Supporting Information

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Two heterodinuclear NiFe-based sulfenate complexes mimicking an S-oxygenated intermediate of an O_2-tolerant [NiFe]-H_2ase: synthesis, structures, and reactivity

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Contents:

1. Selected bond lengths (Å) and angles (°) for complexes 2–5 and 7

Table S1 Selected bond lengths (Å) and angles (°) for complexes **2–5** and **7**

	2	**3**	**4**[a]	**5**	**7**
Ni1–S1	2.1440(10)	2.1147(9)	2.1513(13)	2.1533(5)	2.1520(15)
Ni1–S2	2.1358(12)	2.1344(12)	2.1512(13)	2.1742(5)	2.1536(16)
Ni1–N1	1.950(3)	1.953(2)	1.930(4)	1.9439(16)	1.921(5)
Ni1–N2	1.945(3)	1.936(2)	1.930(4)	1.9668(17)	1.921(5)
S1–Ni1-S2	93.43(4)	96.04(4)	92.53(7)	98.84(2)	90.27(6)
N1–Ni1–S1	90.56(9)	87.89(7)	91.77(13)	89.15(5)	92.60(15)
N1–Ni1–S2	175.97(9)	175.65(7)	173.29(13)	171.96(5)	174.34(15)
S1–Ni1–N2	174.04(9)	171.35(7)	173.29(13)	171.70(5)	173.41(15)
N2–Ni1–S2	92.36(10)	92.54(7)	91.77(13)	89.23(5)	92.66(16)
N1–Ni1–N2	83.64(13)	83.58(10)	83.5(2)	82.81(7)	84.0(2)

[a] For complex **4** the corresponding bond lengths and angles are Ni1–S1, Ni1–S1a, Ni1–N1, Ni1–N1a, S1–Ni1-S1a, N1–Ni1–S1, N1–Ni1–S1a, S1–Ni1–N1a, N1a–Ni1–S1a, N1–Ni1–N1a, respectively.

