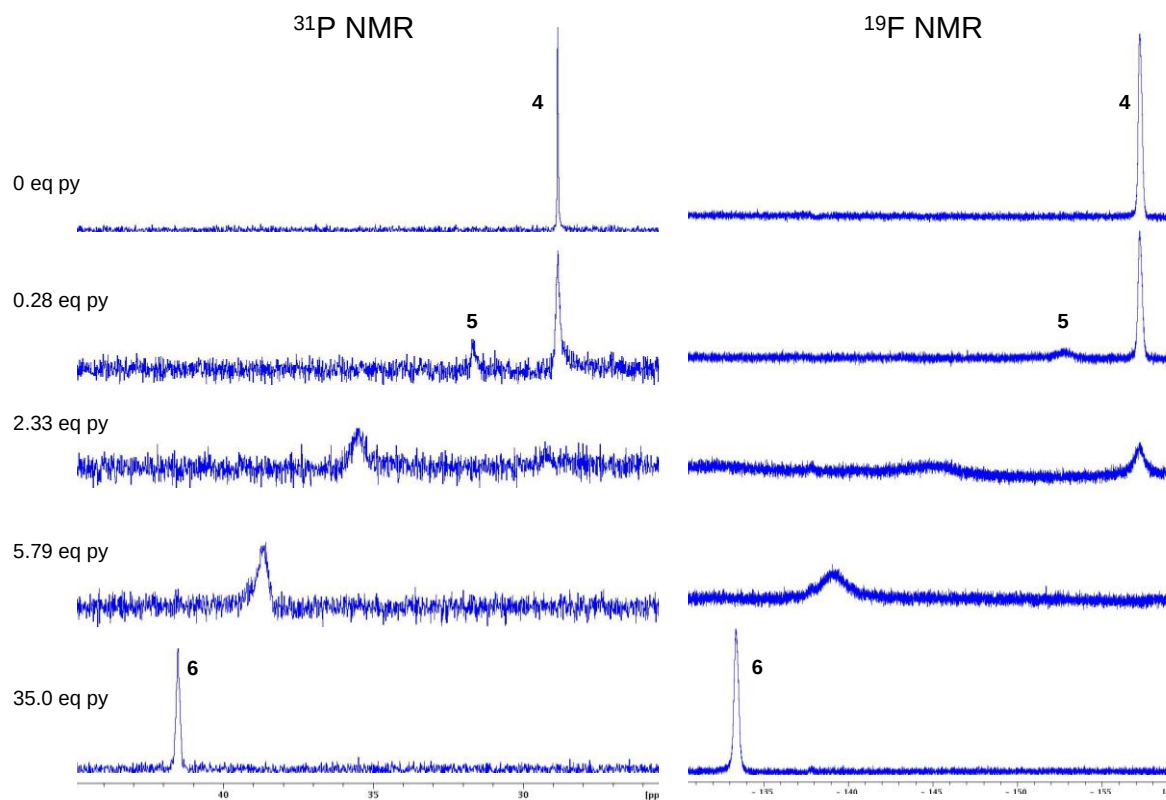


Figure S2. $^{31}\text{P}\{^1\text{H}\}$ and $^{19}\text{F}\{^1\text{H}\}$ NMR spectra of **4** in the presence of varying amounts of pyridine (CD_2Cl_2 , 23 $^\circ\text{C}$).

