

Supplementary Material

Ligand Effects on Structural, Protophilic and Reductive Features of Stannylated Dinuclear Iron Dithiolato Complexes

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Figure S1. Overlay of the x-ray structures of compounds **1**, **2** and **3**.

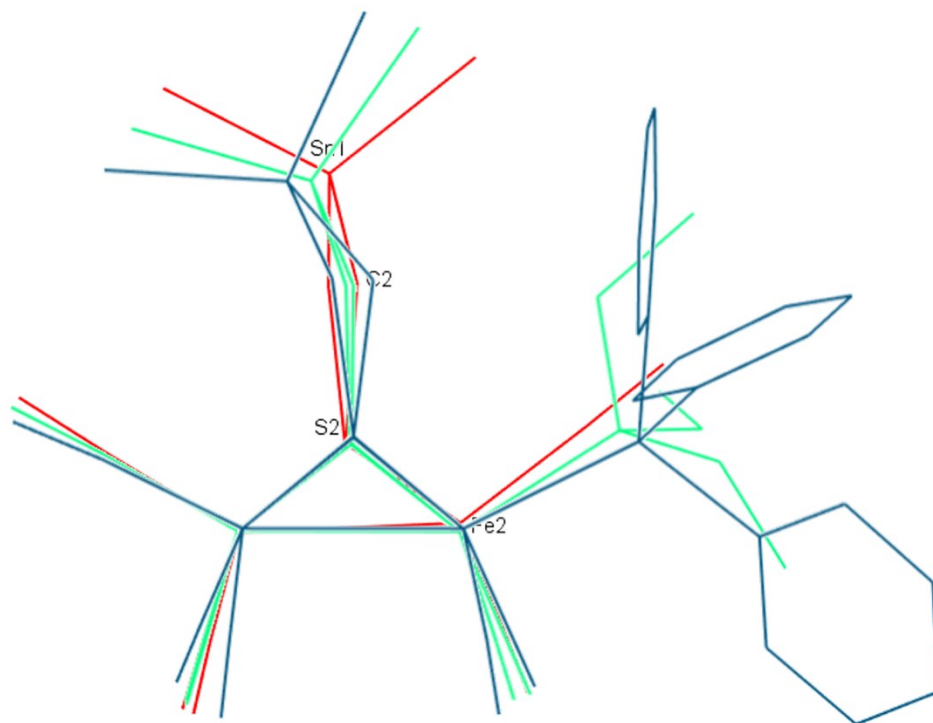


Figure S2. IR spectra of **2** and **3** do not suggest S-protonation in the presence of HBF₄. Panels (A) and (C) depict the IR spectrum from 2800 – 1800 cm⁻¹ including the CN stretches of acetonitrile (solvent, very strong bands at 2295 cm⁻¹ and 2255 cm⁻¹) and the CO stretches of **2** and **3** between 2150 – 1850 cm⁻¹. The IR regime of the SH stretches (2500 ± 50 cm⁻¹) is highlighted. Panels (B) and (D) depict the IR regime of the SH stretches in greater details. Neither **2** (B) nor **3** (C) show a significant increase of signals around 2500 cm⁻¹ upon acidification in the presence of HBF₄ (red and blue traces, respectively). The SH stretching frequency is typically observed around 2500 cm⁻¹.

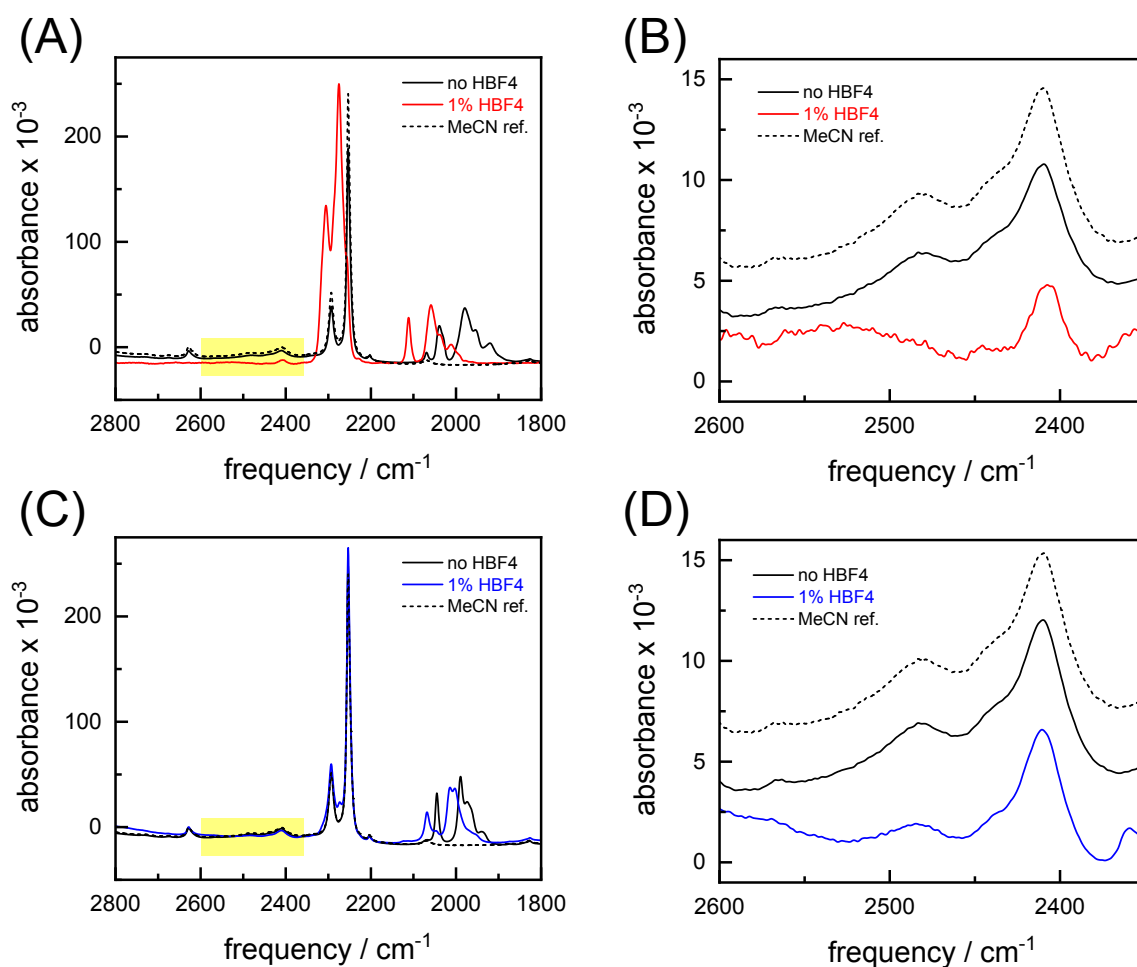


Figure S3. ^1H NMR spectrum (CD_2Cl_2) of **2** at 298 K.

