Supporting Information

for

Carbene−carbanion equilibrium

for tris(2-pyridylthio)methanido Fe(II) complexes

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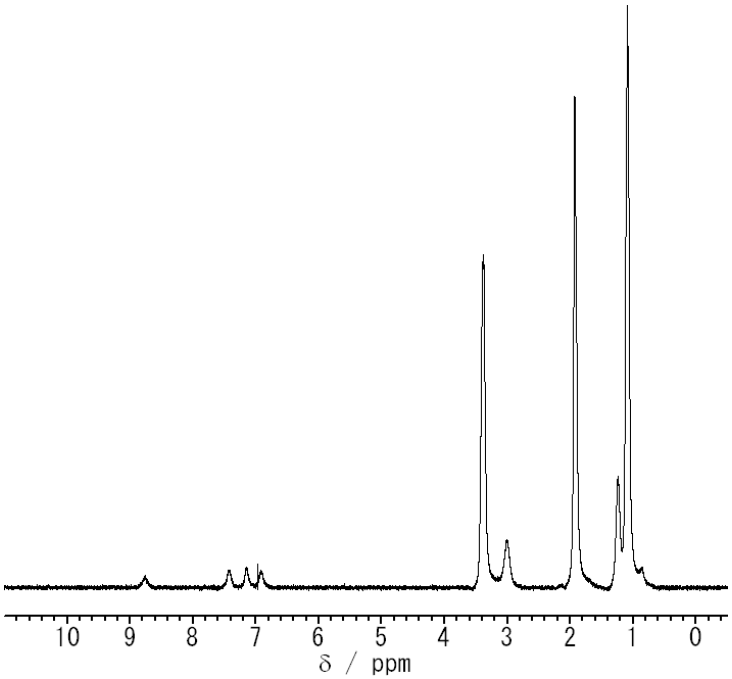

Fig. S1 The ^{1}H NMR spectrum of complex **1** in CD_3CN.

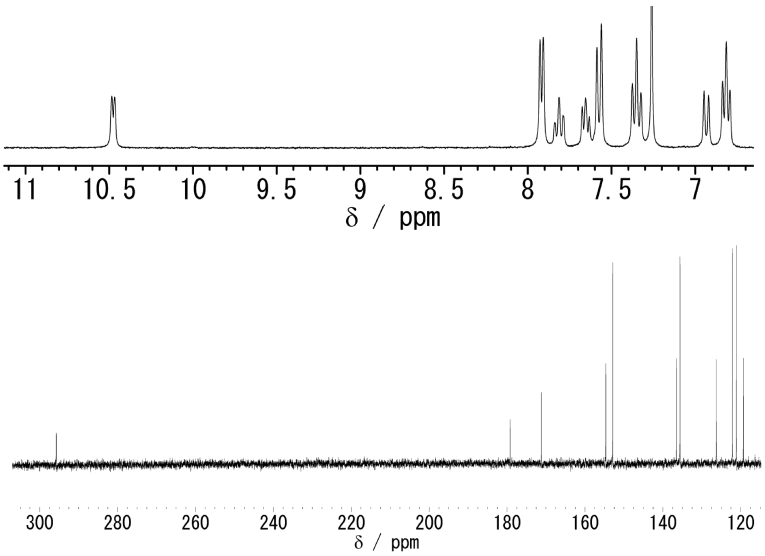

Fig. S2 The ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of complex **2** in $CDCl_3$.

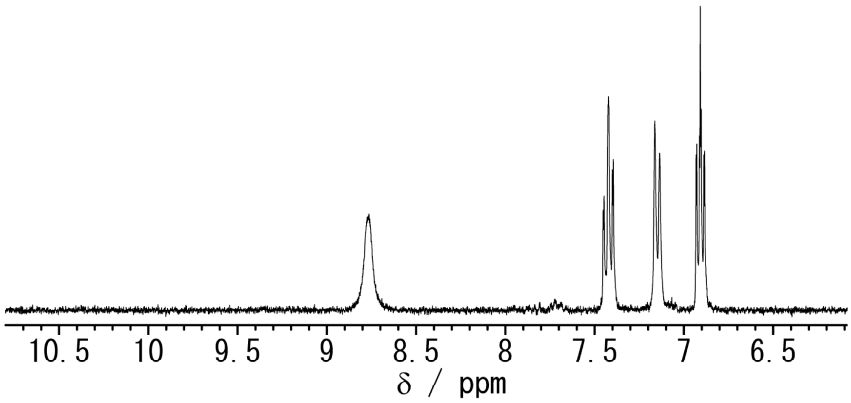

Fig. S3 The ^{1}H NMR spectrum of complex **2** in CD_3CN.

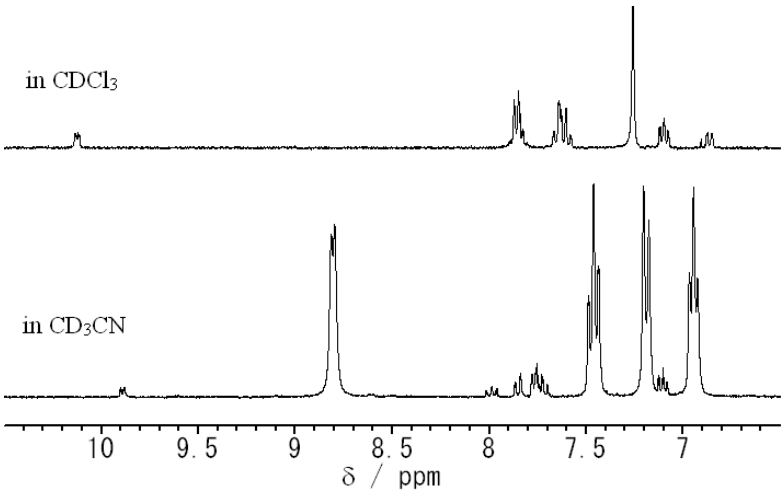

Fig. S4 ^{1}H NMR spectra of the carbanion complex **3** in $CDCl_3$ (top) and CD_3CN (bottom).