2. IR and $^{1}H(^{13}C)$ NMR spectra of 1

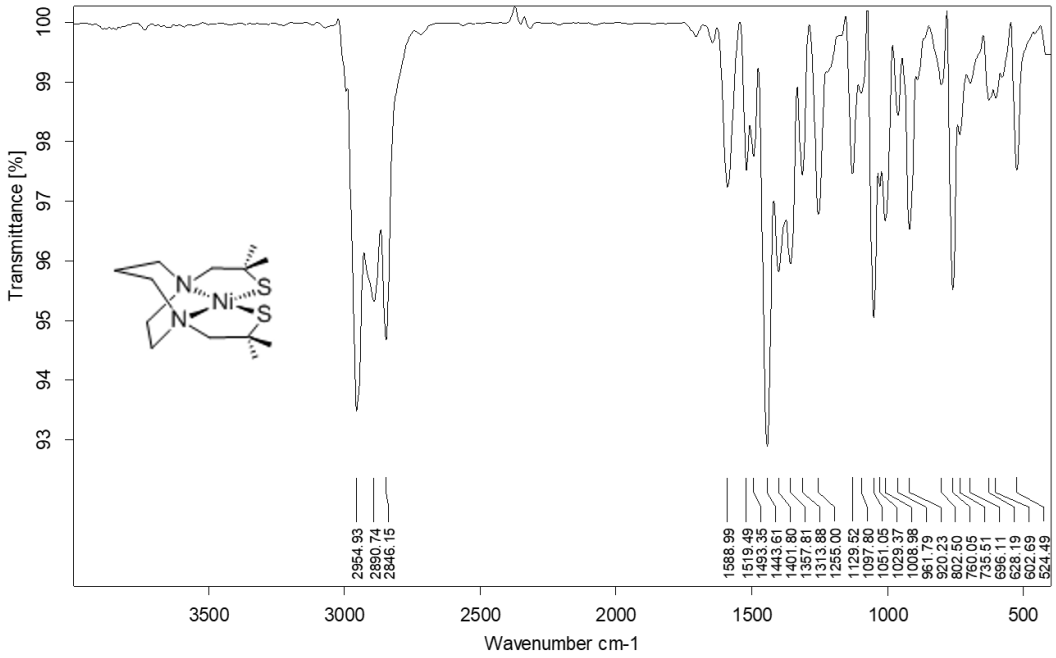

Fig. S1 IR spectrum of **1**

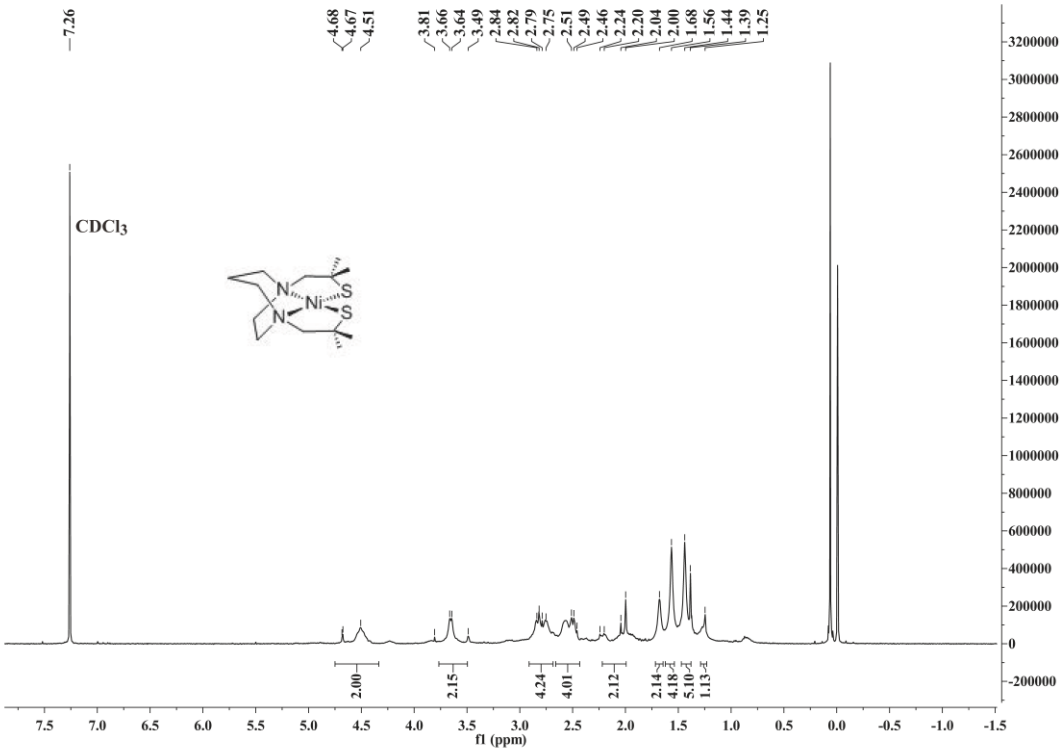

Fig. S2 ^{1}H NMR spectrum of **1**

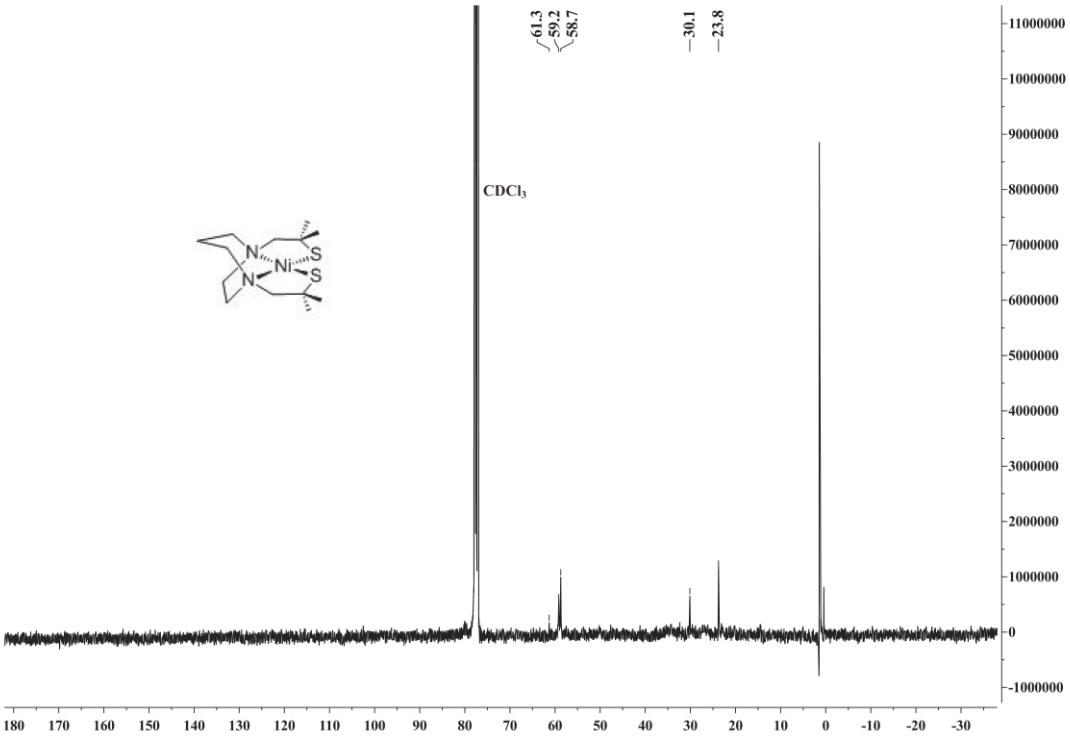

Fig. S3 ^{13}C NMR spectrum of **1**