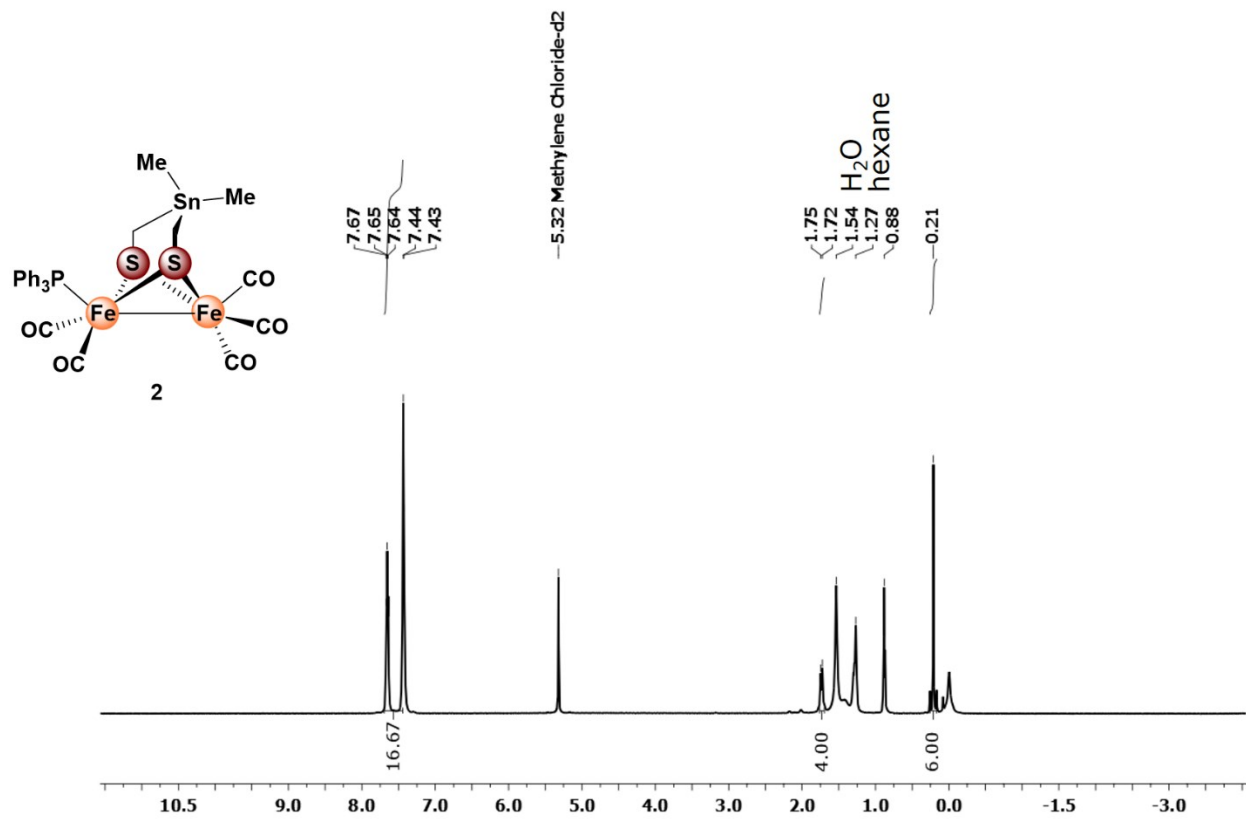


Figure S4. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CD_2Cl_2) of **2** at 298 K.