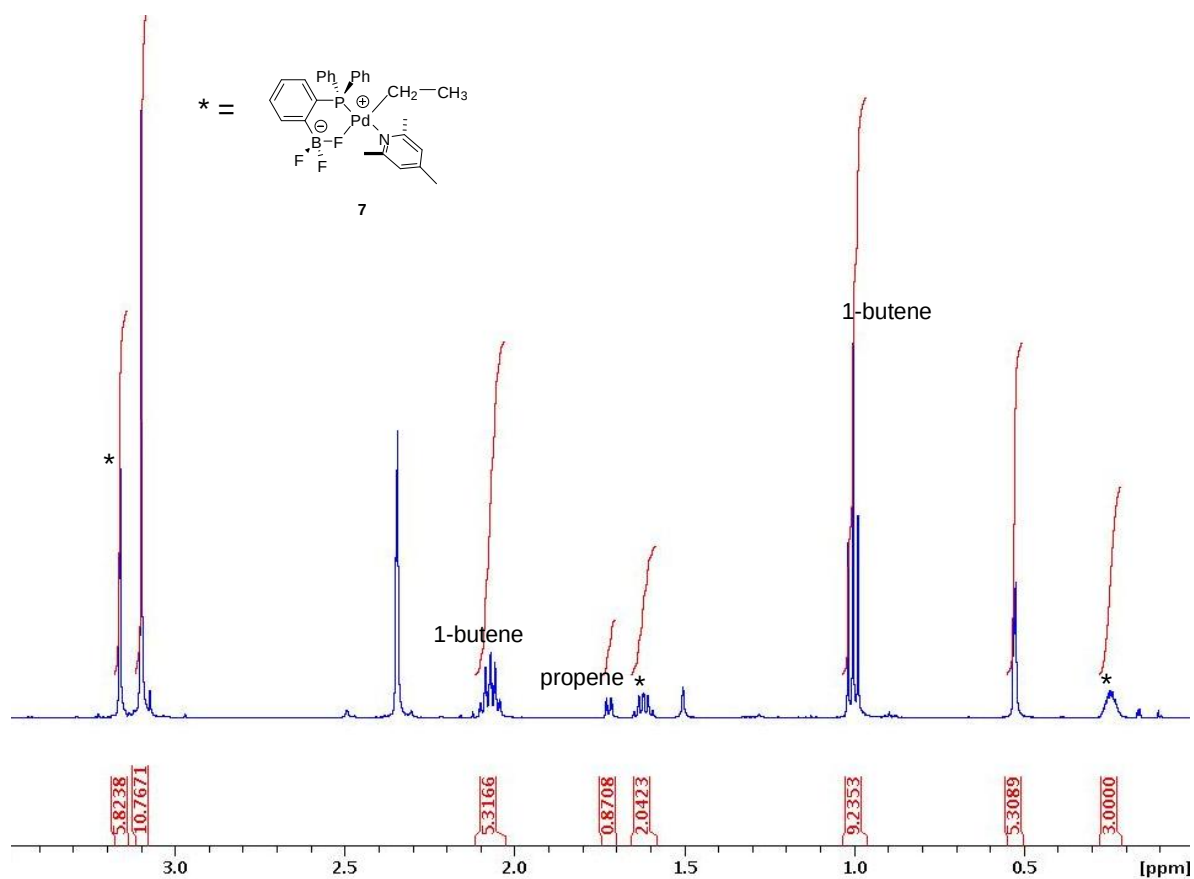


Figure S3. ^1H NMR spectrum of **4** in CD_2Cl_2 in the presence of ethylene (150 psi) at 23 °C for 3 h. Resonances for **4**: δ 3.10 (s, 3H, *o*-col- CH_3), 2.35 (s, 3H, *p*-col- CH_3), 0.53 (d, $J_{\text{H-P}}=2$, 3H, PdCH_3)

