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Supporting Information

Heterodinuclear nickel(II)-iron(II) azadithiolates as structural and functional models for the active site of [NiFe]-hydrogenases

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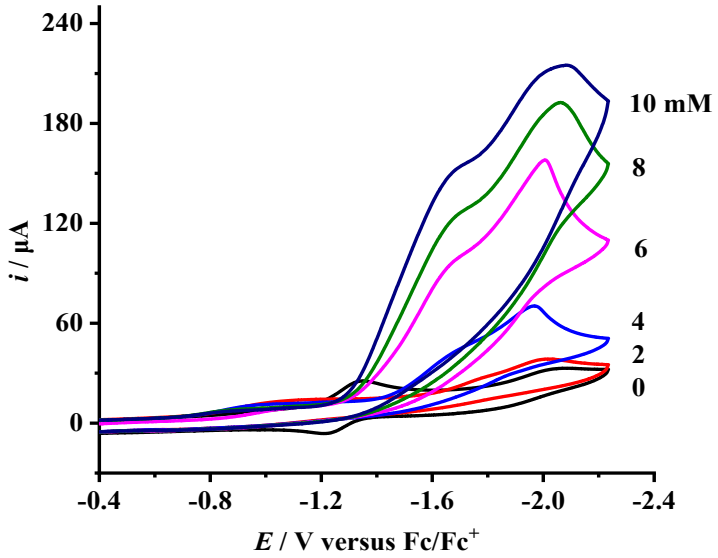

Fig. S1 Cyclic voltammograms of TFA (0−10 mM) without **7** or **9** in 0.1 M *n*-Bu_4NPF_6/MeCN at a scan rate of 0.1 Vs^{-1}.

TFA/mM	**7**		**9**		TFA without **7** or **9**	
	E_{pc}/V	i_p/μA	E_{pc}/V	i_p/μA	E_{pc}/V	i_p/μA
2	–1.85	72.6	–1.53	64.1	–2.02	38.5
4	–1.89	120	–1.59	88.8	–1.97	70.4
10	–2.01	240	–1.79	220	–2.08	214

All potentials are versus Fc/Fc^+ in 0.1 M *n*-Bu_4NPF_6/MeCN at a scan rate of 0.1 Vs^{-1}.

3. Cyclic voltammograms of precursor 3 (1.0 mM) with TFA (0−10 mM) in 0.1 M *n*-Bu_4NPF_6/MeCN at a scan rate of 0.1 Vs^{-1}

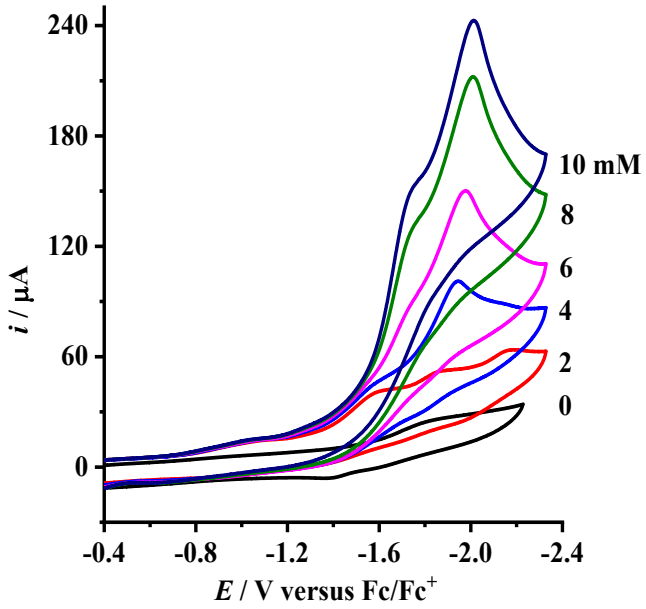

Fig. S2 Cyclic voltammograms of precursor **3** (1.0 mM) with TFA (0−10 mM) in 0.1 M *n*-Bu_4NPF_6/MeCN at a scan rate of 0.1 Vs^{-1}.

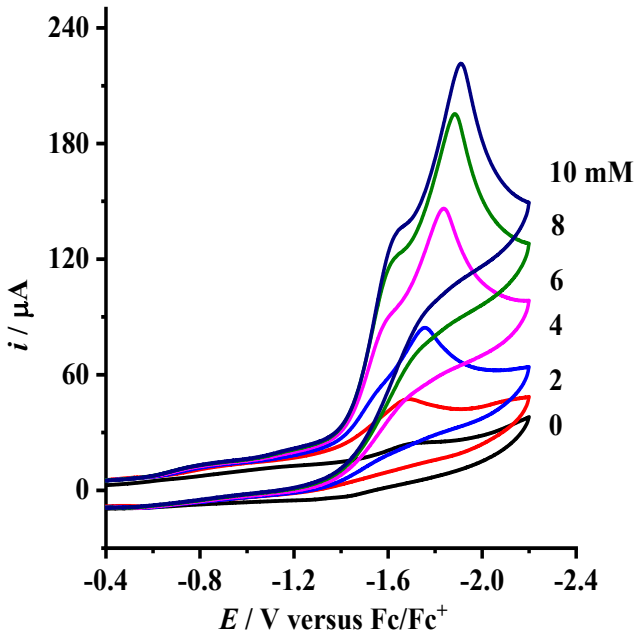

Fig. S3 Cyclic voltammograms of precursor **4** (1.0 mM) with TFA (0−10 mM) in 0.1 M *n*-Bu_4NPF_6/MeCN at a scan rate of 0.1 Vs^{-1}.