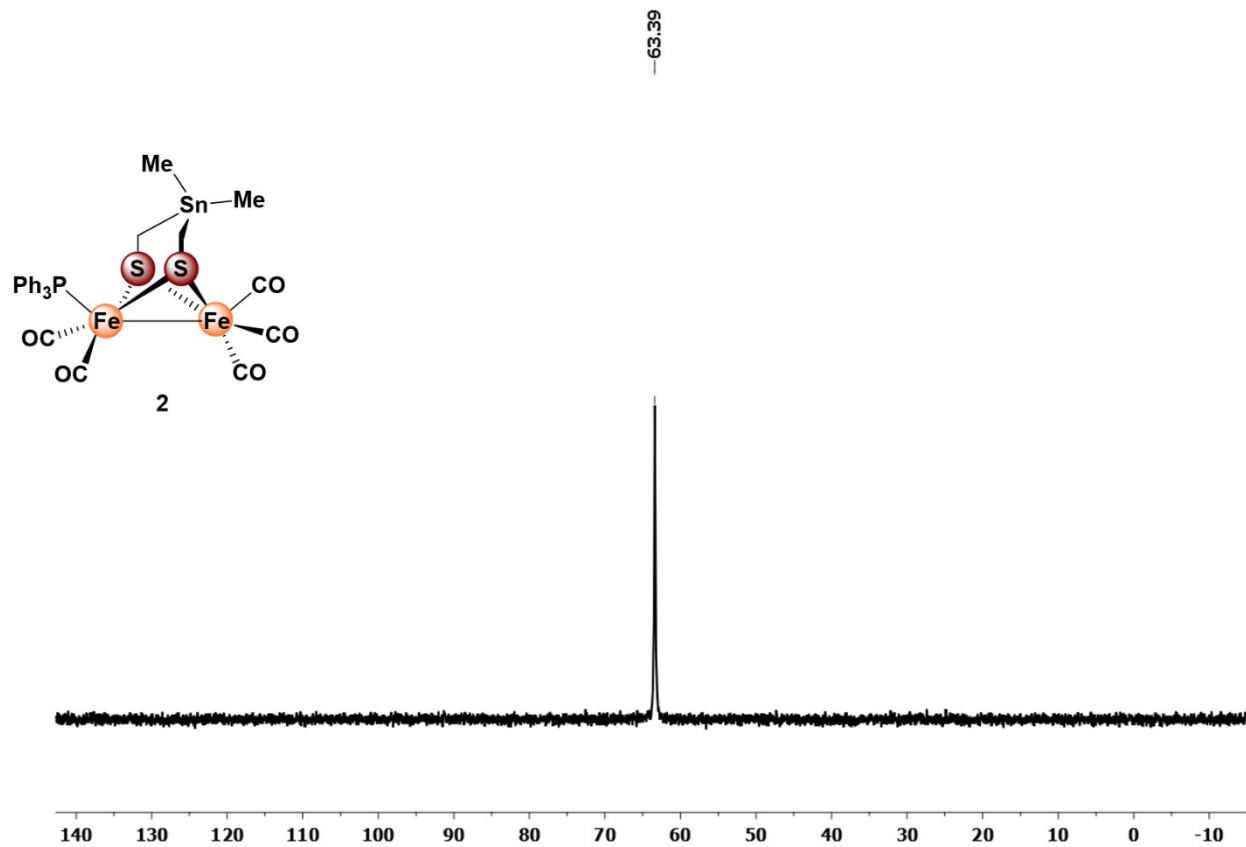


Figure S5. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3) of **2** at 298 K.

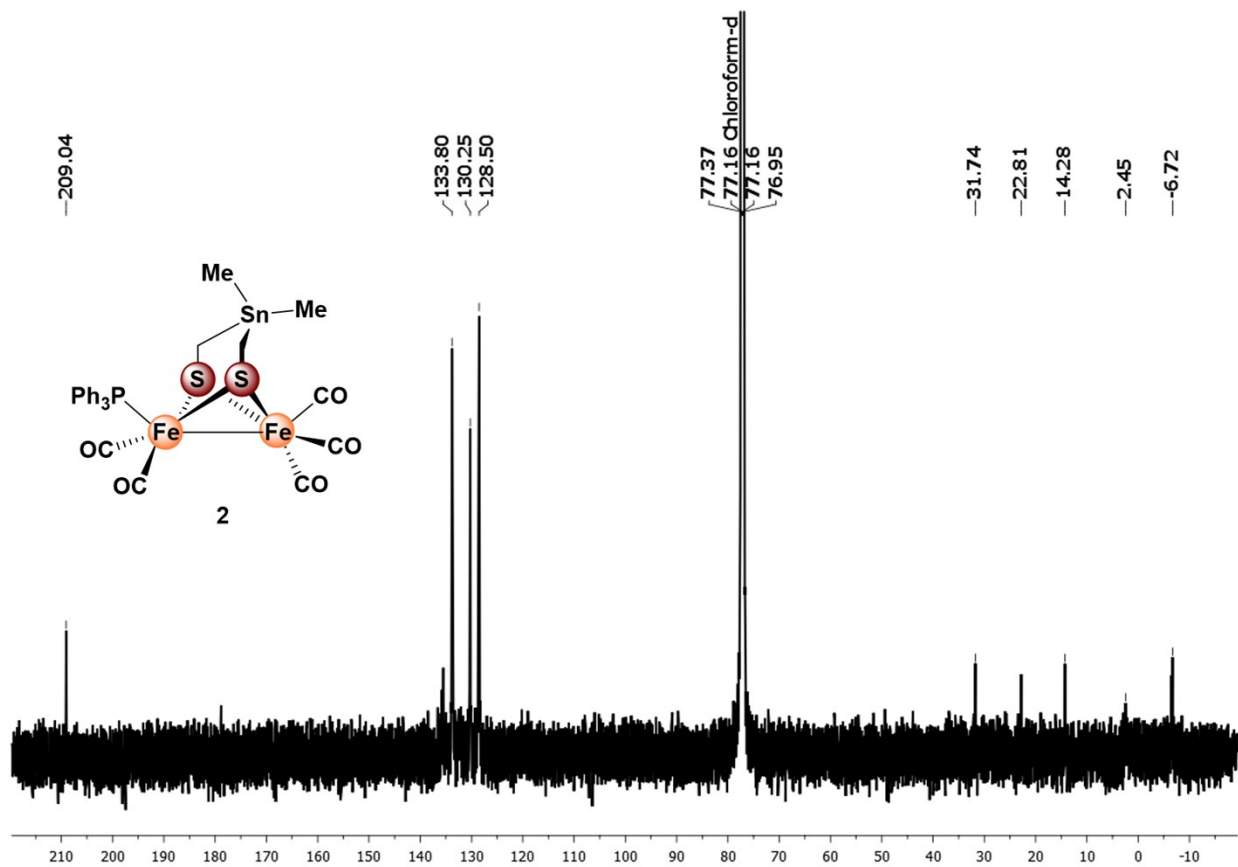


Figure S6. ^1H NMR spectrum (CDCl_3) of **3** at 298 K.

