

Supplementary Information for

**Structural, Magnetic, and Mössbauer Spectral Study of the Electronic  
Spin-State Transition in {Fe[HC(3-Mepz)<sub>2</sub>(5-Mepz)]<sub>2</sub>}(BF<sub>4</sub>)<sub>2</sub>**

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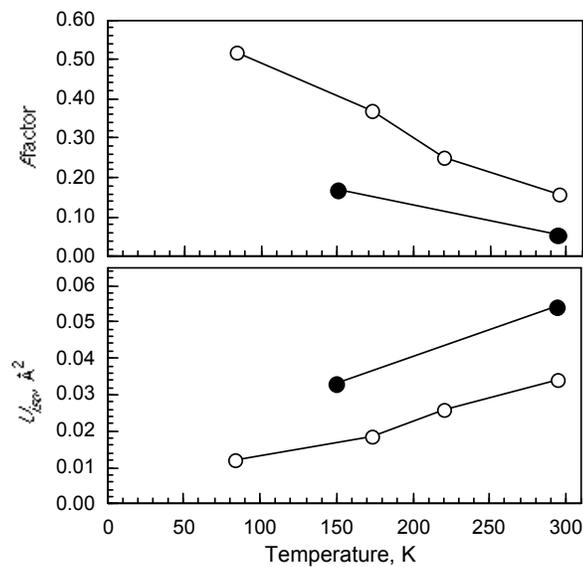
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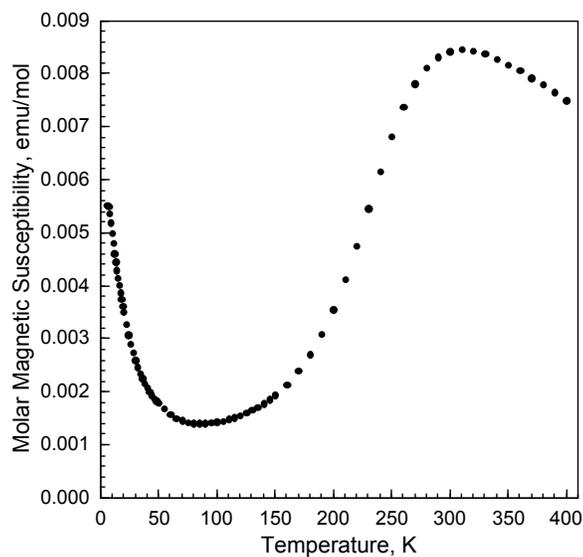
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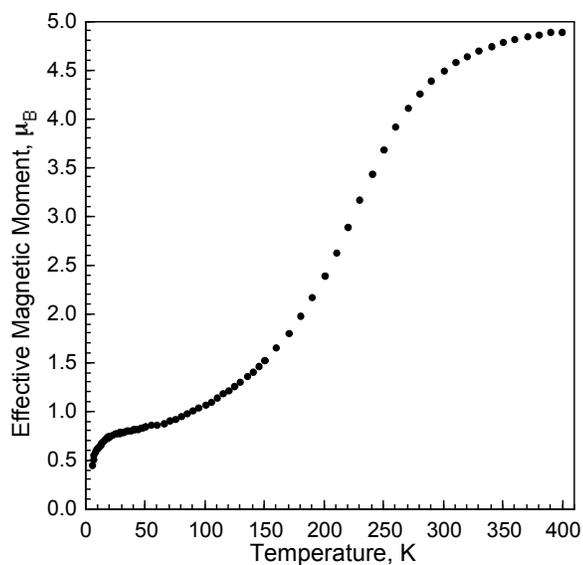
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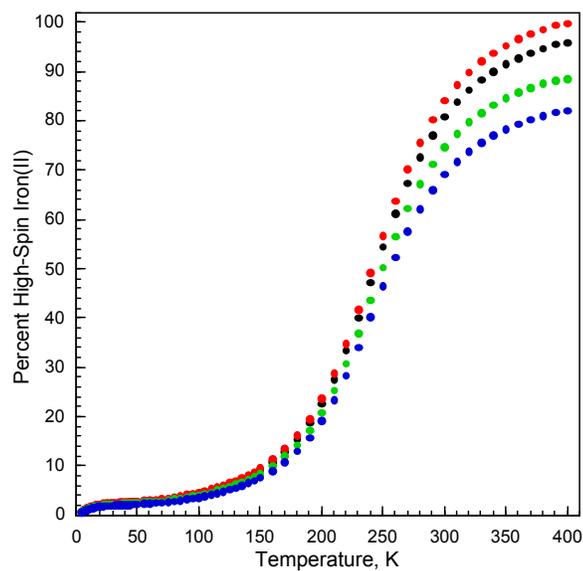
**Figure S1.** The temperature dependence of the thermal factor,  $U_{iso}$ , and the equivalent recoil-free fraction, the  $f$ -factor, of **1**, solid points, and of  $\{\text{Fe}[\text{HC}(3,5\text{-Me}_2\text{pz})_3]_2\}(\text{BF}_4)_2$ , open points.<sup>6a,c</sup> The error bars are smaller than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



**Figure S2.** The temperature dependence of  $\chi_M$  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  $\mu_{eff}$  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  $\mu_{eff}$  values, respectively, of 0.0 and 4.9  $\mu_B$ , red, 0.1 and 5.0  $\mu_B$ , black, 0.2 and 5.2  $\mu_B$ , green, and 0.4 and 5.4  $\mu_B$ , blue.