5. IR and ^{1}H (^{13}C, ^{31}P) NMR spectra of 2

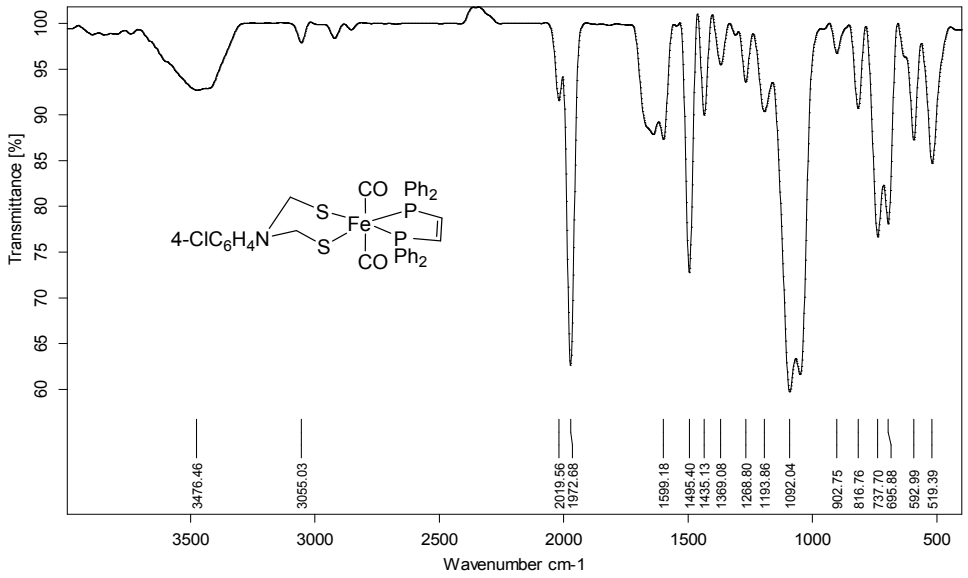

Fig. S4 IR spectrum of **2**

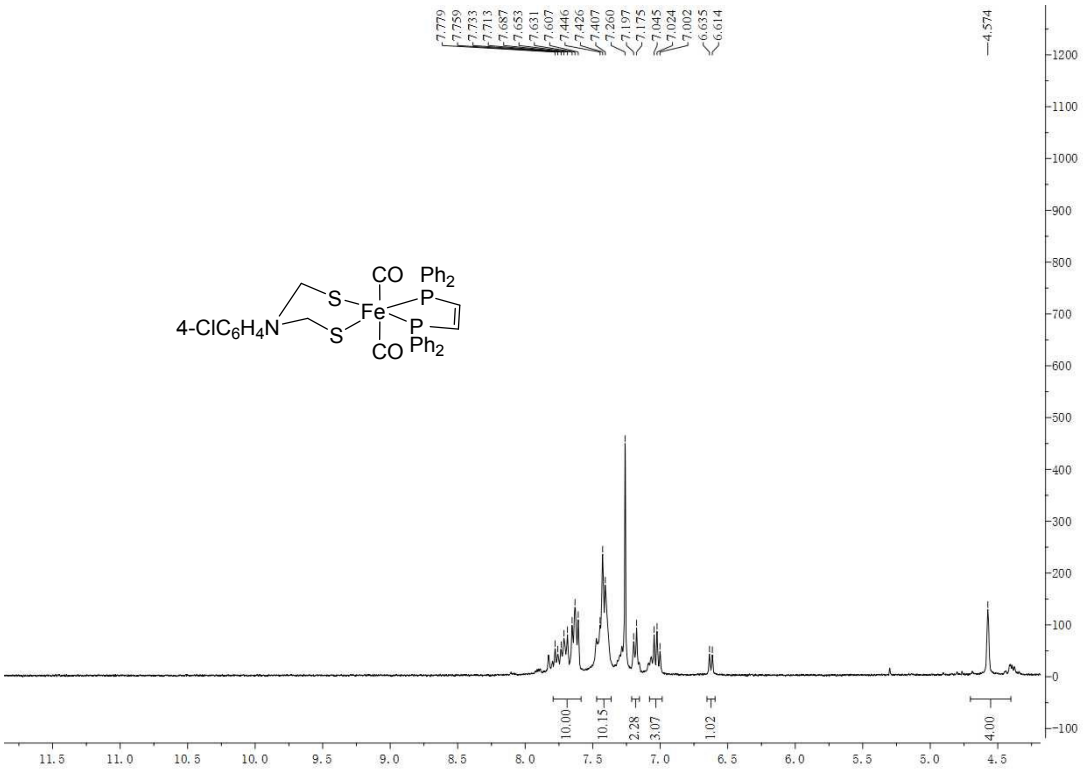

Fig. S5 ^{1}H NMR spectrum of **2** in $CDCl_3$

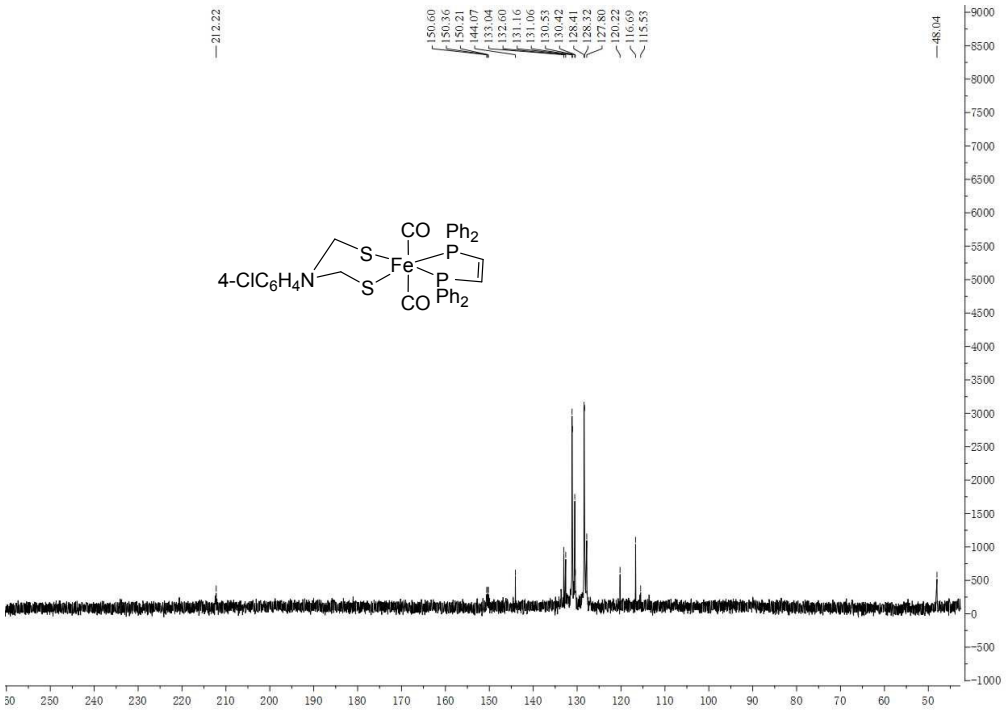

Fig. S6 ^{13}C NMR spectrum of **2** in DMSO-d_6