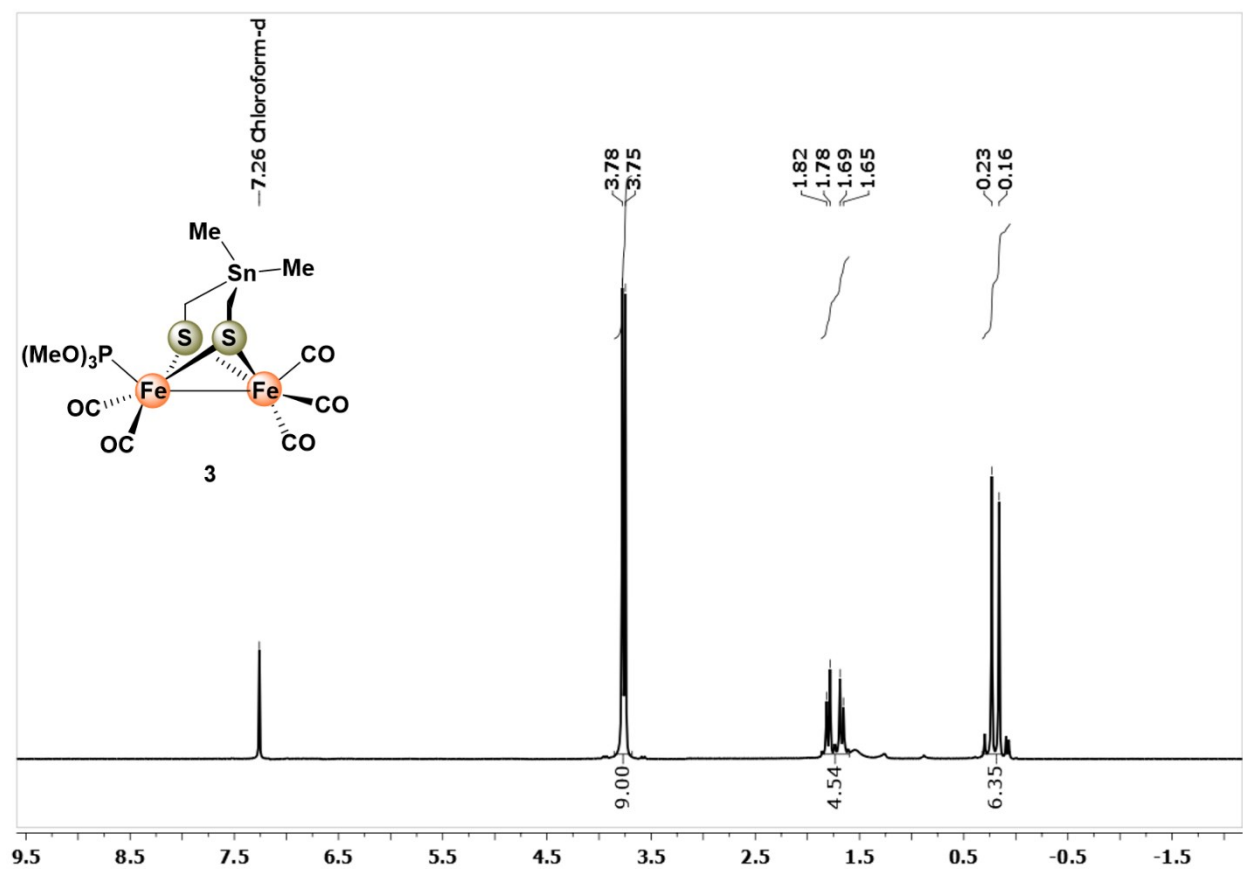


Figure S7. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3) of **3** at 298 K.

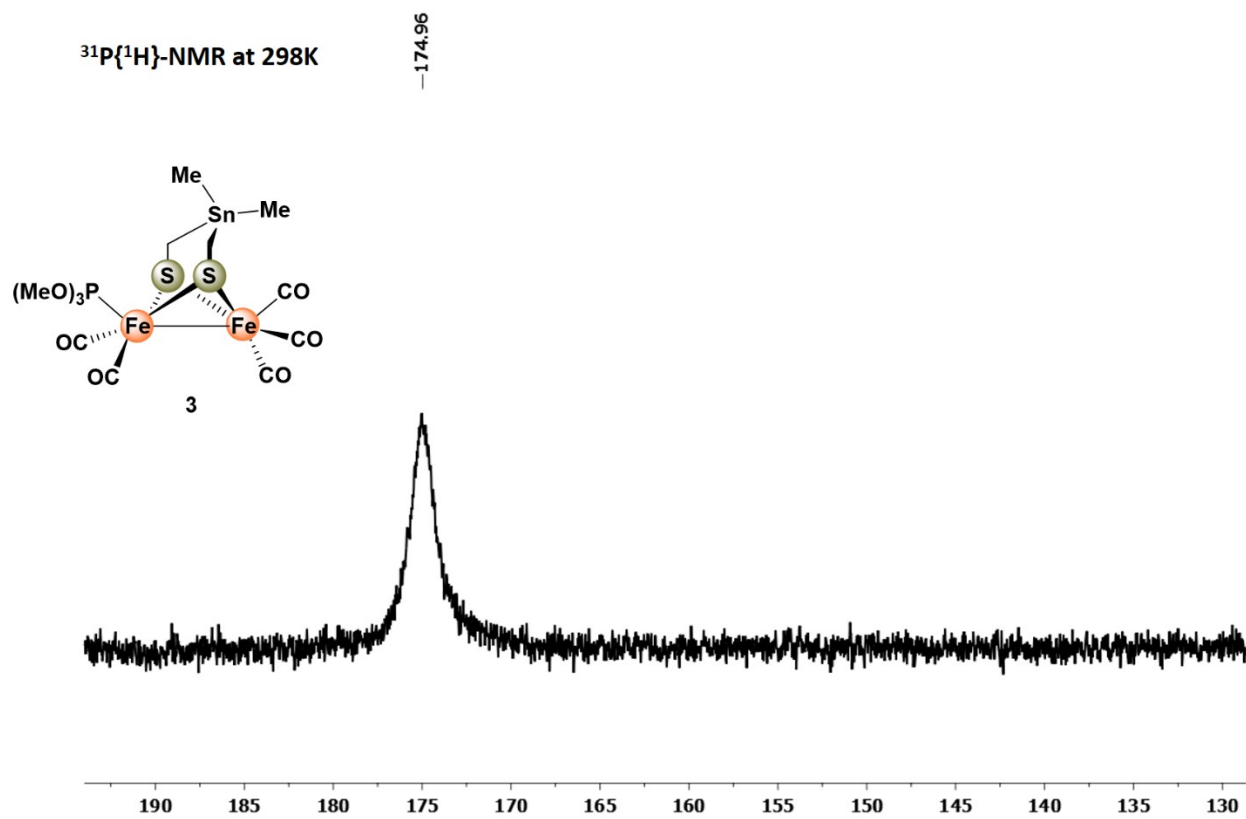


Figure S8. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (CDCl_3) of **3** at 223 K.