3. IR and $^{1}H(^{13}C)$ NMR spectra of 2

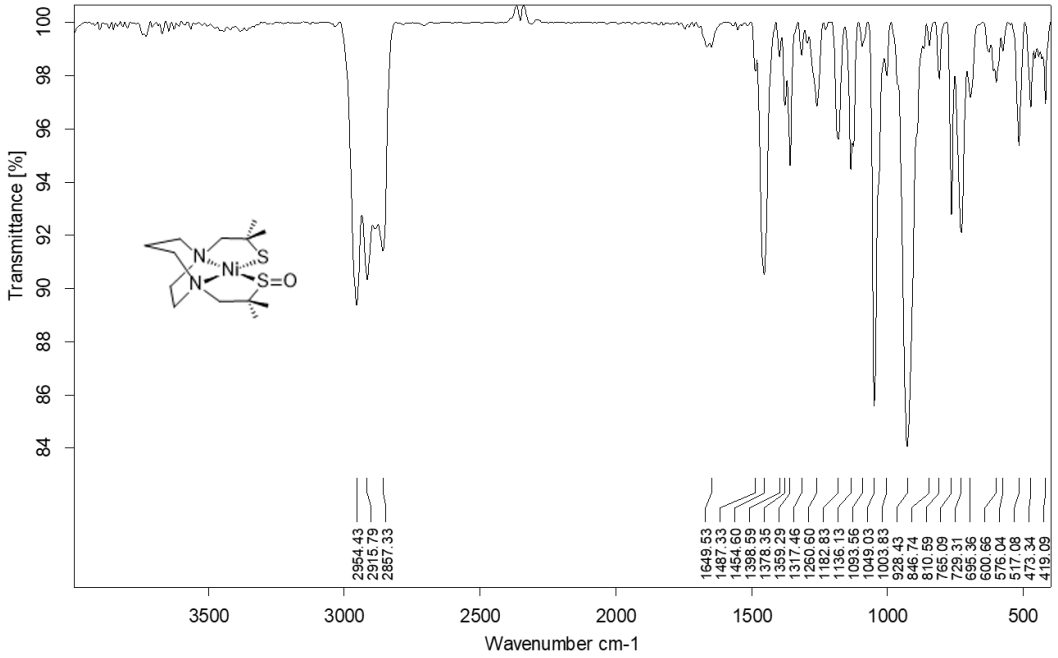

Fig. S4 IR spectrum of **2**

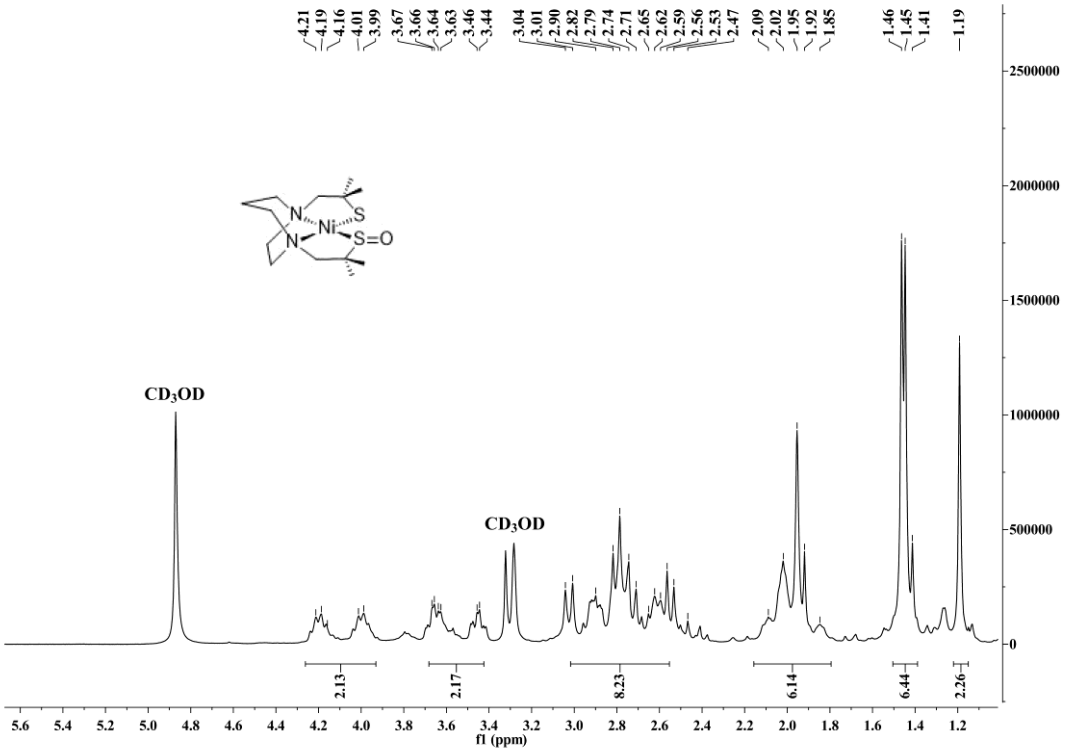

Fig. S5 ^{1}H NMR spectrum of **2**

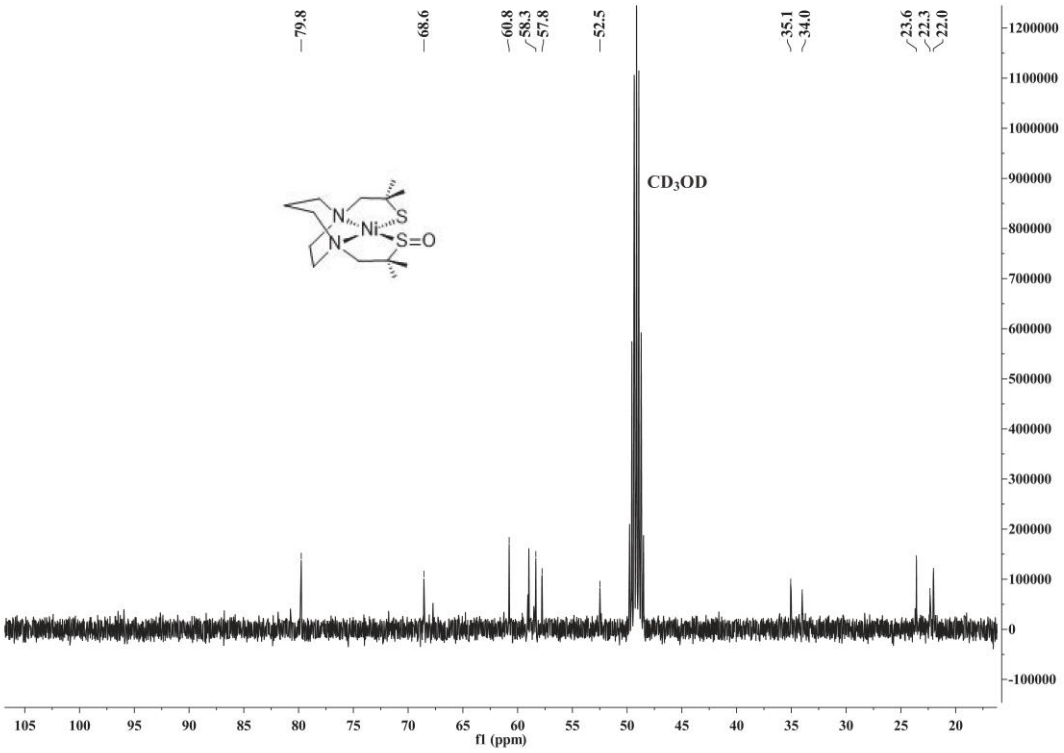

Fig. S6 ^{13}C NMR spectrum of **2**