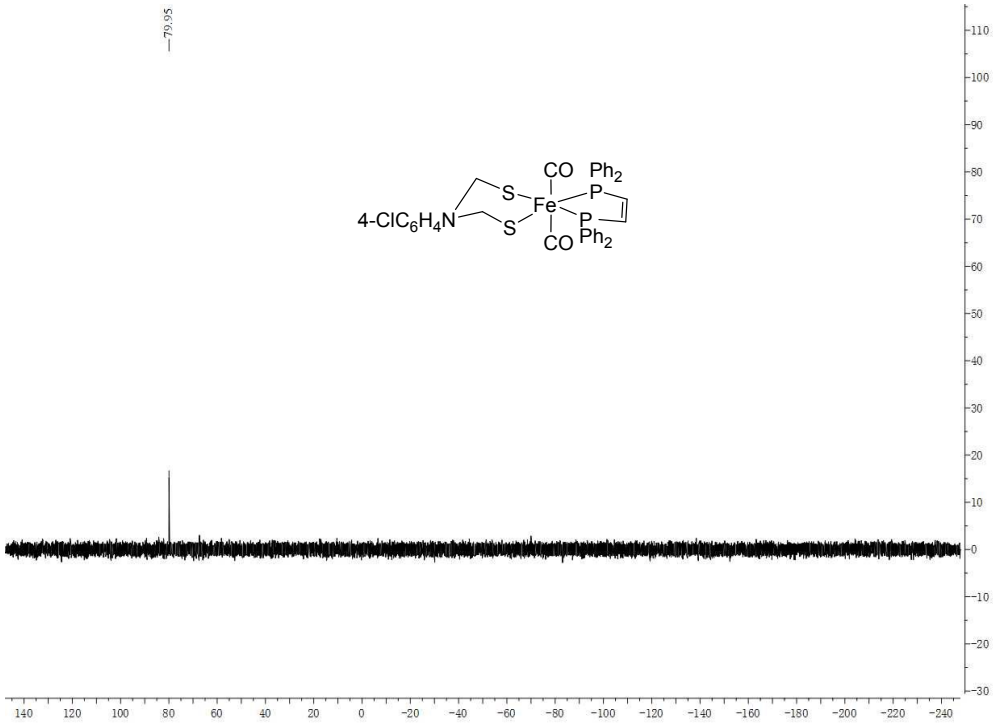

Fig. S7 ^{31}P NMR spectrum of **2** in $CDCl_3$

6. IR and ^{1}H (^{13}C, ^{31}P) NMR spectra of 4

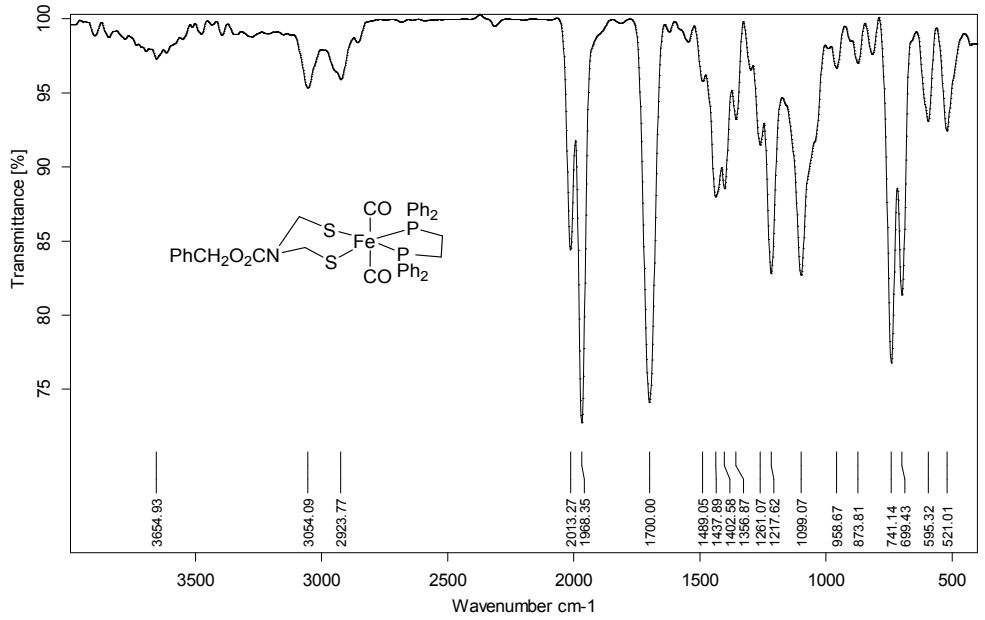

Fig. S8 IR spectrum of **4**

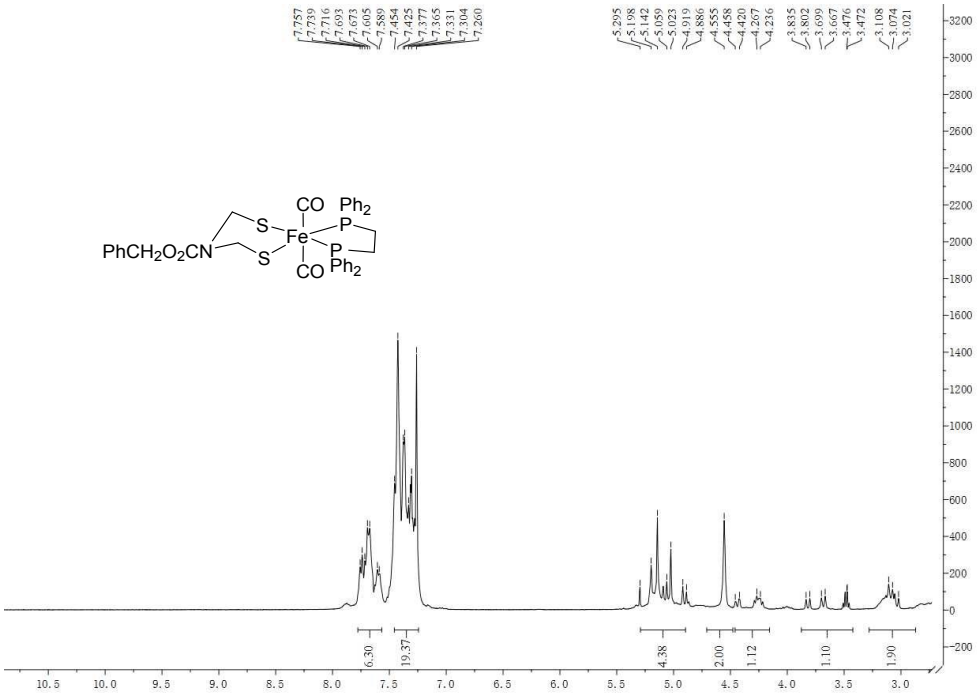