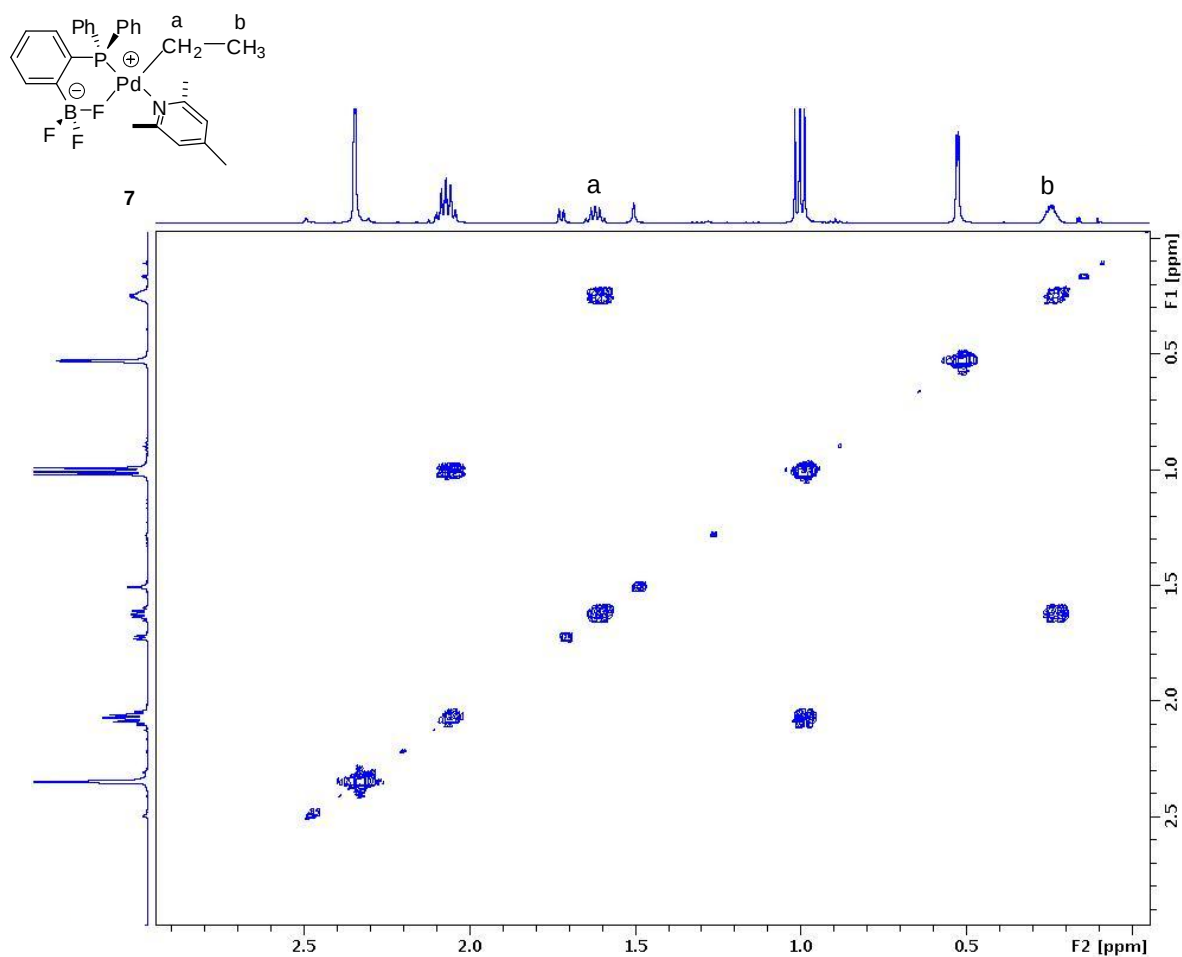


Figure S4. COSY-NMR of **7** in CD₂Cl₂ at 23 °C.