4. IR and $^{1}H(^{13}C)$ NMR spectra of 3

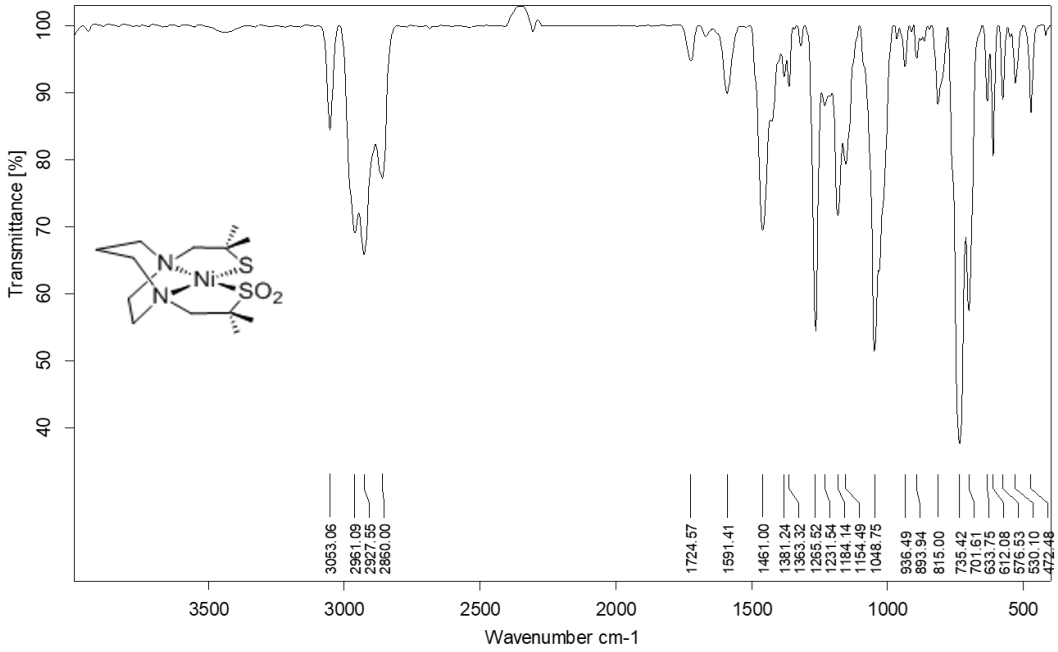

Fig. S7 IR spectrum of **3**

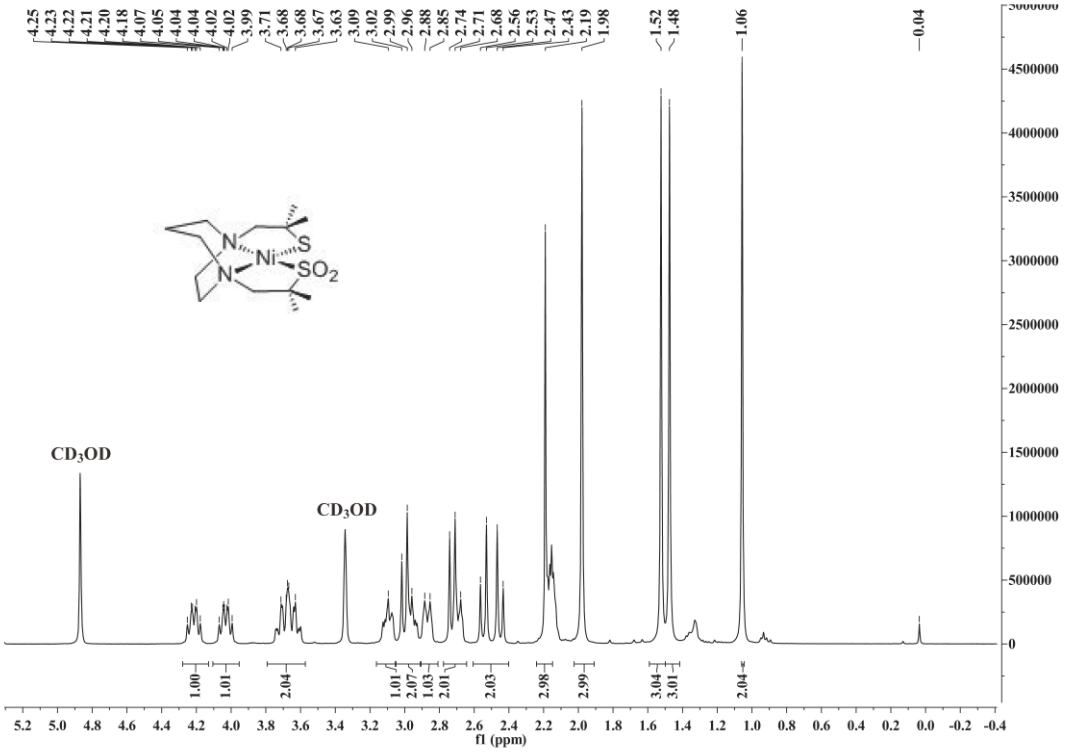

Fig. S8 ^{1}H NMR spectrum of **3**

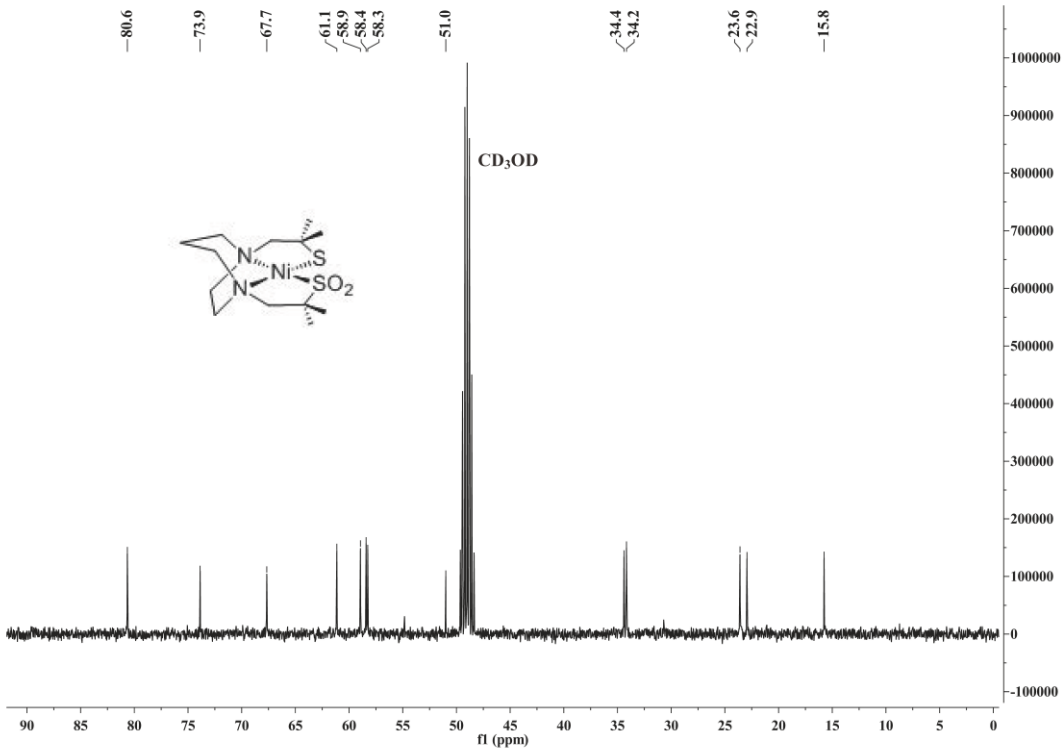

Fig. S9 ^{13}C NMR spectrum of **3**