Fig. S9 ^{1}H NMR spectrum of **4** in $CDCl_3$

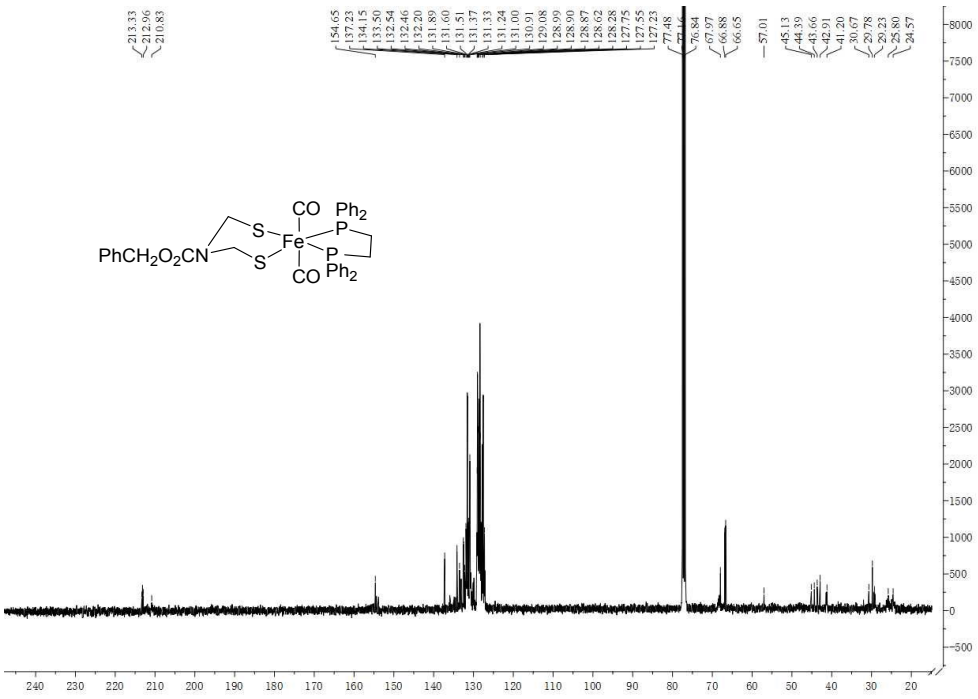

Fig. S10 ^{13}C NMR spectrum of **4** in $CDCl_3$

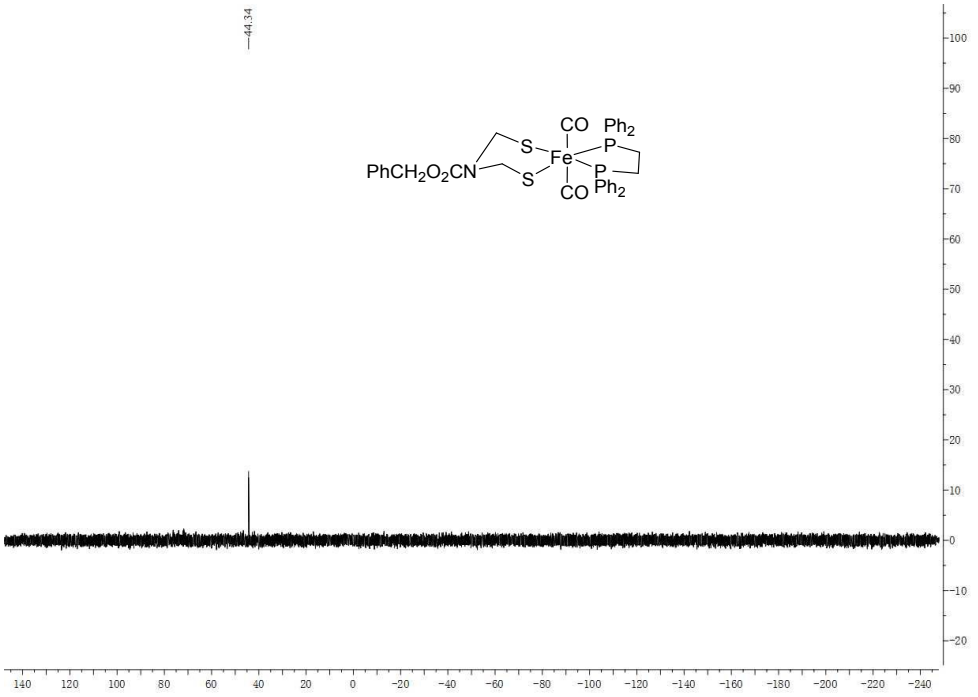

Fig. S11 ^{31}P NMR spectrum of **4** in $CDCl_3$

7. IR and ^{1}H (^{13}C, ^{31}P) NMR spectra of 6