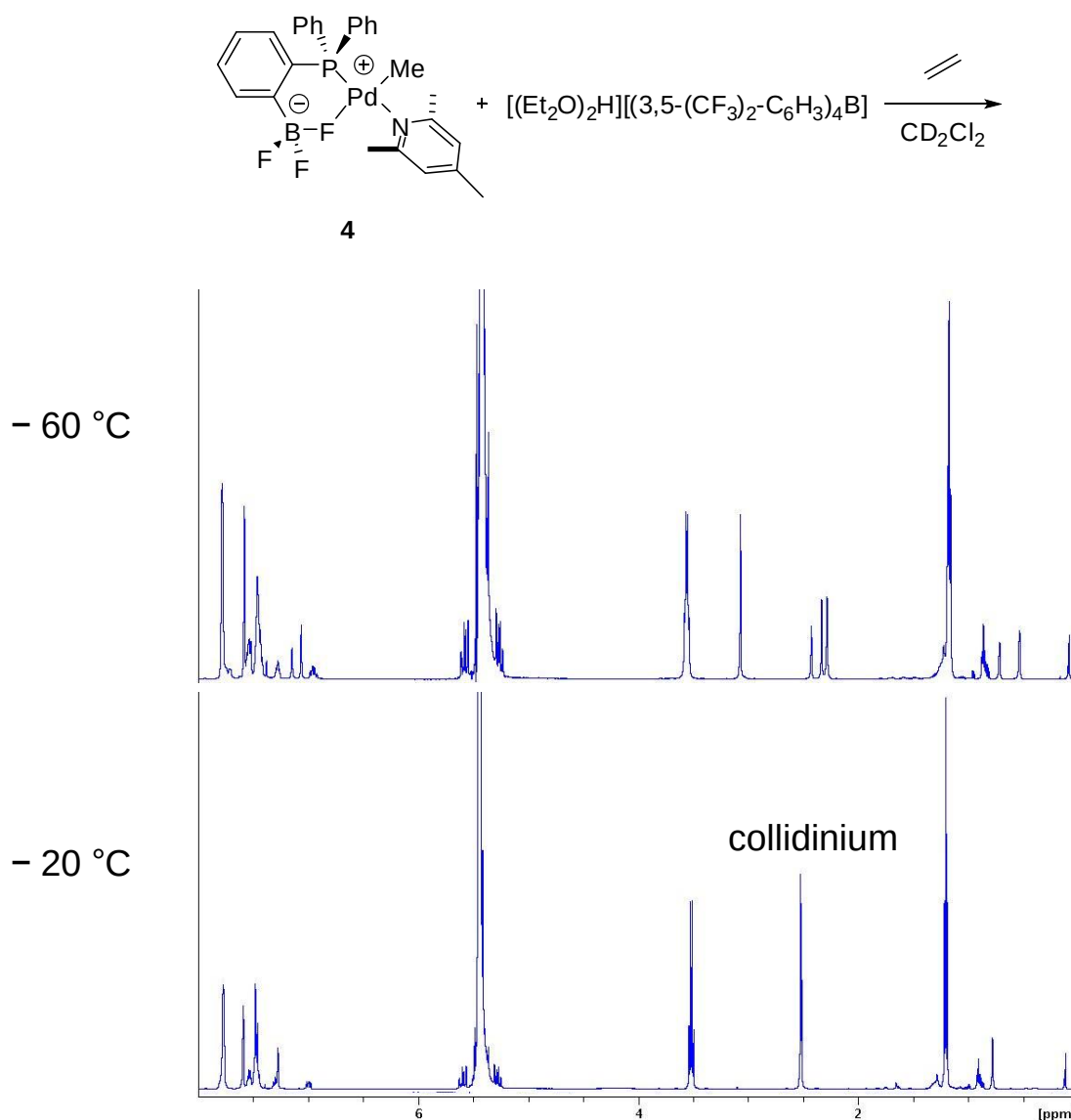


Figure S5. ^1H NMR spectra of **4** in the presence 1 equiv of $[\text{H}(\text{OEt}_2)_2][\text{B}(3,5\text{-(CF}_3)_2\text{-C}_6\text{H}_3)_4]$ and ethylene in CD_2Cl_2 at $-60\text{ }^\circ\text{C}$ and then warmed to $-20\text{ }^\circ\text{C}$ showing the formation of $[\text{collidinium}][\text{B}(3,5\text{-(CF}_3)_2\text{-C}_6\text{H}_3)_4]$ and $(\text{PF})\text{PdMe}(\text{ethylene})$.