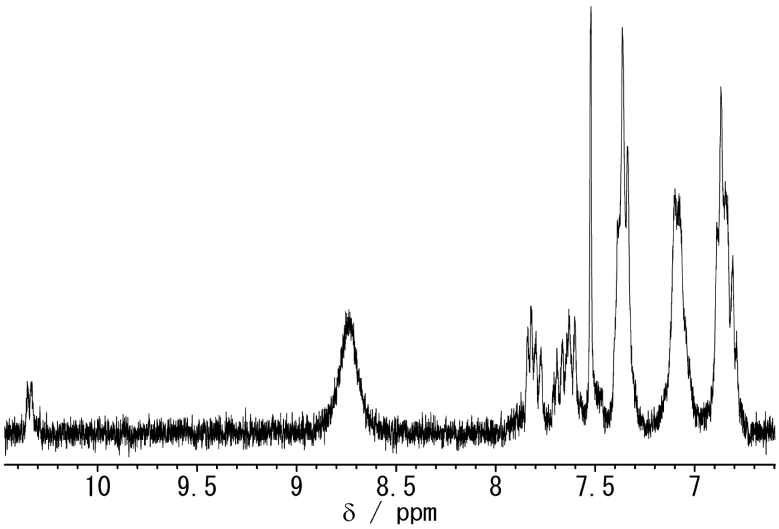

Fig. S5 The ^{1}H NMR spectrum of complex **2** in $CDCl_3$:CD_3CN (1:1).

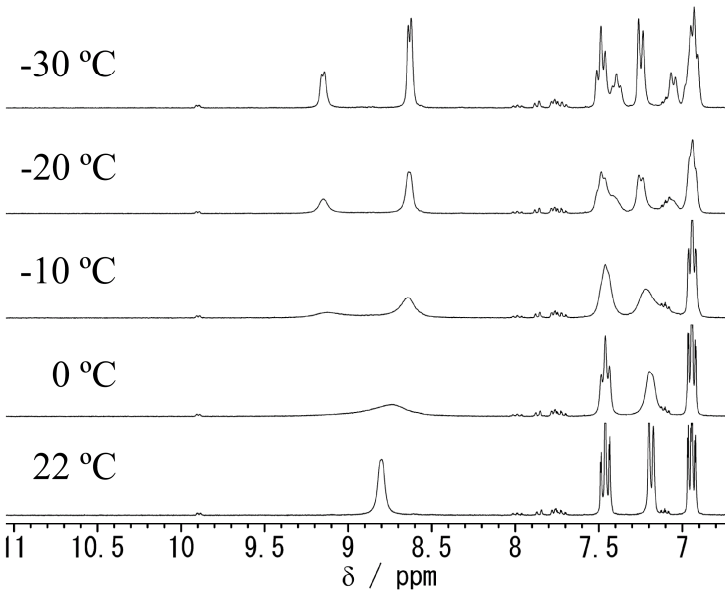

Fig. S6 The ^{1}H NMR spectral changes of complex **3** in CD_3CN with various temperature conditions (from 22 ºC to –30 ºC).

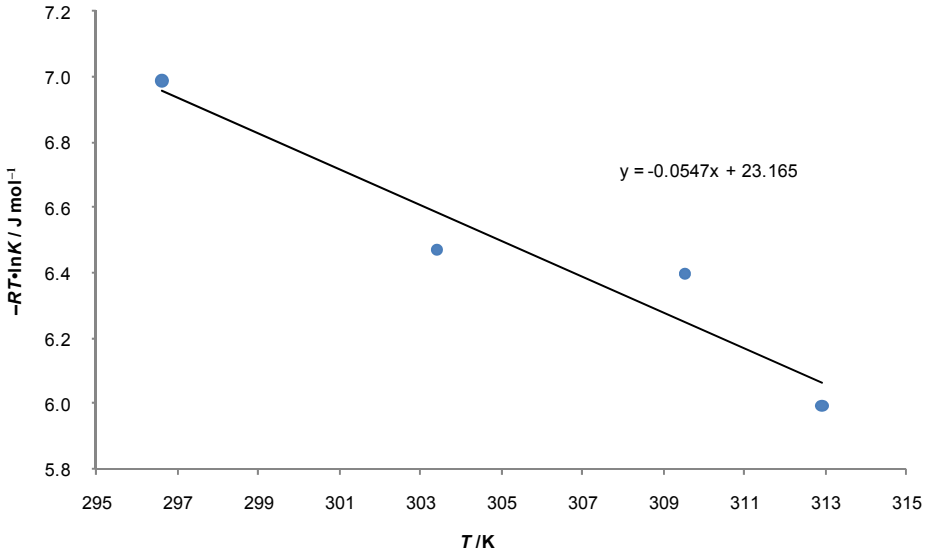

Fig. S7 The plot of ΔG vs T for the equilibrium between carbanion (**3**) and carbene (**3'**).

Chemical transformation of complex 3 to complex 1

Solid KI was added to a solution of **3** (10 mg) in acetonitrile (5 mL) and the mixture was stirred for 20 min. Ether (20 mL) was put onto the resulted red solution to give red crystals of **1** (2 mg, 24%).