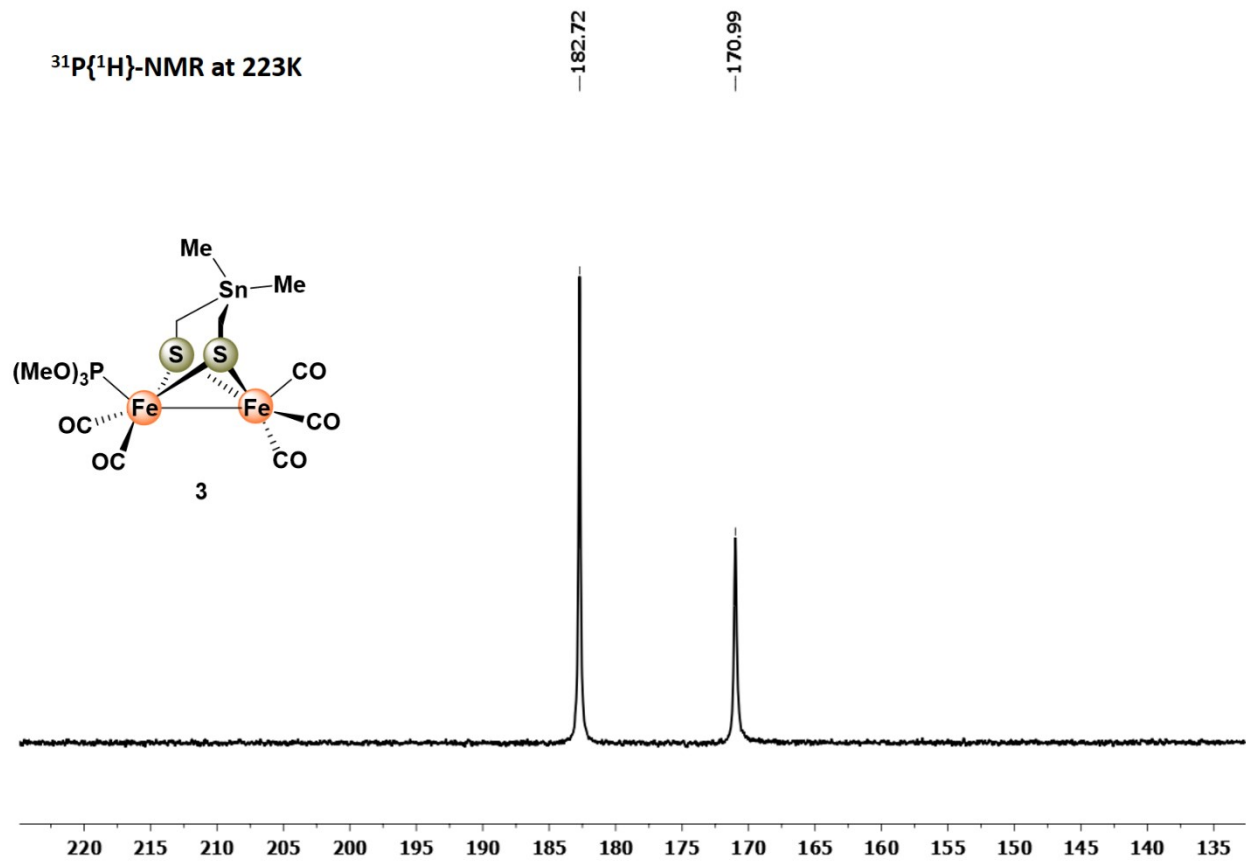


Figure S9. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl_3) of **3** at 298 K.