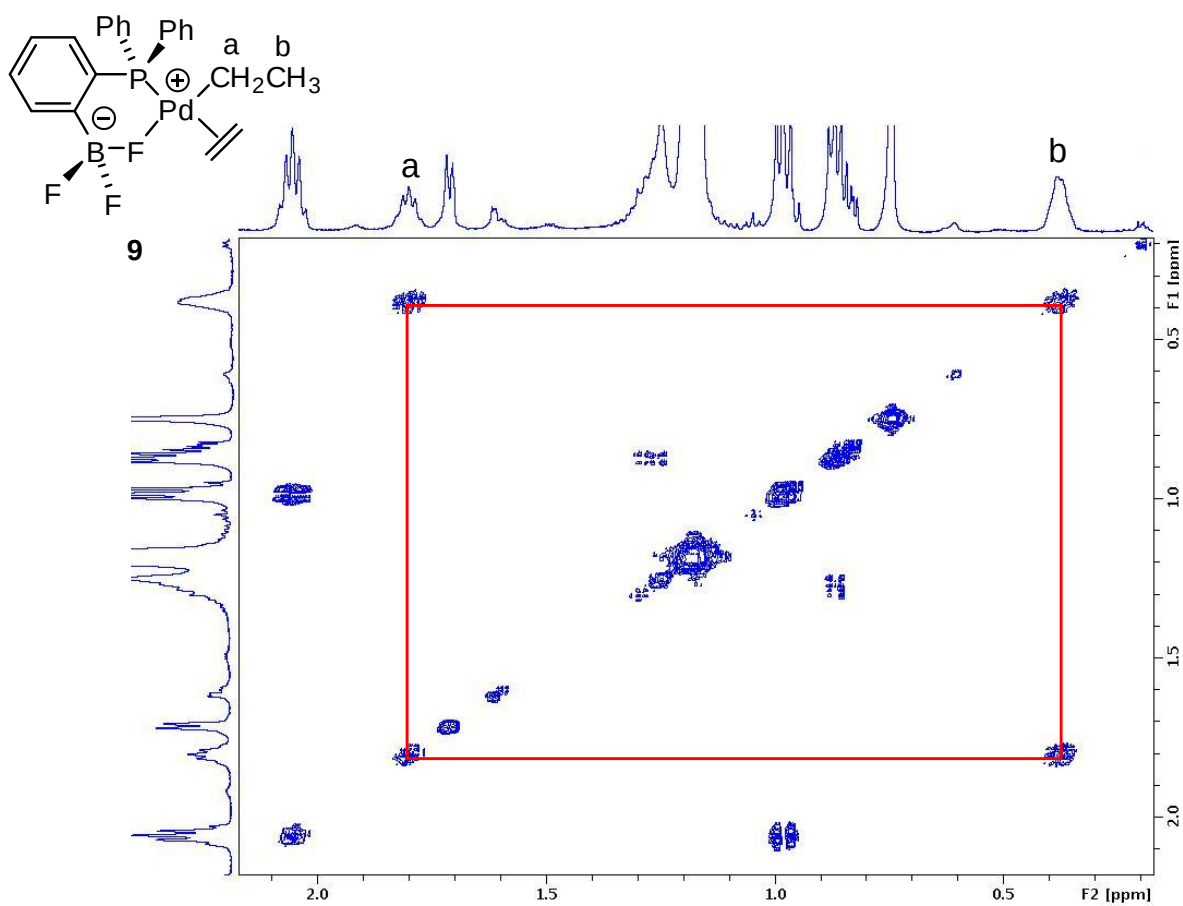


Figure S7. COSY-NMR of **9** in CD₂Cl₂ at -10 °C for 30 min.

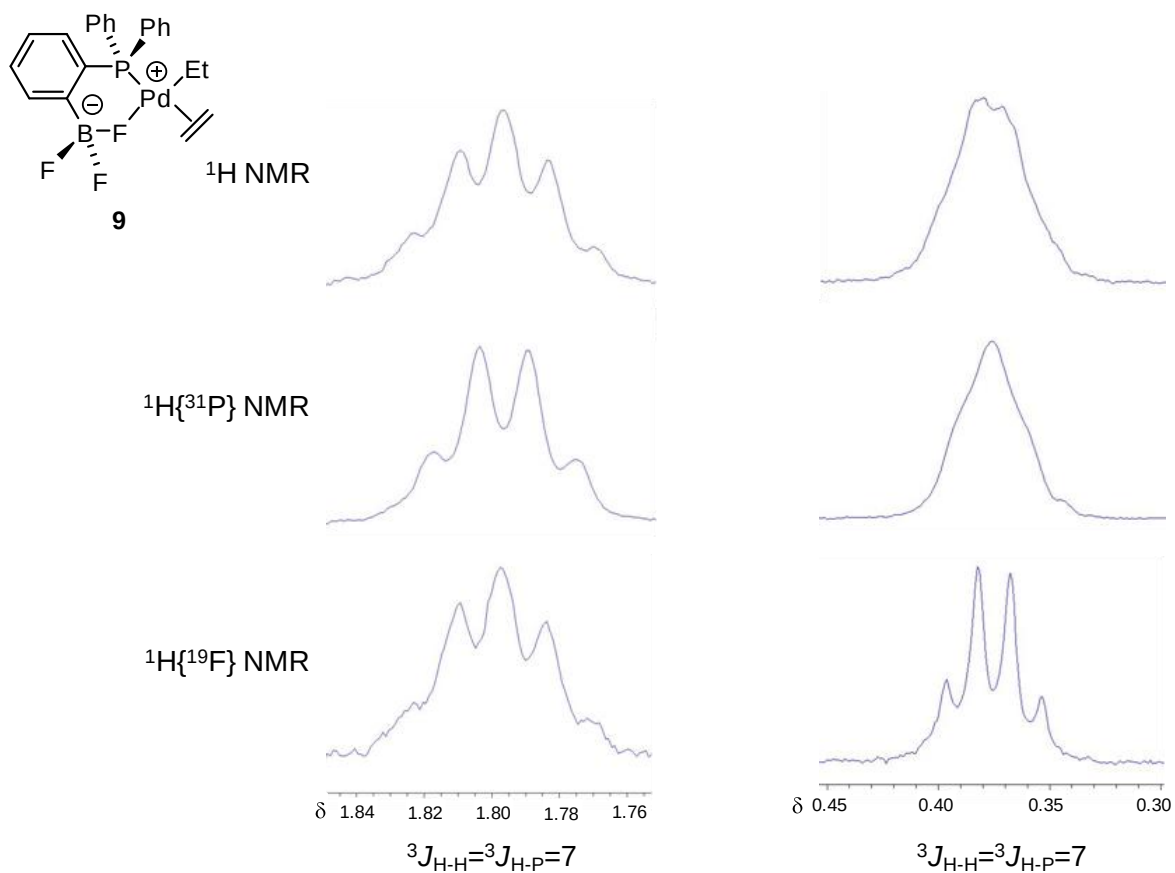


Figure S8. ¹H, ¹H{³¹P} and ¹H{¹⁹F} NMR spectra of **9** in CD₂Cl₂ at -10 °C. The PdCH₂CH₃ (left) and PdCH₂CH₃ (right) resonances are shown.