5. IR and $^{1}H(^{13}C)$ NMR spectra of 4

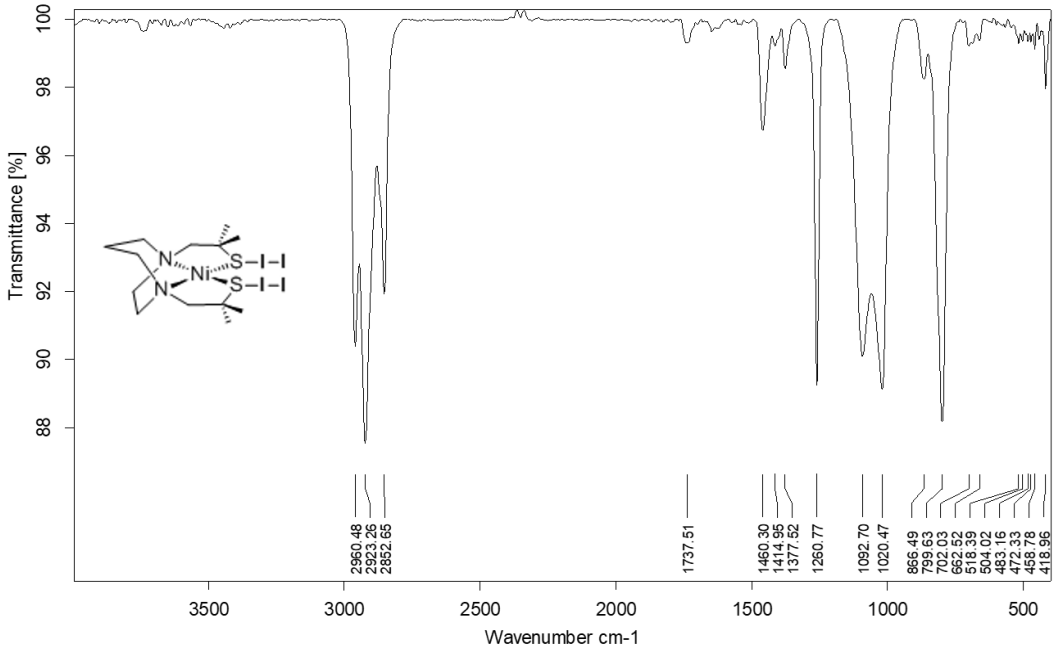

Fig. S10 IR spectrum of **4**

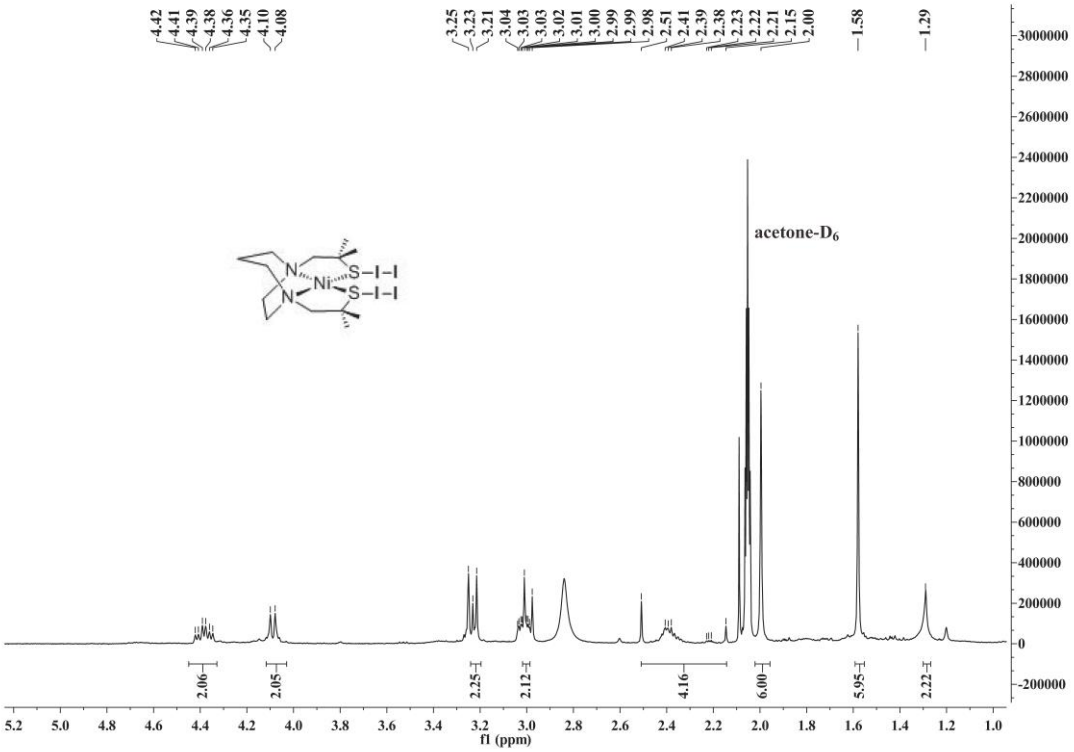

Fig. S11 ^{1}H NMR spectrum of **4**

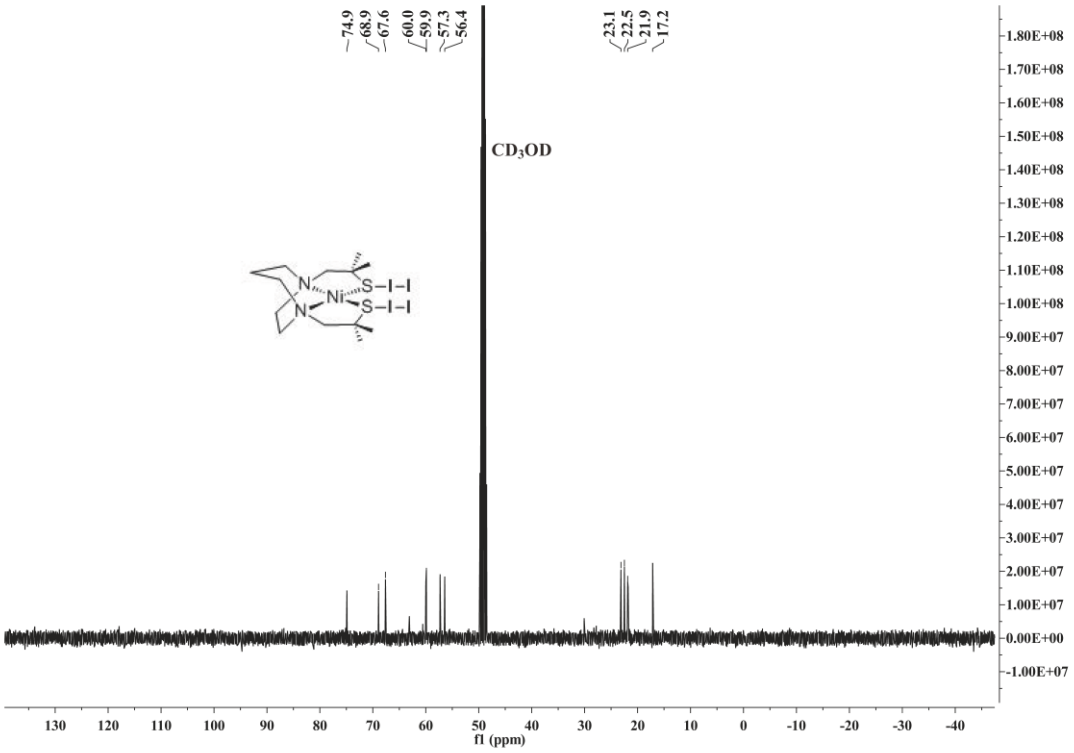

Fig. S12 ^{13}C NMR spectrum of **4**

