

Ferrous and Cobaltous Chlorides Bearing 2,8-Bis(imino)quinolines: Highly Active Catalysts for Ethylene Polymerization at High Temperature [*Organometallics* 2010, 29, 1168. DOI: 10.1021/om9010142]. Shu Zhang, Wen-Hua Sun,* Tianpengfei Xiao, and Xiang Hao

It was recently discovered that the ^1H NMR spectra of paramagnetic complexes of iron (**Fe1** and **Fe2**) and cobalt (**Co1** and **Co2**) in CD_3OD were incorrect and showed the presence of the dissociated ligands. Therefore, these complexes were additionally measured in CD_2Cl_2 for their NMR spectra; moreover, the temperature-dependent magnetic susceptibility measurements were also carried out. Herein we adjusted the NMR data appearing on pages 1172 and 1173 for **Fe1**, **Fe2**, **Co1**, and **Co2** along with the ^1H NMR spectra in the Supporting Information. The signal assignments were made on the basis of integration and proximity to the paramagnetic center according to the literature.^{1,2} In addition, the charts of their paramagnetic properties are also added for further references.

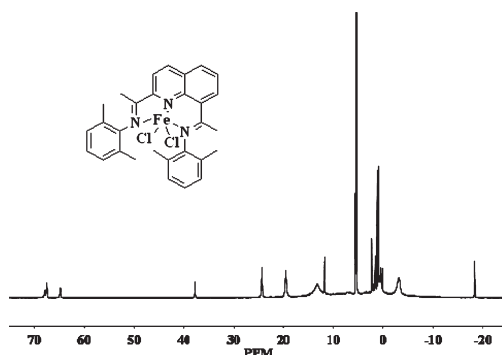


Figure 1. ^1H NMR spectrum of **Fe1** (600 MHz, 20 °C, CD_2Cl_2).

^1H NMR for complex **Fe1** (Figure 1; 600 MHz, CD_2Cl_2): δ 67.9 (s, 1H, quino *H*), 67.4 (s, 1H, quino *H*), 64.8 (s, 1H, quino *H*), 37.7 (s, 1H, quino *H*), 24.3 (s, 3H, CH_3), 19.4 (s, 3H, CH_3), 13.2 (s, 3H, CH_3), 11.8 (s, 2H, Ar *H*), 2.3 (s, 1H, quino *H*), 1.6 (s, 1H, Ar *H*), 1.3 (s, 3H, CH_3), 0.9 (s, 2H, Ar *H*), 0.4 (s, 3H, CH_3), -3.0 (s, 3H, CH_3), -18.4 (s, 1H, Ar *H*).

^1H NMR for complex **Fe2** (Figure 2; 600 MHz, CD_2Cl_2): δ 69.1 (s, 1H, quino *H*), 68.7 (s, 1H, quino *H*), 66.9 (s, 1H, quino *H*), 37.6 (s, 1H, quino *H*), 24.0 (s, 3H, CH_3), 23.7 (s, 3H, CH_3), 20.8 (s, 3H, CH_3), 17.2 (s, 3H, CH_3), 13.3 (s, 3H, CH_3), 11.3 (s, 2H, Ar *H*), 2.3 (s, 1H, quino *H*), 1.3 (s, 3H, CH_3), 0.9 (s, 2H, Ar *H*), 0.5 (s, 3H, CH_3), -2.5 (s, 3H, CH_3).

^1H NMR for complex **Co1** (Figure 3; 600 MHz, CD_2Cl_2): δ 72.9 (s, 1H, quino *H*), 43.2 (s, 1H, quino *H*), 25.0 (s, 1H,

(1) Britovsek, G. J. P.; Bruce, M.; Gibson, V. C.; Kimberley, B. S.; Maddox, P. J.; Mastroianni, S.; McTavish, S. J.; Redshaw, C.; Solan, G. A.; Strömberg, S.; White, A. J. P.; Williams, D. J. *J. Am. Chem. Soc.* **1999**, 121, 8728.