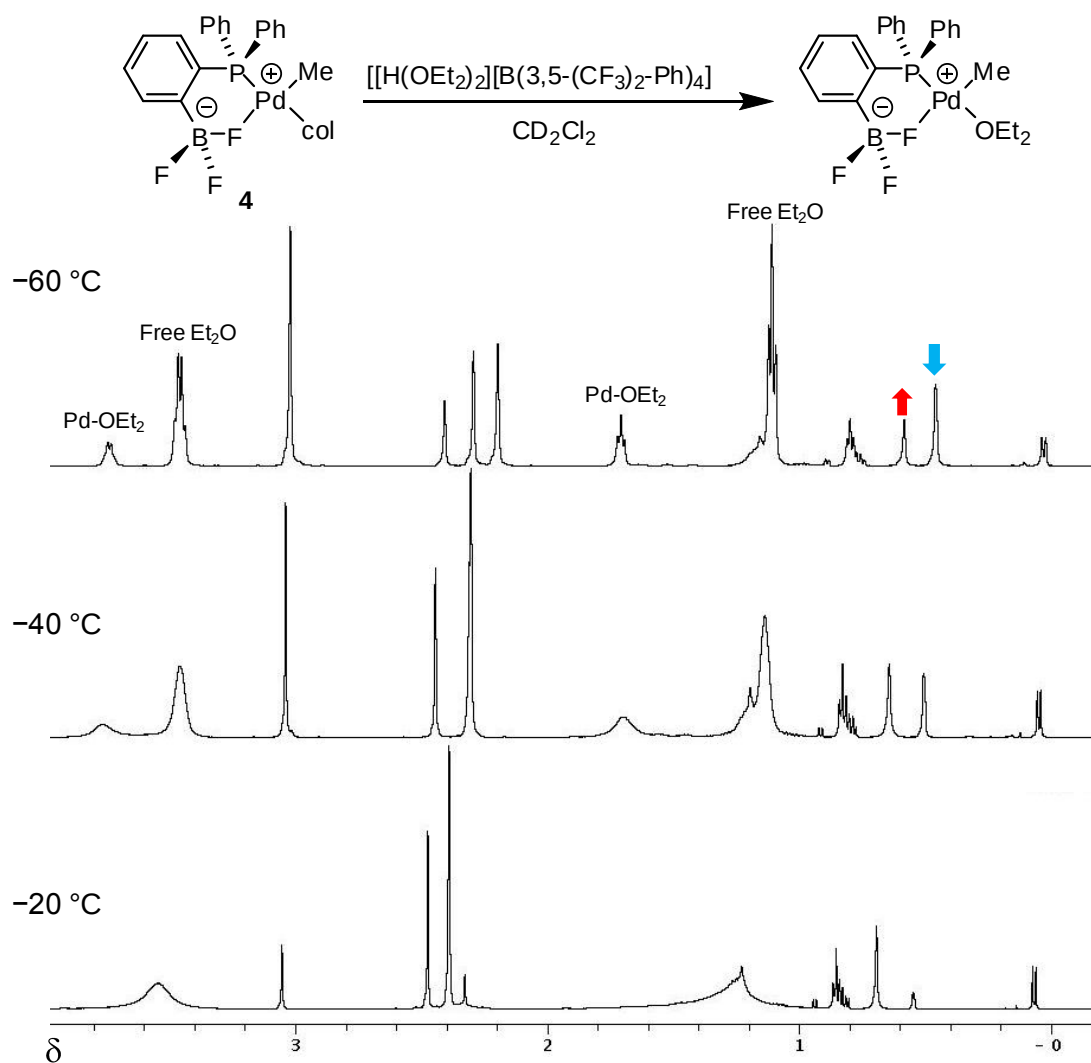


Figure S9. ^1H NMR spectra of **4** in the presence 1 equiv of $[[\text{H}(\text{OEt}_2)_2][\text{B}(3,5\text{-(CF}_3)_2\text{-C}_6\text{H}_3)_4]$ in CD_2Cl_2 at -60°C and then warmed to -20°C showing the formation of $[\text{collidinium}][\text{B}(3,5\text{-(CF}_3)_2\text{-C}_6\text{H}_3)_4]$ and $(\text{PF})\text{PdMe}(\text{OEt}_2)$.