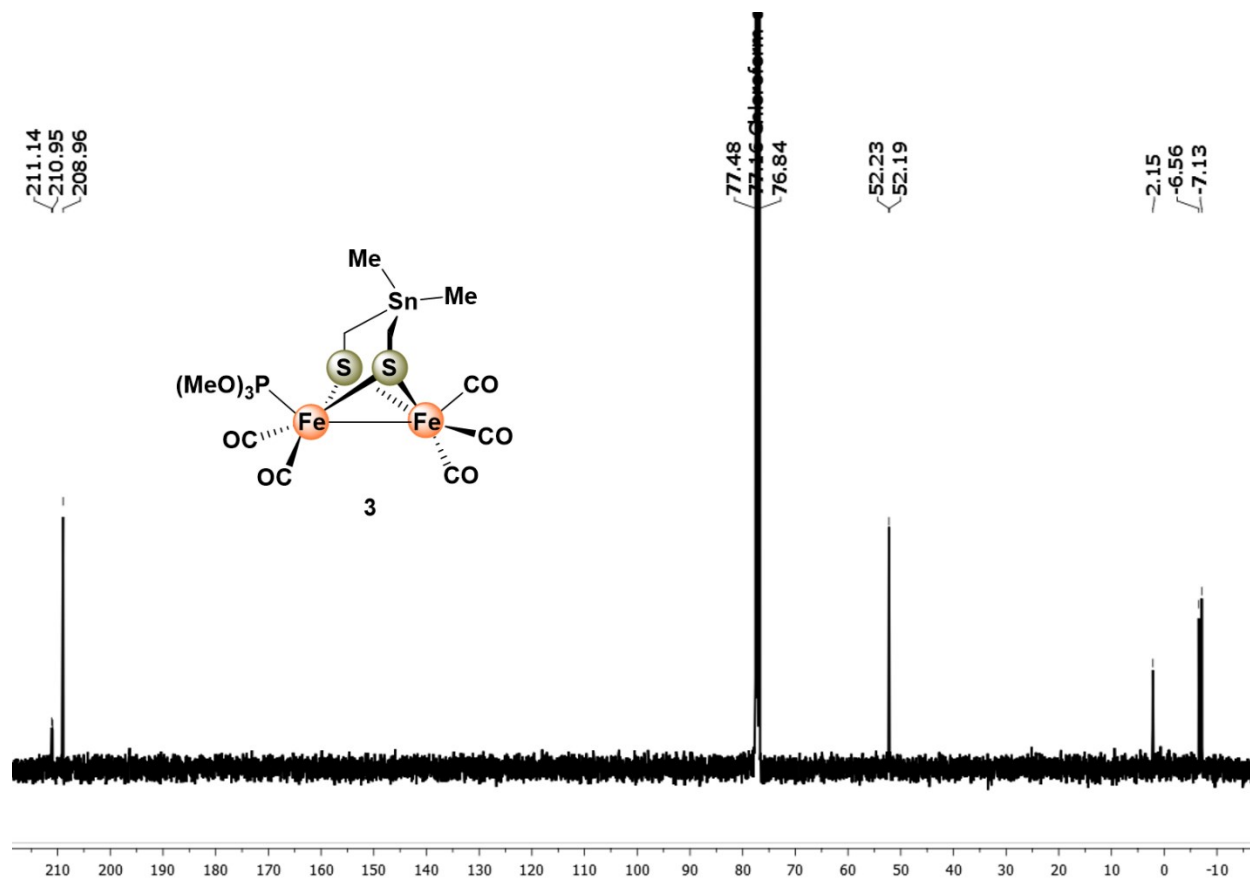


Figure S10. In situ ^1H NMR spectrum (CD_2Cl_2) of complex **3** with $\text{HBF}_4\cdot\text{Et}_2\text{O}$ at 298 K

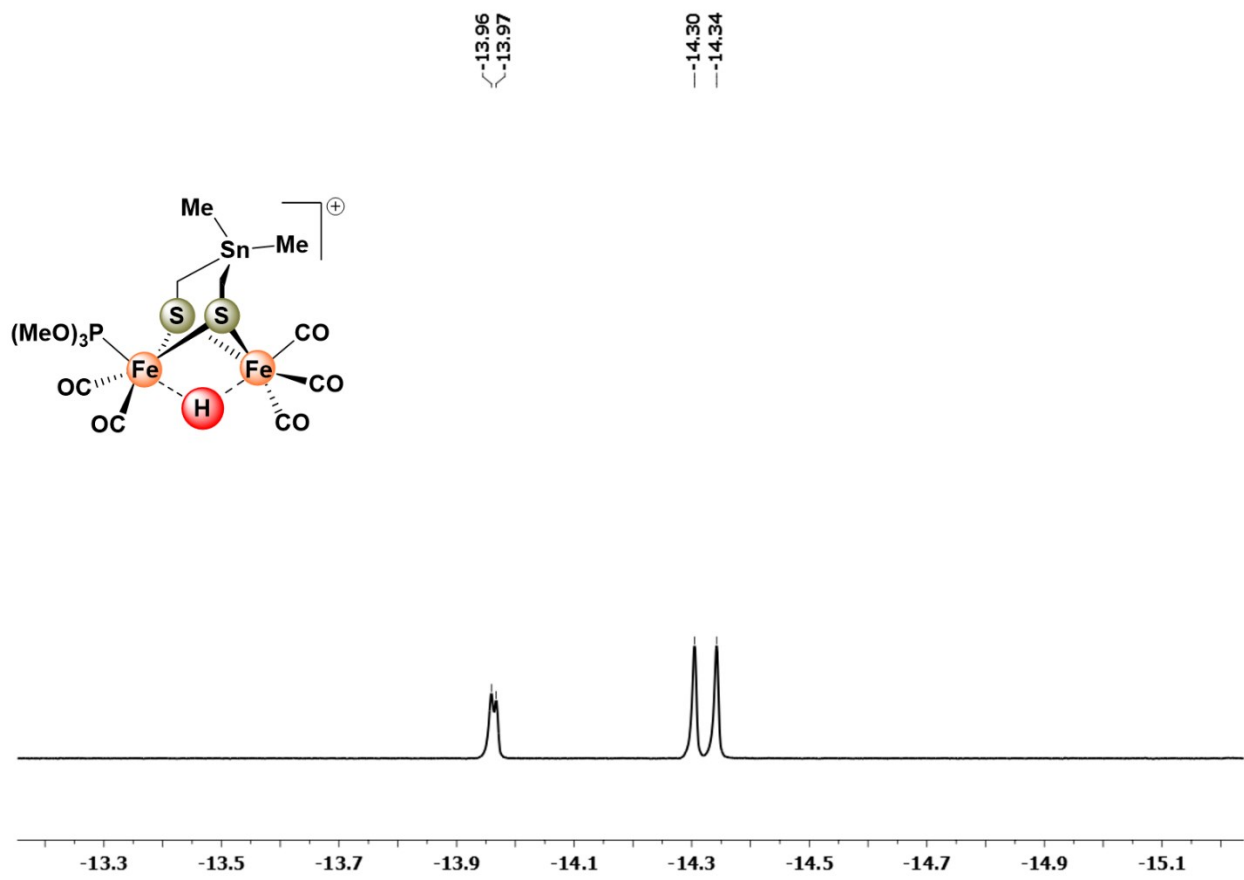


Figure S11. In situ ^{31}P NMR spectrum (CD_2Cl_2) of complex **3** with $\text{HBF}_4 \cdot \text{Et}_2\text{O}$ at 298 K