(2) Bianchini, C.; Mantovani, G.; Meli, A.; Migliacci, F.; Zanolini, F.; Laschi, F.; Sommaczi, A. *Eur. J. Inorg. Chem.* **2003**, 1620.

quino *H*), 23.0 (s, 1H, quino *H*), 17.6 (s, 3H, CH₃), 15.4 (s, 2H, Ar *H*), 14.8 (s, 6H, CH₃), 2.4 (s, 1H, quino *H*), 1.3 (s, 9H, CH₃), 0.9 (s, 2H, Ar *H*), -3.8 (s, 1H, Ar *H*), -4.1 (s, 1H, Ar *H*).

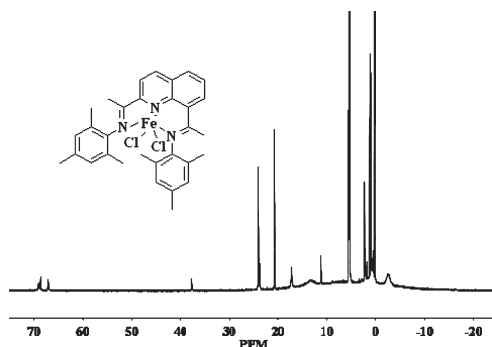


Figure 2. ¹H NMR spectrum of **Fe2** (600 MHz, 20 °C, CD₂Cl₂).

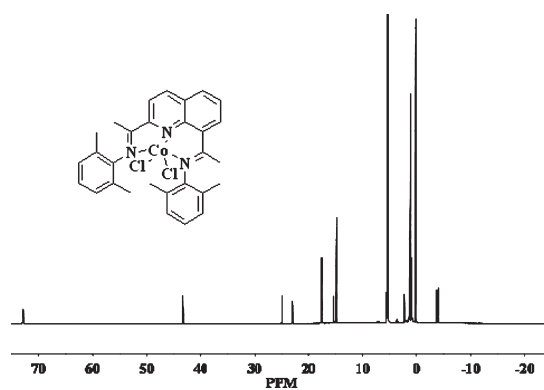


Figure 3. ¹H NMR spectrum of **Co1** (600 MHz, 20 °C, CD₂Cl₂).

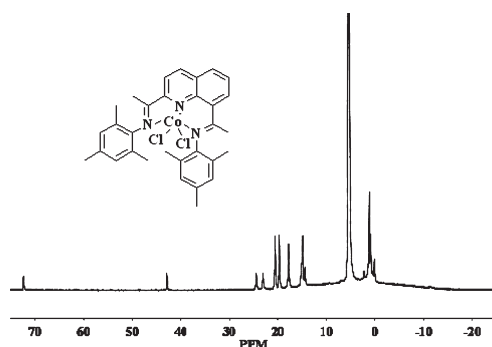


Figure 4. ¹H NMR spectrum of **Co2** (600 MHz, 20 °C, CD₂Cl₂).

¹H NMR for complex **Co2** (Figure 4; 600 MHz, CD₂Cl₂):
 δ 72.2 (s, 1H, quino *H*), 42.7 (s, 1H, quino *H*), 24.3 (s, 1H, quino *H*), 23.0 (s, 1H, quino *H*), 20.6 (s, 3H, CH₃), 19.6 (s, 3H, CH₃), 17.8 (s, 3H, CH₃), 14.8 (s, 6H, CH₃), 14.3 (s, 2H, Ar *H*), 2.3 (s, 1H, quino *H*), 1.3 (s, 9H, CH₃), 0.9 (s, 2H, Ar *H*).

Magnetic Susceptibility Measurements

The paramagnetic properties of these complexes were also proved by checking the temperature-dependent magnetic susceptibility measurements for four compounds (**Fe1**, **Fe2**, **Co1**, and **Co2**) over a temperature range from 2 to 300 K at 1000 Oe.

The plots of χ and $1/\chi$ versus T are shown in Figures 5–8. All four compounds obey the Curie–Weiss law in the temperature range of 2–300 K. At 300 K, the χT values of 3.416 and 2.555 $\text{emu mol}^{-1} \text{K}$ (5.23 and $4.52 \mu_{\text{B}}$), respectively, for **Fe1** and **Fe2** are comparable with the expected magnetic moment value for one isolated Fe^{2+} ($4.9 \mu_{\text{B}}$ for $3d^6$, $S = 2$, for $g = 2$) ion. Furthermore, the χT values of 2.789 and 2.379 $\text{emu mol}^{-1} \text{K}$ (4.72 and $4.36 \mu_{\text{B}}$), respectively, for **Co1** and **Co2** are also in good agreement with the theoretical value for one isolated Co^{2+} ion ($4.65 \mu_{\text{B}}$ for $3d^7$, $S = 3/2$, for $g = 2.4$).