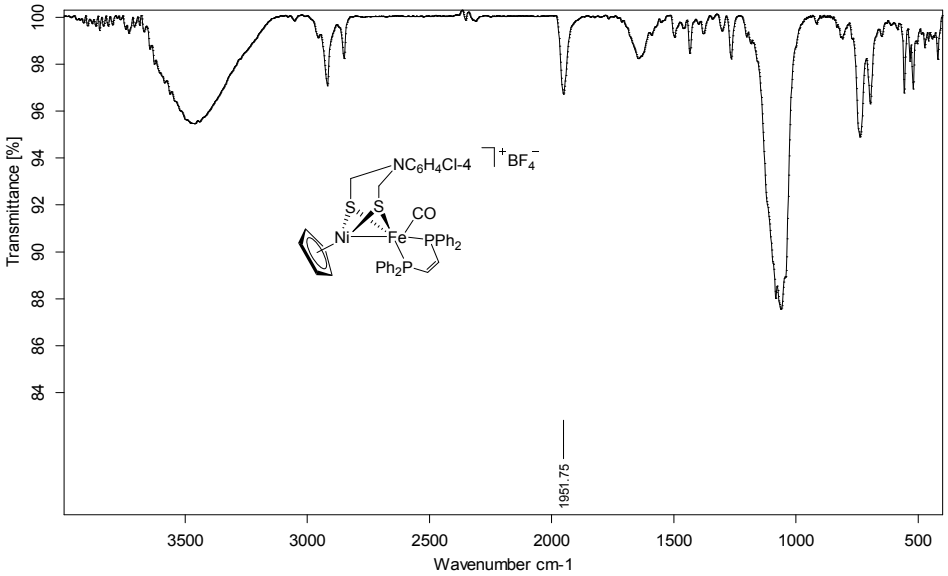

Fig. S12 IR spectrum of **6**

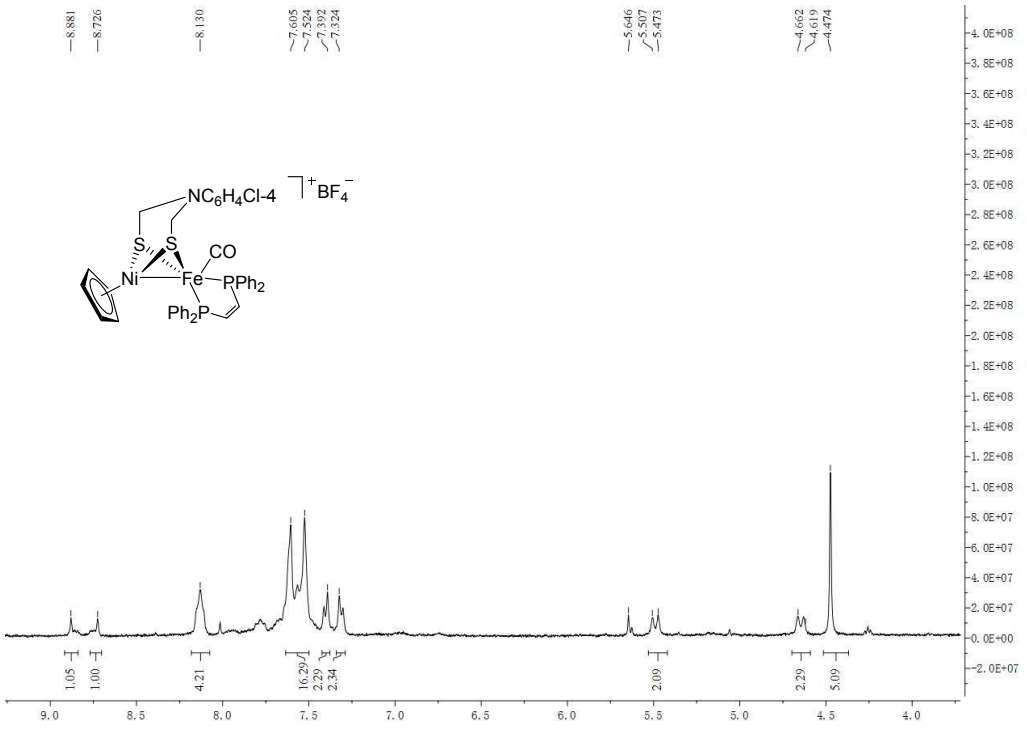

Fig. S13 ^{1}H NMR spectrum of **6** in acetone-d_6

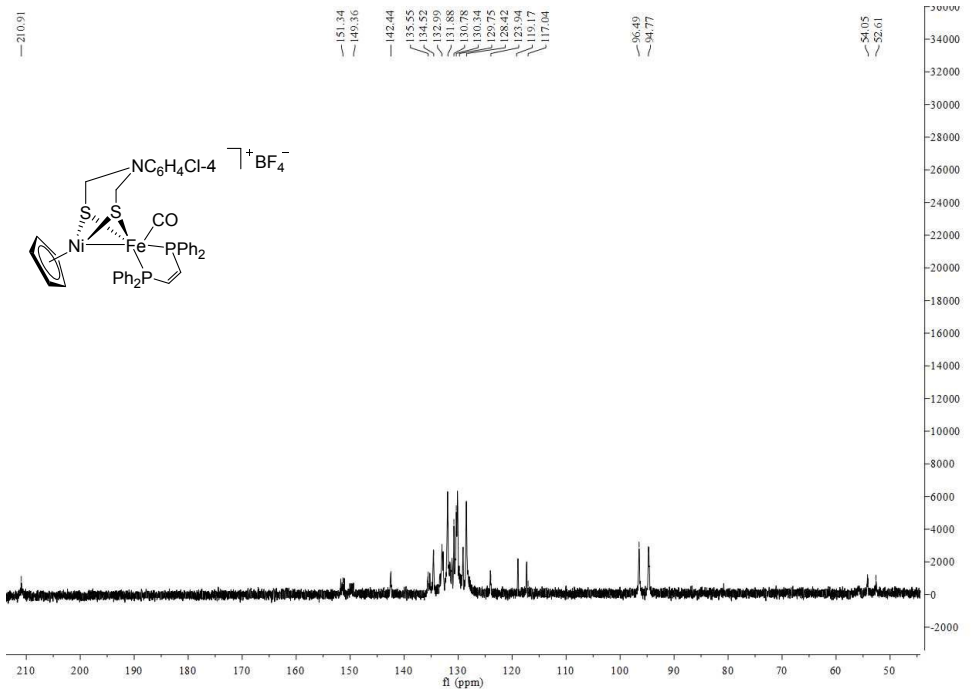

Fig. S14 ^{13}C NMR spectrum of **6** in CD_2Cl_2

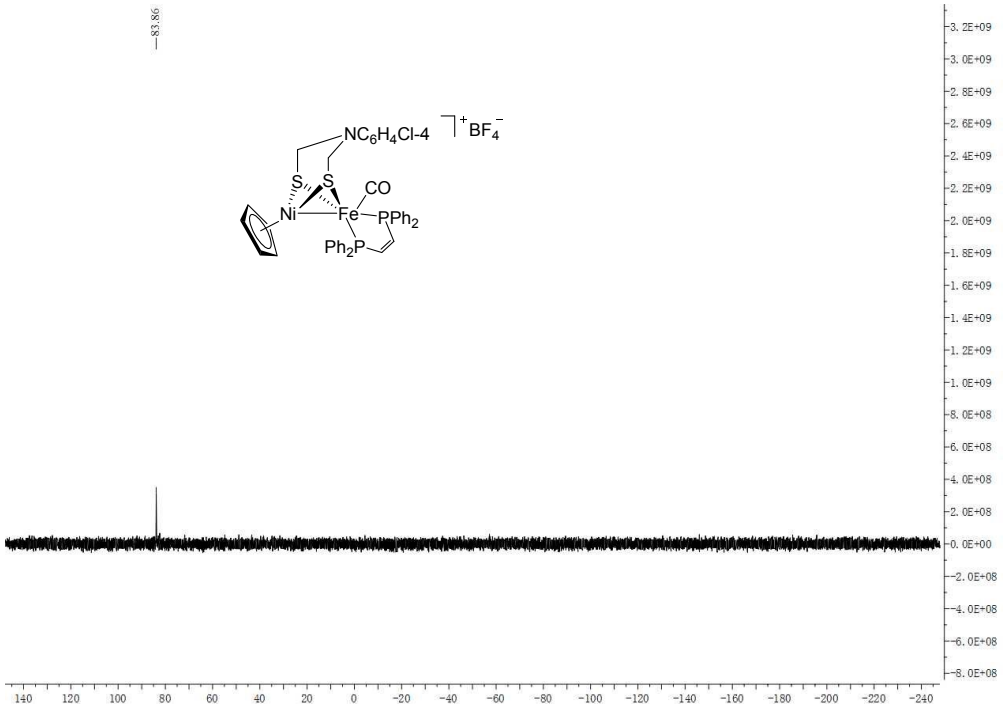