6. IR and $^{1}H(^{13}C)$ NMR spectra of 5

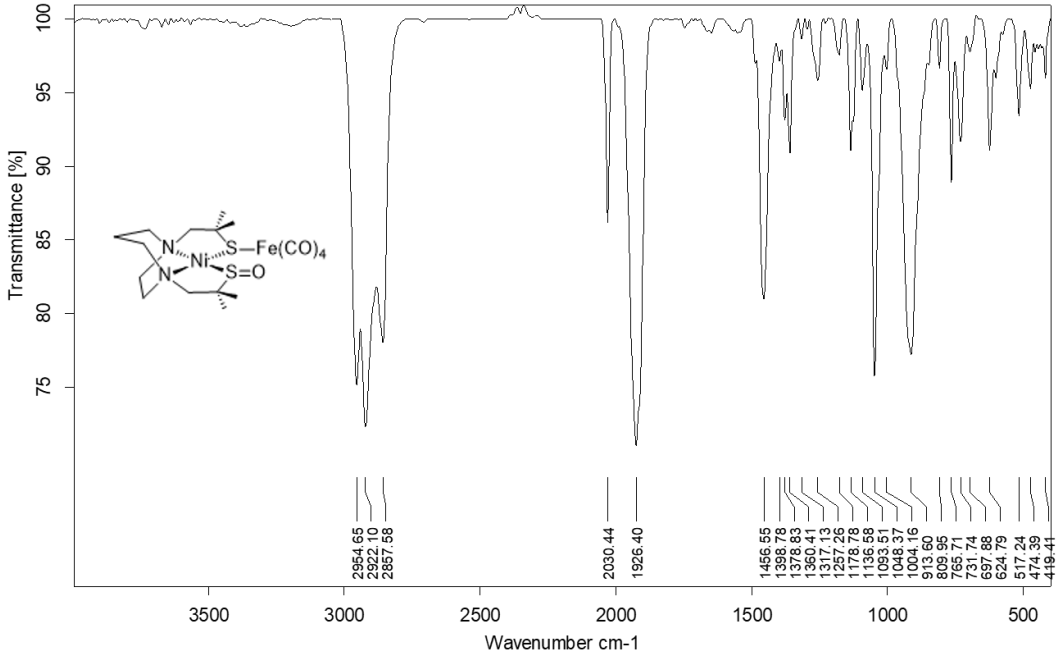

Fig. S13 IR spectrum of **5**

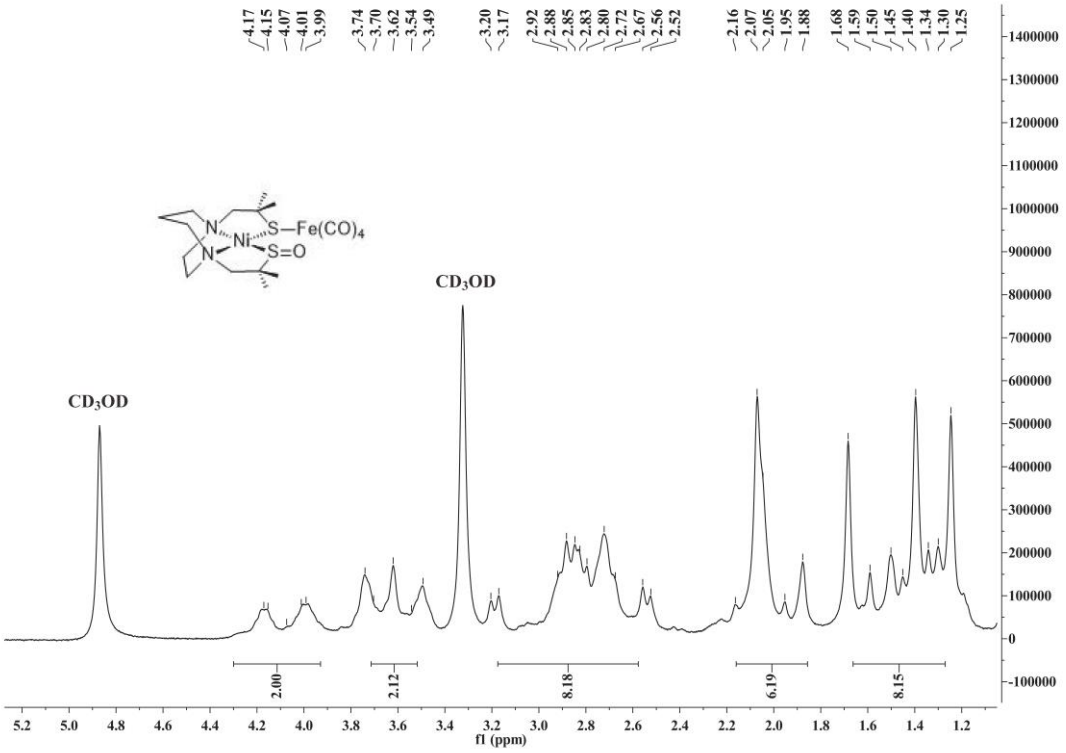

Fig. S14 ^{1}H NMR spectrum of **5**

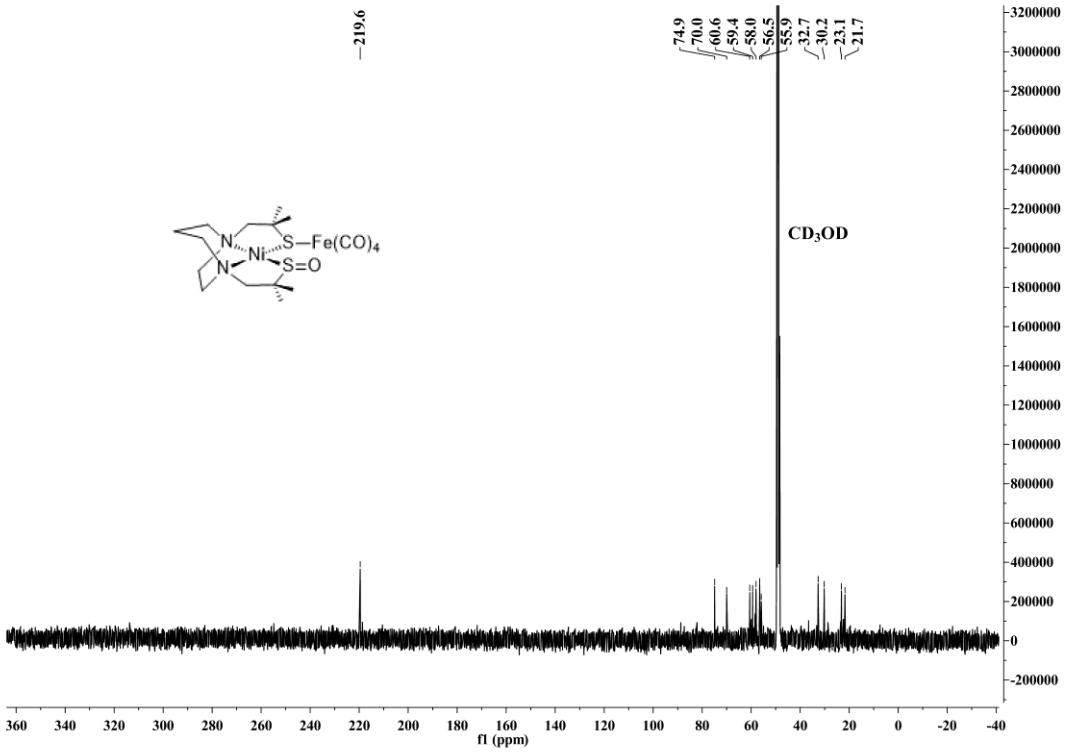

Fig. S15 ^{13}C NMR spectrum of **5**