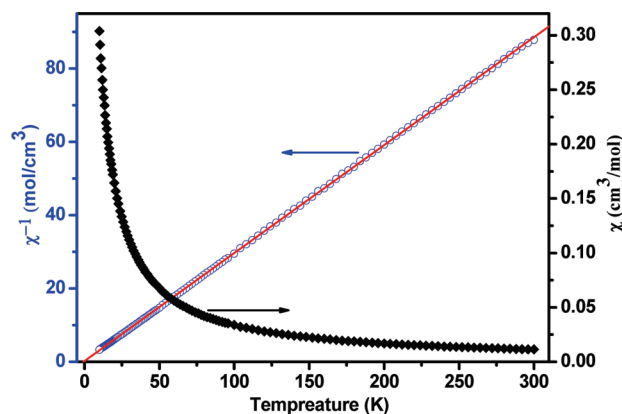


Figure 5. Temperature-dependent magnetic susceptibility measurements for **Fe1**.

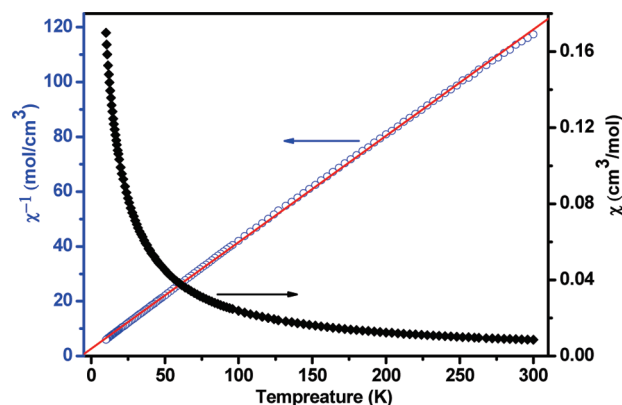


Figure 6. Temperature-dependent magnetic susceptibility measurements for **Fe2**.

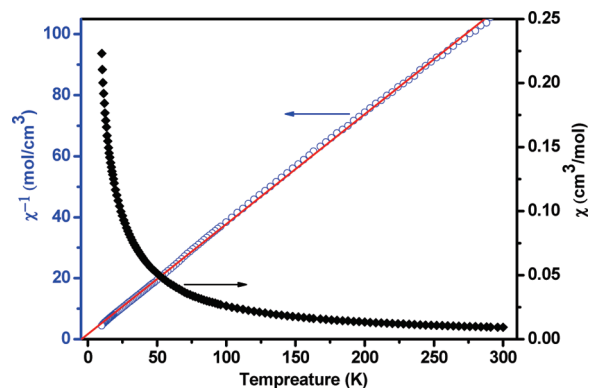


Figure 7. Temperature-dependent magnetic susceptibility measurements for **Co1**.

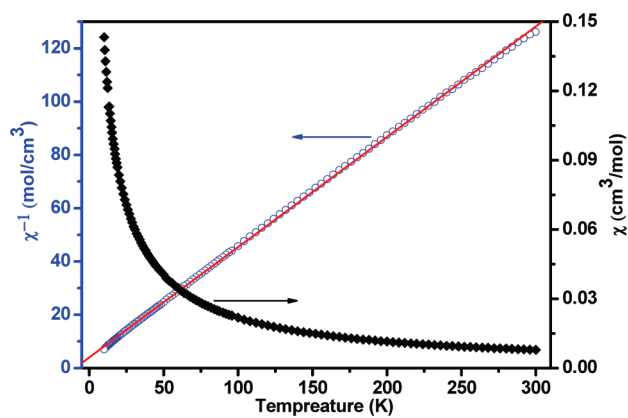


Figure 8. Temperature-dependent magnetic susceptibility measurements for Co₂.

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