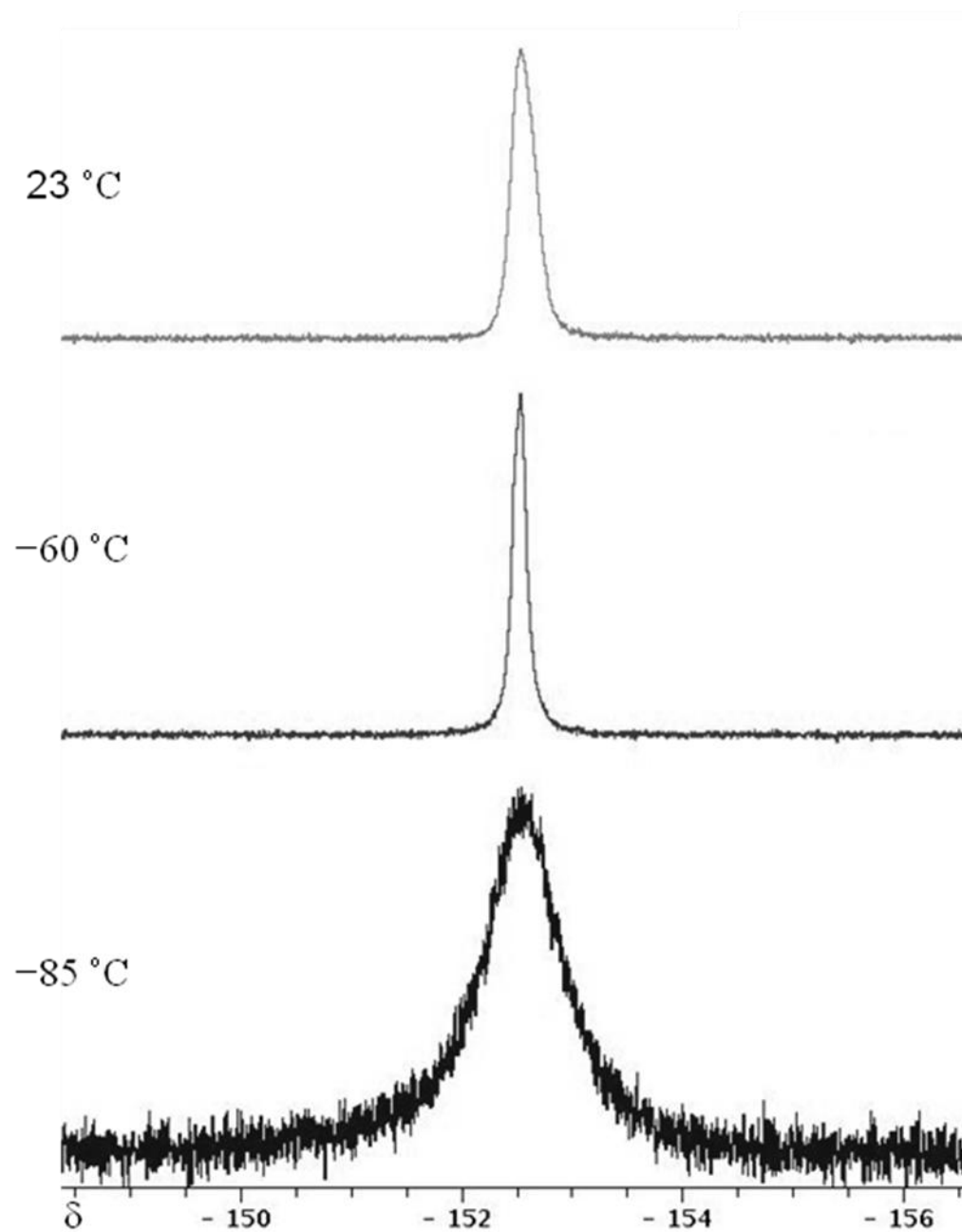


Figure S10. Variable-temperature $^{19}\text{F}\{^1\text{H}\}$ NMR spectra of **3** in CD_2Cl_2 .