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

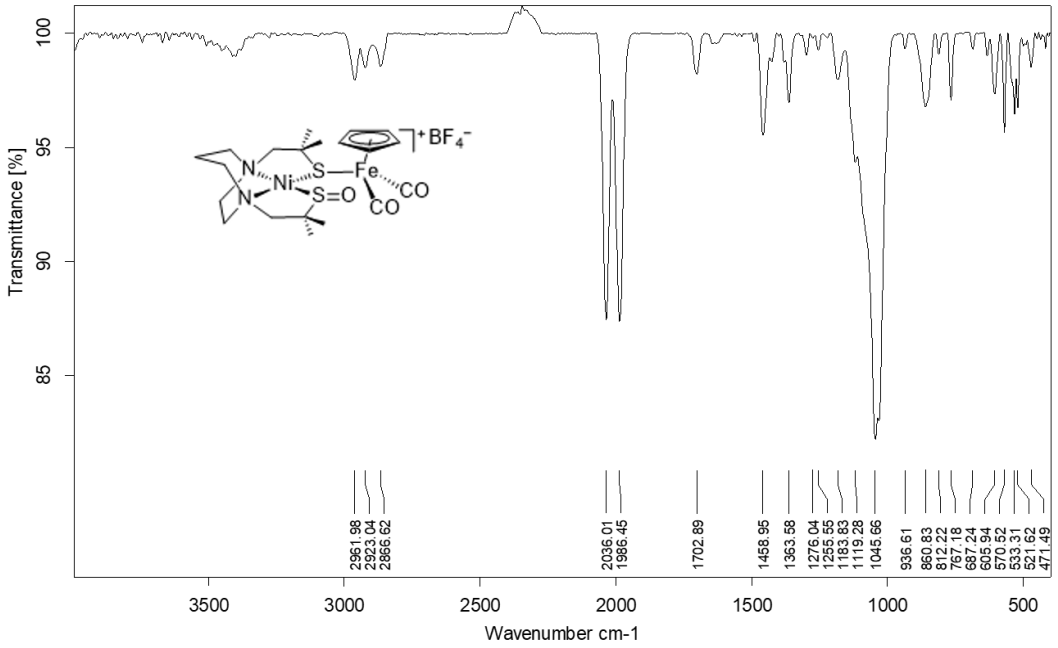

Fig. S16 IR spectrum of **6**

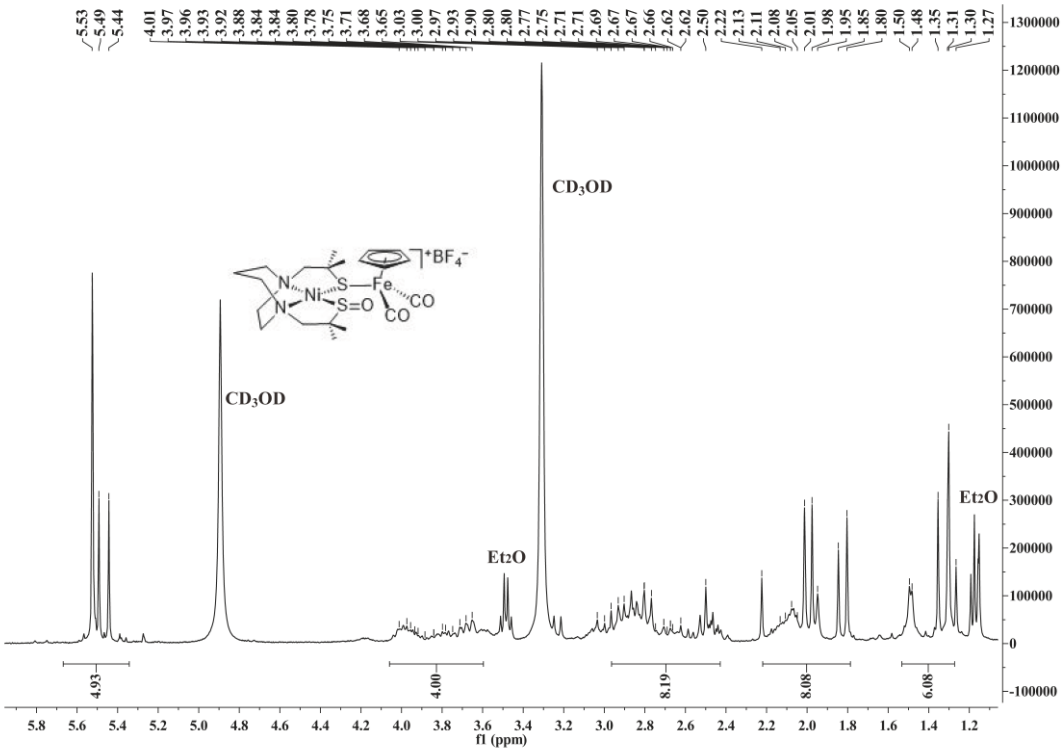

Fig. S17 ^{1}H NMR spectrum of **6**

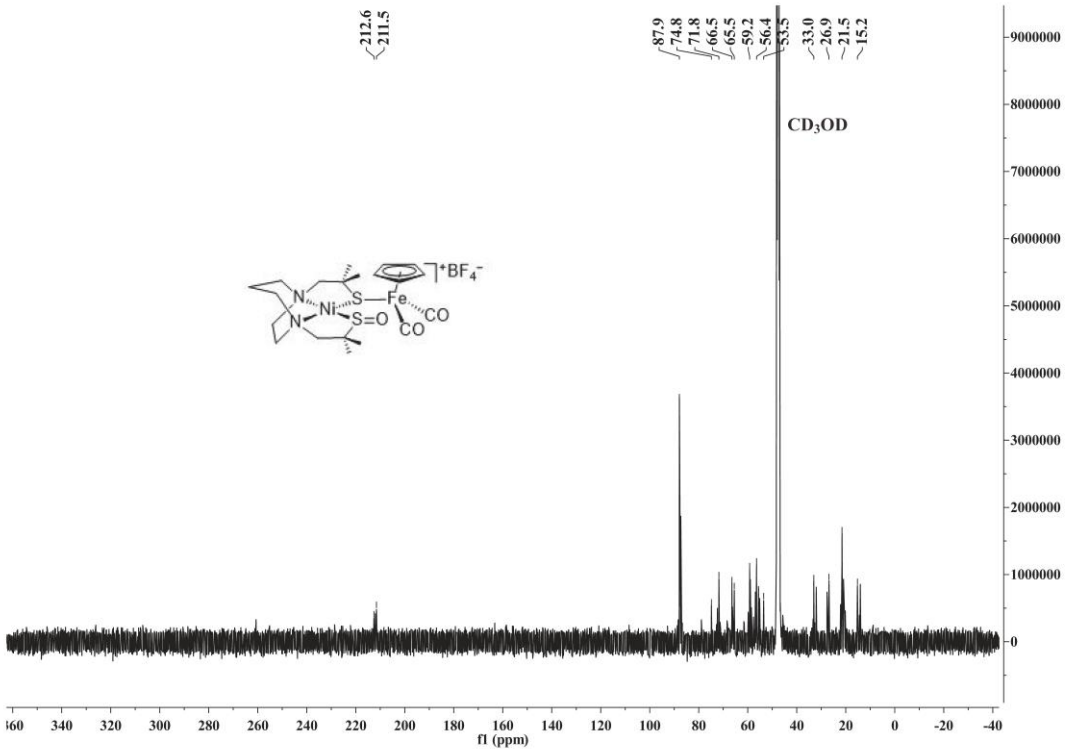

Fig. S18 ^{13}C NMR spectrum of **6**

