Supporting Information

Insertion Reactions of a Two-Coordinate Iron Diaryl with Dioxygen and Carbon Monoxide

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1. Magnetic Determination of 1 and 2 by Evans' method.

3.00 mg of **1** was dissolved in exactly 0.80 mL mixture of C_6H_6 and C_6D_6 (c = 4.407 $\times 10^{-3}$ mol/L) and some solution was transferred into an NMR tube. Into the NMR tube, a sealed capillary that contained the C_6H_6/C_6D_6 solvent mixture was placed. The NMR spectra were recorded on a Varian spectrometer operating at 300.077 MHz at 292.75 K. Two peaks were identified for C_6H_6 protons, which have a chemical shift difference of 0.183 ppm. Based on the theory of Evans method,[1,2] the magnetic susceptibility was calculated to be 9.905 $\times 10^{-3}$ cm^3mol^{-1}, which corresponds to an effective magnetic moment of 4.82 μ_B per molecule for **1**.

5.18 mg of **2** was dissolved in exactly 0.80 mL mixture of C_6H_6 and C_6D_6 (c = 7.330 $\times 10^{-3}$ mol/L) and some solution was transferred into an NMR tube. Into the NMR tube, a sealed capillary that contained the C_6H_6/C_6D_6 solvent mixture was placed. The NMR spectra were recorded on a Varian spectrometer operating at 300.077 MHz at 292.75 K. Two peaks were identified for C_6H_6 protons, which have a chemical shift difference of 0.366 ppm. Based on the theory of Evans method,[1,2] the magnetic susceptibility was calculated to be 1.191 $\times 10^{-2}$ cm^3mol^{-1}, which corresponds to an effective magnetic moment of 5.28 μ_B per molecule for **2**.

References:
1. Evans, D. F., *J. Chem. Soc.* **1959**, 2003.
2. Schubert, E. M., *J. Chem. Educ.* **1992,** *69*, 62.