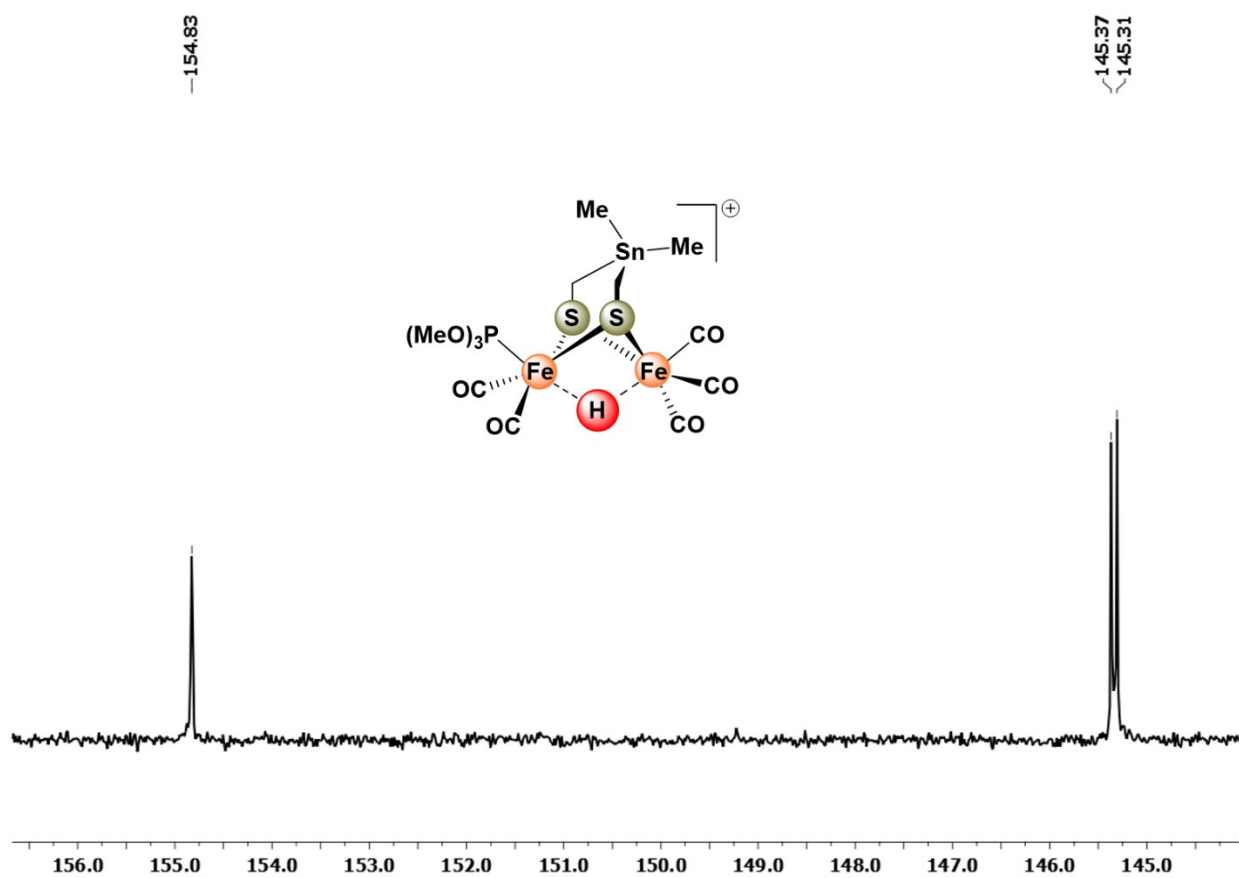


Figure S12. Cyclic voltammetry of 1.0 mM $\text{Fe}_2(\text{CO})_5(\text{PPh}_3)\{\mu\text{-(SCH}_2)_2\}\text{SnMe}_2$ (**2**) in CH_2Cl_2 -[*n*- $\text{Bu}_4\text{N}][\text{BF}_4]$ (0.1 M) at various scan rates. Glassy carbon electrode. Potential E is given in volts (V) and referenced to Fc^+/Fc couple. The arrows indicate the scan direction.

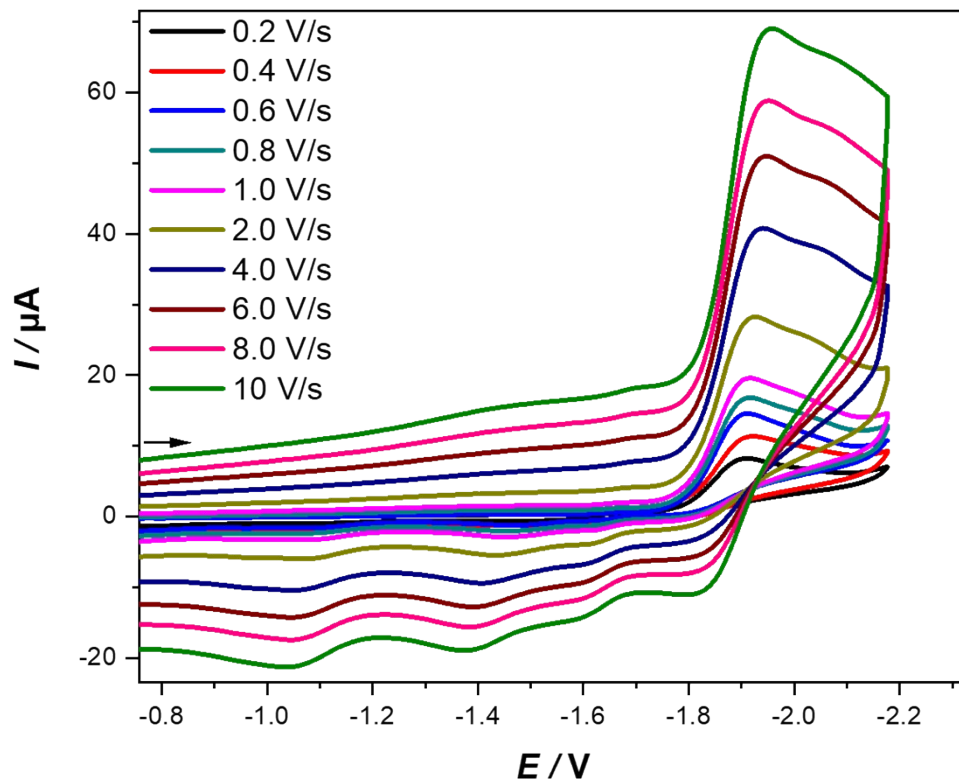


Figure S13. Cyclic voltammetry of 1.0 mM $\text{Fe}_2(\text{CO})_5(\text{P}(\text{OMe})_3)\{\mu\text{-(SCH}_2)_2\}\text{SnMe}_2$ (**3**) in CH_2Cl_2 - $[\textit{n}\text{-Bu}_4\text{N}][\text{BF}_4]$ (0.1 M) at $v = 0.2\text{-}1$ V/s. Glassy carbon electrode. Potential E is given in volts (V) and referenced to Fc^+/Fc couple. The arrows indicate the scan direction.