Fig. S15 ^{31}P NMR spectrum of **6** in $CDCl_3$

8. IR and ^{1}H (^{13}C, ^{31}P) NMR spectra of 7

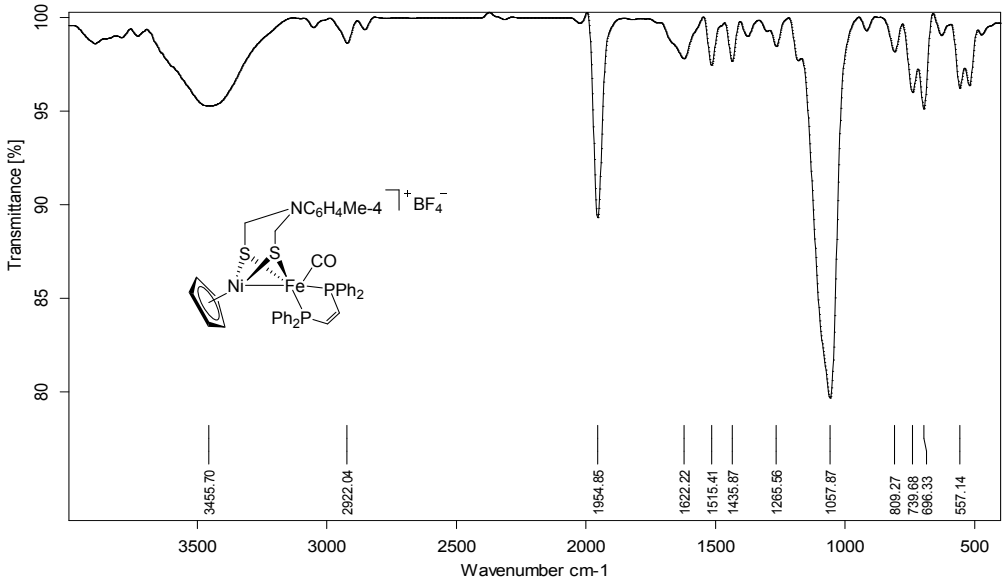

Fig. S16 IR spectrum of **7**

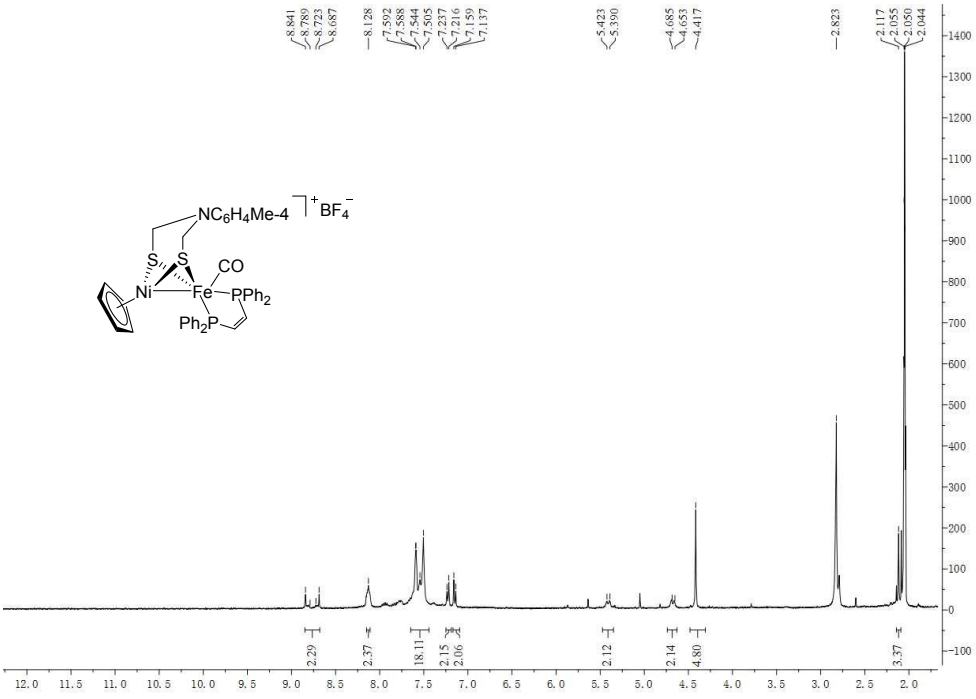

Fig. S17 ^{1}H NMR spectrum of **7** in acetone-d_6

