

Supplementary Information for

**Structural, Magnetic, and Mössbauer Spectral Study of the Electronic
Spin-State Transition in {Fe[HC(3-Mepz)₂(5-Mepz)]₂}(BF₄)₂**

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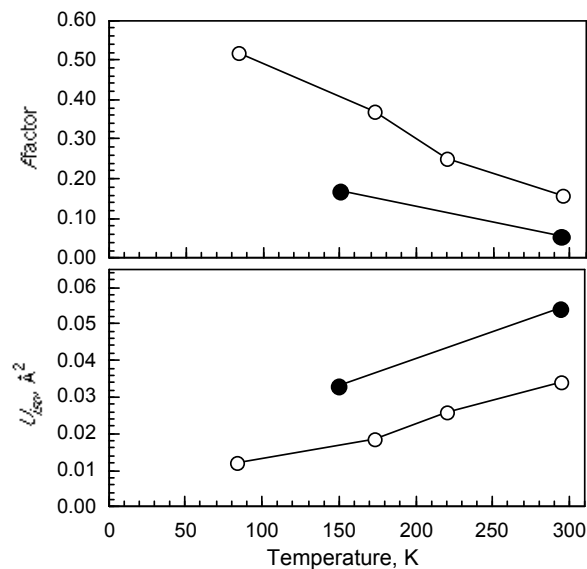


Figure S1. The temperature dependence of the thermal factor, U_{iso} , and the equivalent recoil-free fraction, the f -factor, of **1**, solid points, and of $\{\text{Fe}[\text{HC}(3,5\text{-Me}_2\text{pz})_3]_2\}(\text{BF}_4)_2$, open points.^{6a,c} The error bars are smaller than the data points.

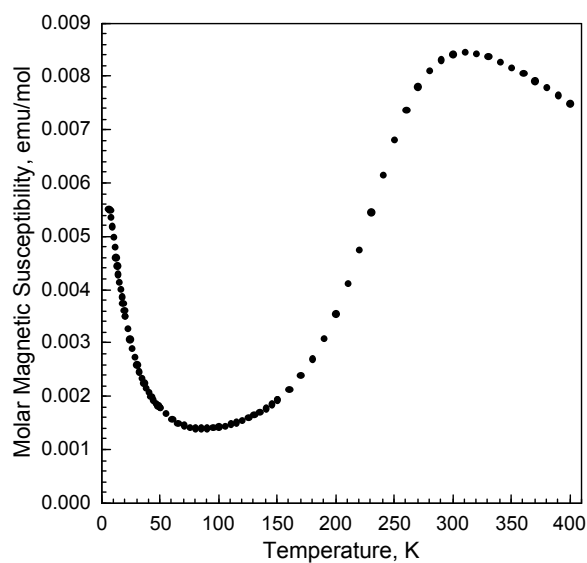


Figure S2. The temperature dependence of χ_M obtained for **1** after zero-field cooling and subsequent warming and cooling in a 0.1 T applied field.

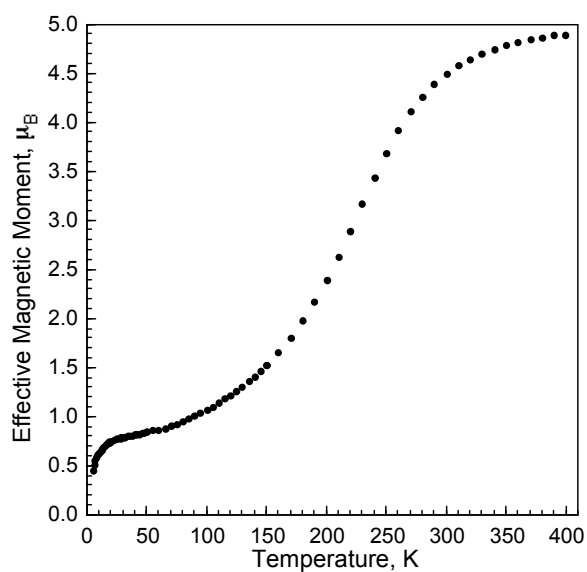


Figure S3. The temperature dependence of μ_{eff} obtained for **1** after zero-field cooling and subsequent warming and cooling in a 0.1 T applied field.

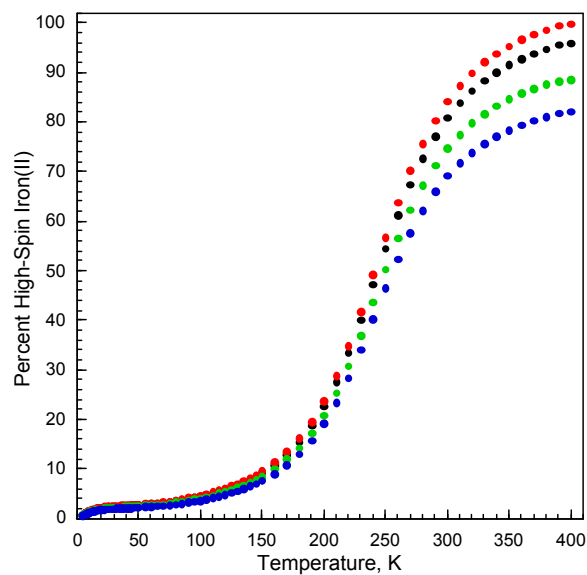


Figure S4. The temperature dependence of the percentage of high-spin iron(II) in **1** obtained with the 300 K low-spin and high-spin μ_{eff} values, respectively, of 0.0 and 4.9 μ_B , red, 0.1 and 5.0 μ_B , black, 0.2 and 5.2 μ_B , green, and 0.4 and 5.4 μ_B , blue.