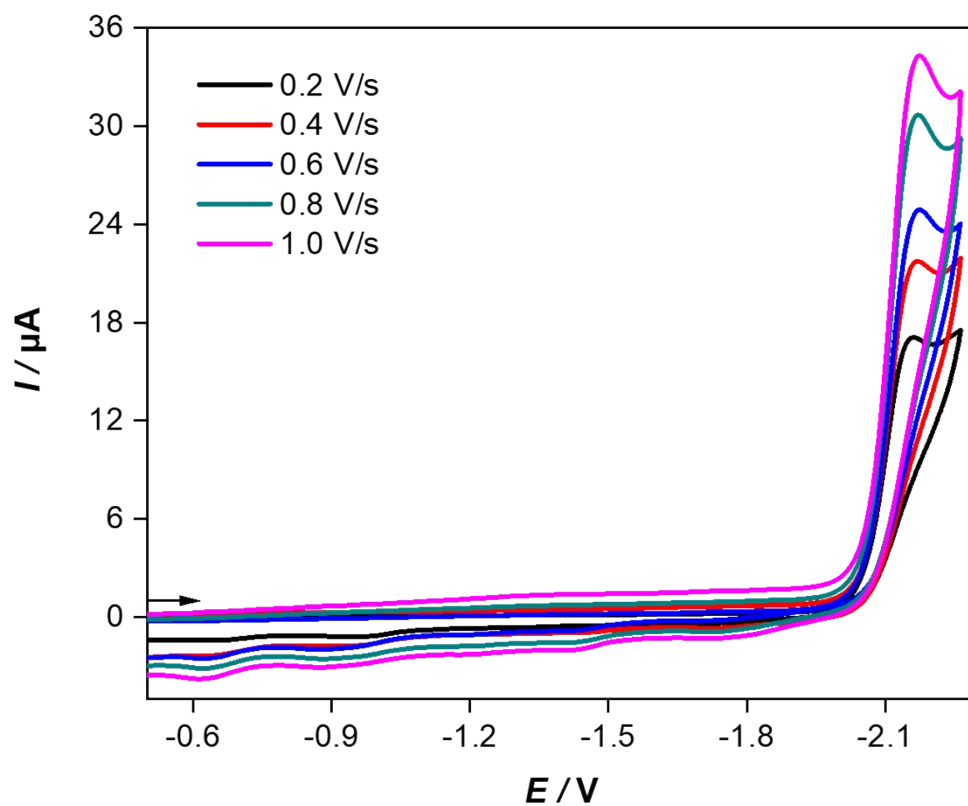


Figure S14. Cyclic voltammetry of 1.0 mM $\text{Fe}_2(\text{CO})_5(\text{P}(\text{OMe})_3)\{\mu\text{-(SCH}_2)_2\}_2\text{SnMe}_2$ (**3**) in CH_2Cl_2 - $[\text{n-Bu}_4\text{N}][\text{BF}_4]$ (0.1 M) at $v = 2$ -10 V/s. Glassy carbon electrode. Potential E is given in volts (V) and referenced to Fc^+/Fc couple. The arrows indicate the scan direction.

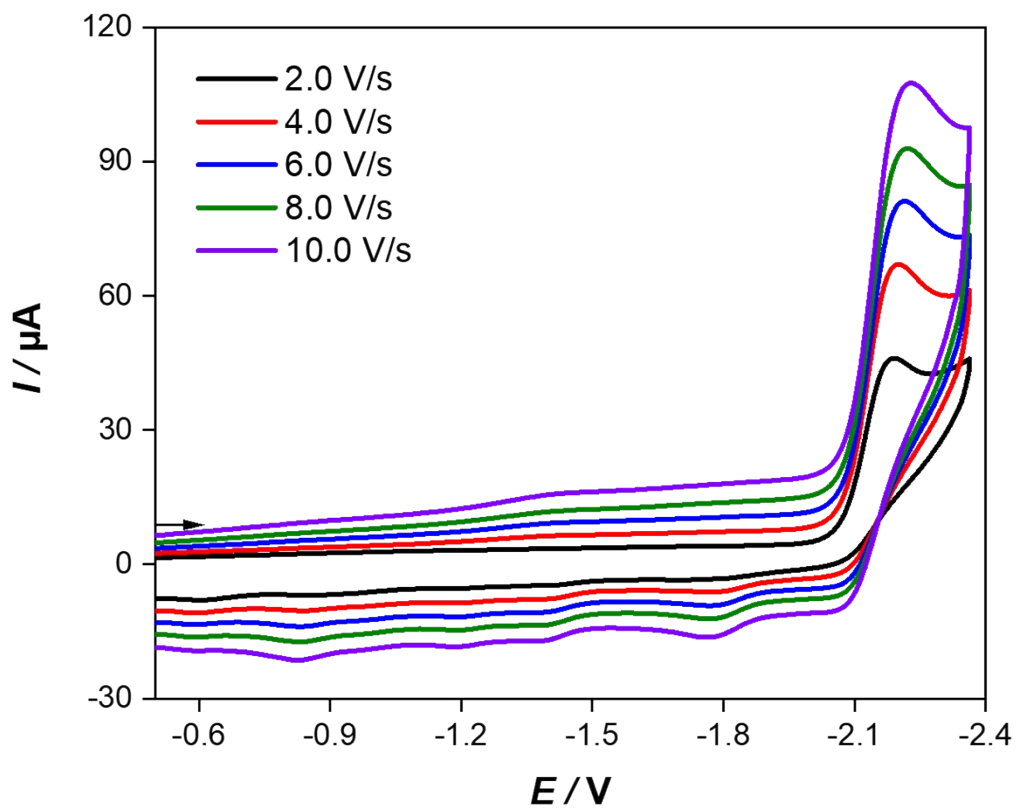


Figure S15. Cyclic voltammetry ($0.2 \text{ V}\cdot\text{s}^{-1}$) of $1.0 \text{ mM Fe}_2(\text{CO})_5(\text{PPh}_3)\{\mu\text{-(SCH}_2)_2\}\text{SnMe}_2$ (**2**) in $\text{CH}_2\text{Cl}_2\text{-}[n\text{-Bu}_4\text{N}][\text{BF}_4]$ (0.1 M) at $[\text{HBF}_4\cdot\text{Et}_2\text{O}]/[\mathbf{2}] = 0\text{-}4$. Glassy carbon electrode (diameter = 1.6 mm). Potential E is given in volts (V) and referenced to Fc^+/Fc couple.