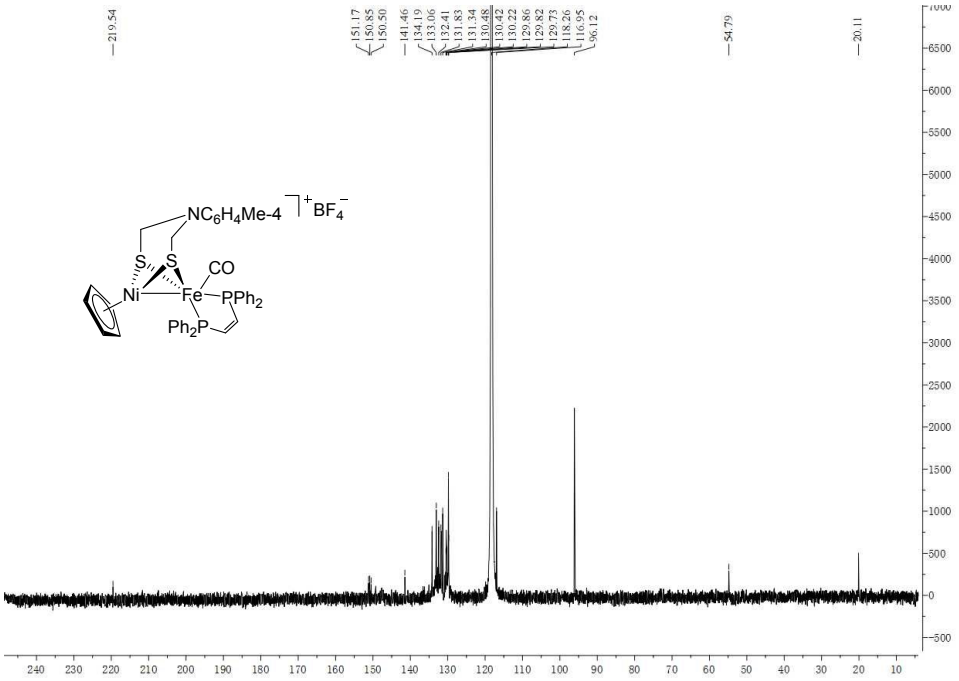

Fig. S18 ^{13}C NMR spectrum of **7** in CD_3CN

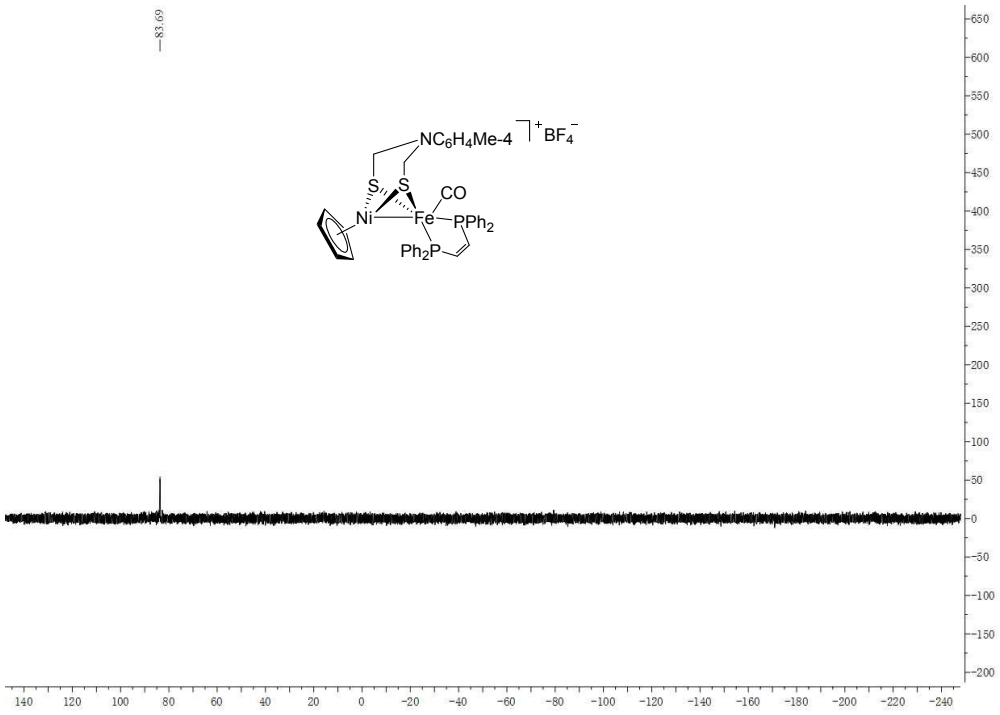

Fig. S19 ^{31}P NMR spectrum of **7** in $CDCl_3$

9. IR and ^{1}H (^{13}C, ^{31}P) NMR spectra of 8

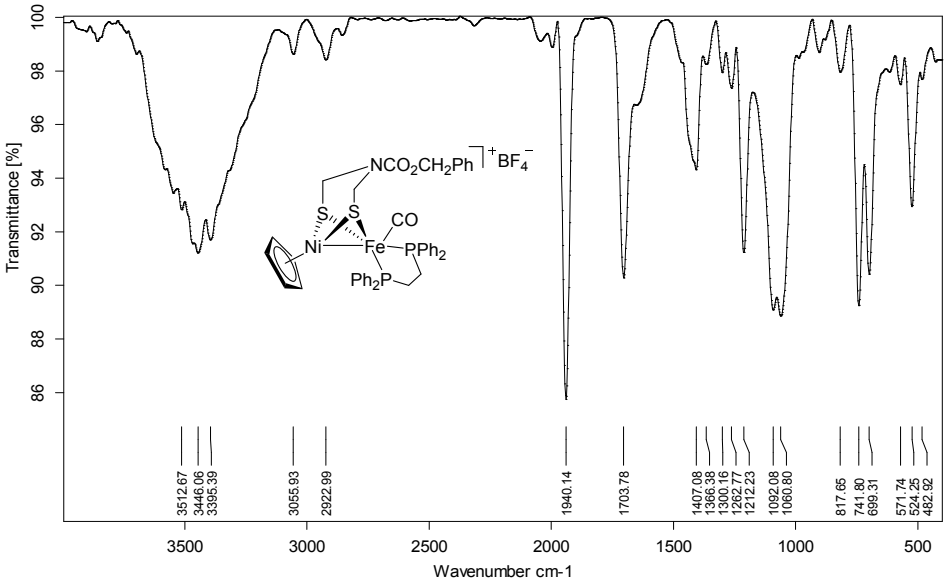

Fig. S20 IR spectrum of **8**