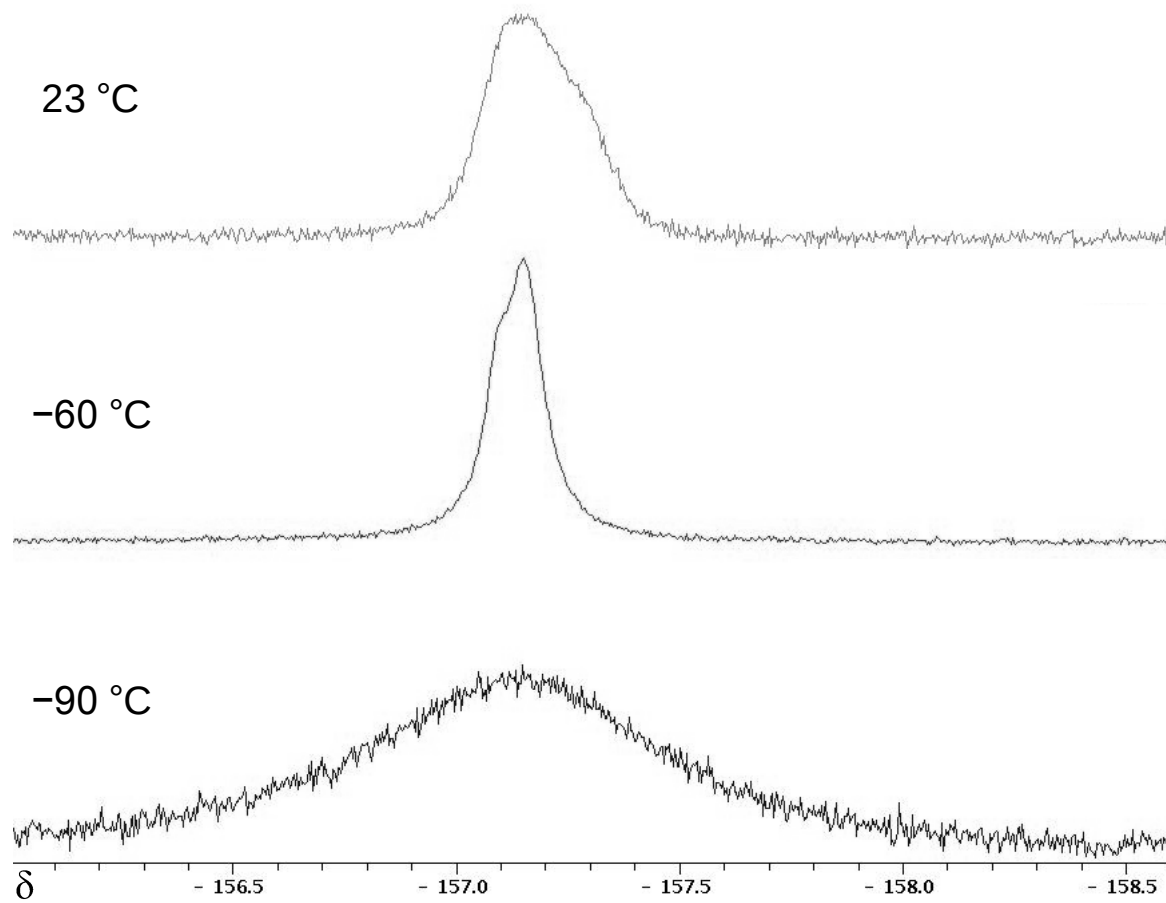


Figure S11. Variable-temperature $^{19}\text{F}\{^1\text{H}\}$ NMR spectra of **4** in CD_2Cl_2 .

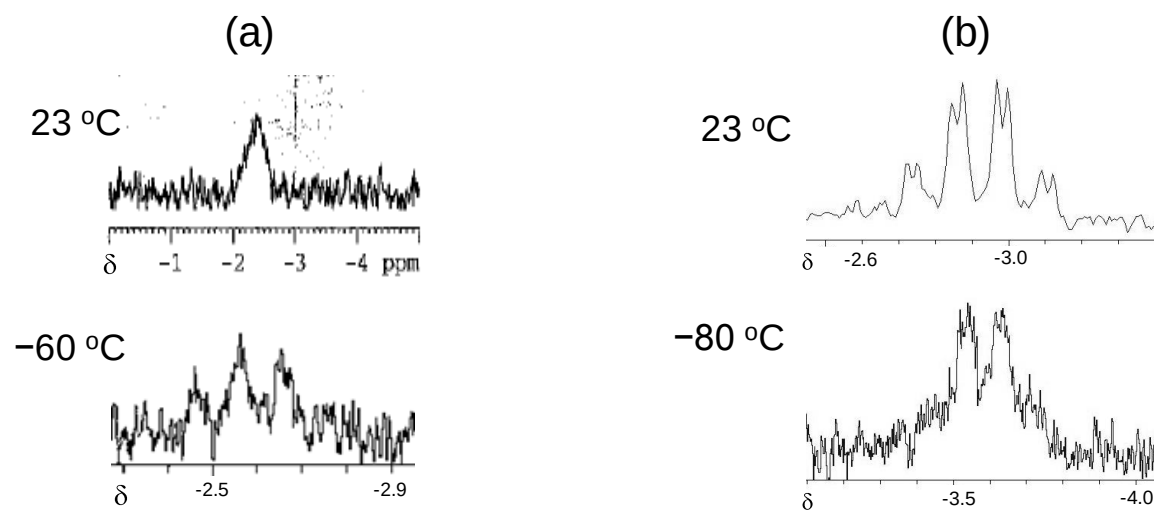


Figure S12. (a) $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of **3** at 23 °C and -60 °C in CD_2Cl_2 . (b) $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of **4** at 23 °C and -80 °C in CD_2Cl_2 .