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

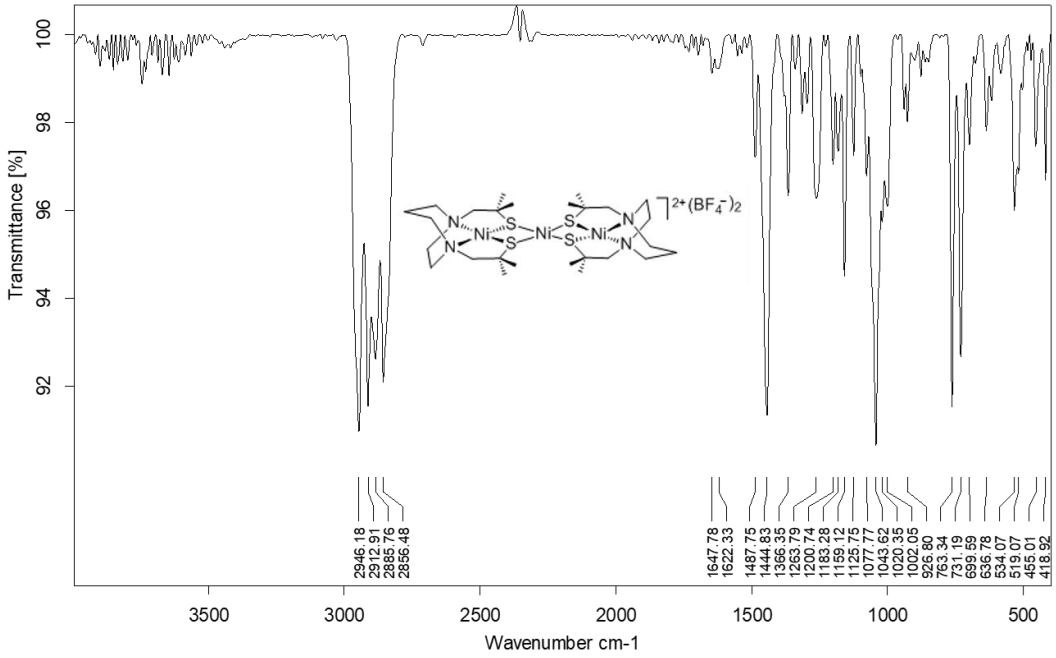

Fig. S19 IR spectrum of **7**

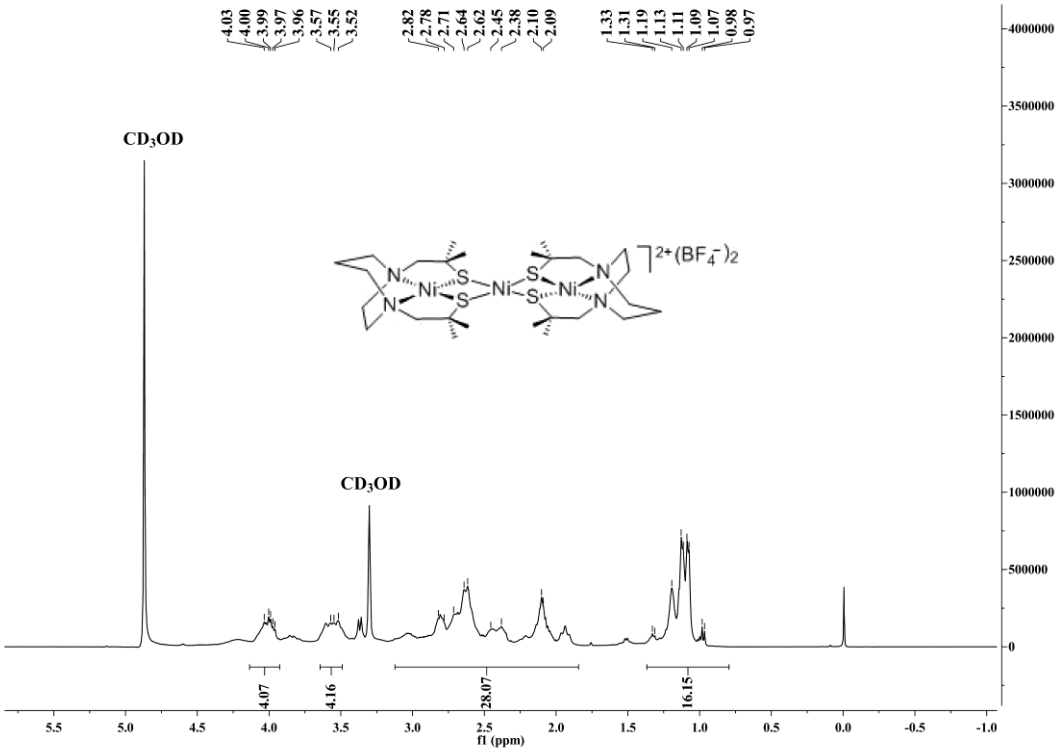

Fig. S20 ^{1}H NMR spectrum of **7**

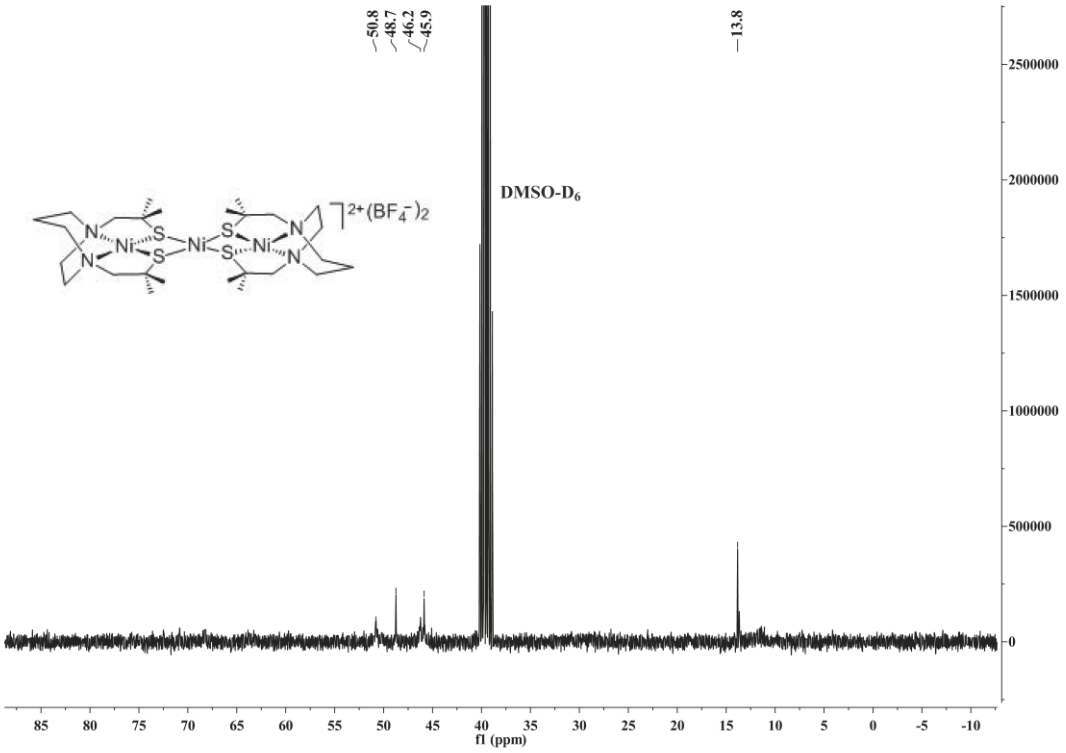

Fig. S21 ^{13}C NMR spectrum of **7**