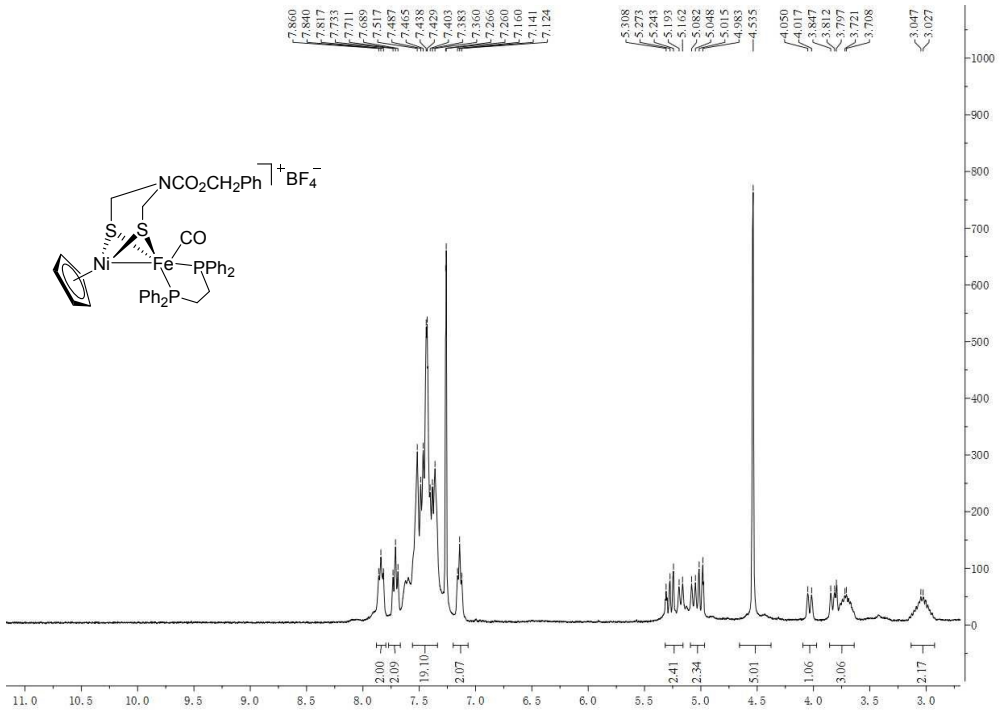

Fig. S21 ^{1}H NMR spectrum of **8** in $CDCl_3$

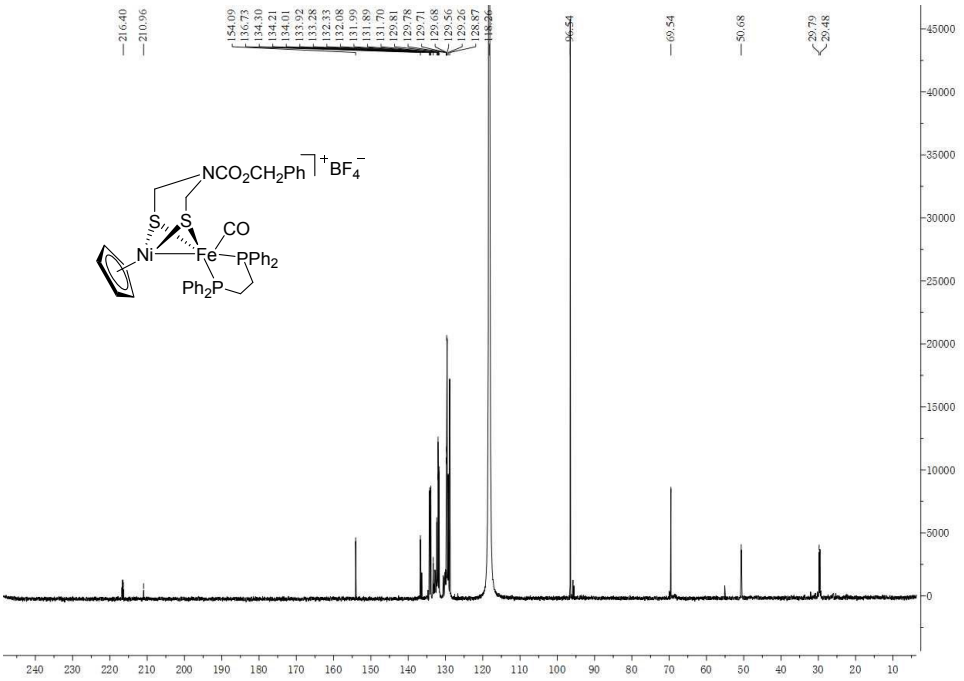

Fig. S22 ^{13}C NMR spectrum of **8** in CD_3CN

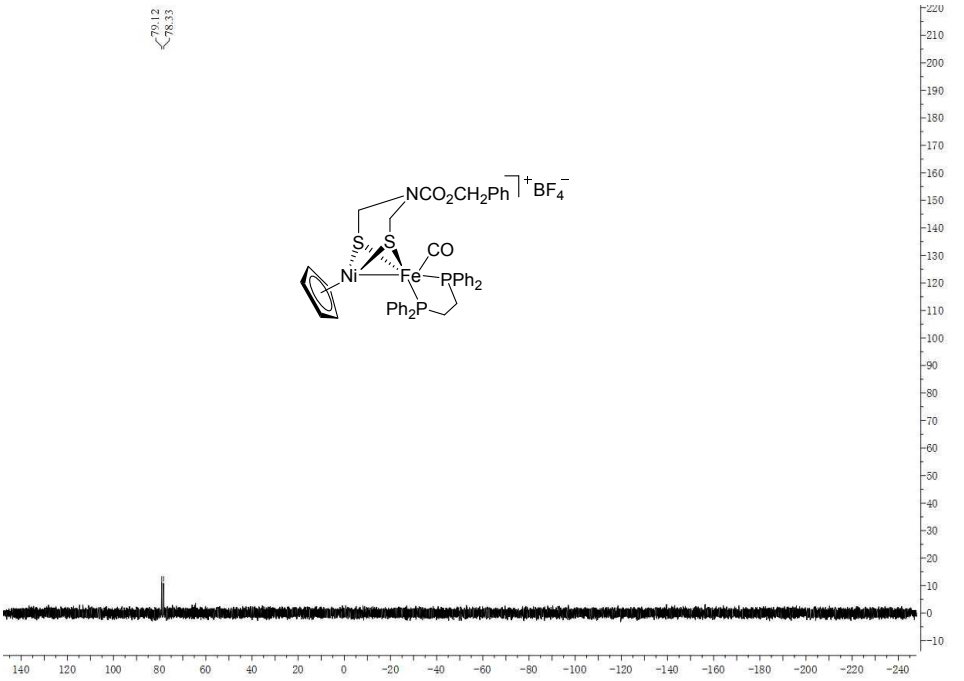

Fig. S23 ^{31}P NMR spectrum of **8** in $CDCl_3$