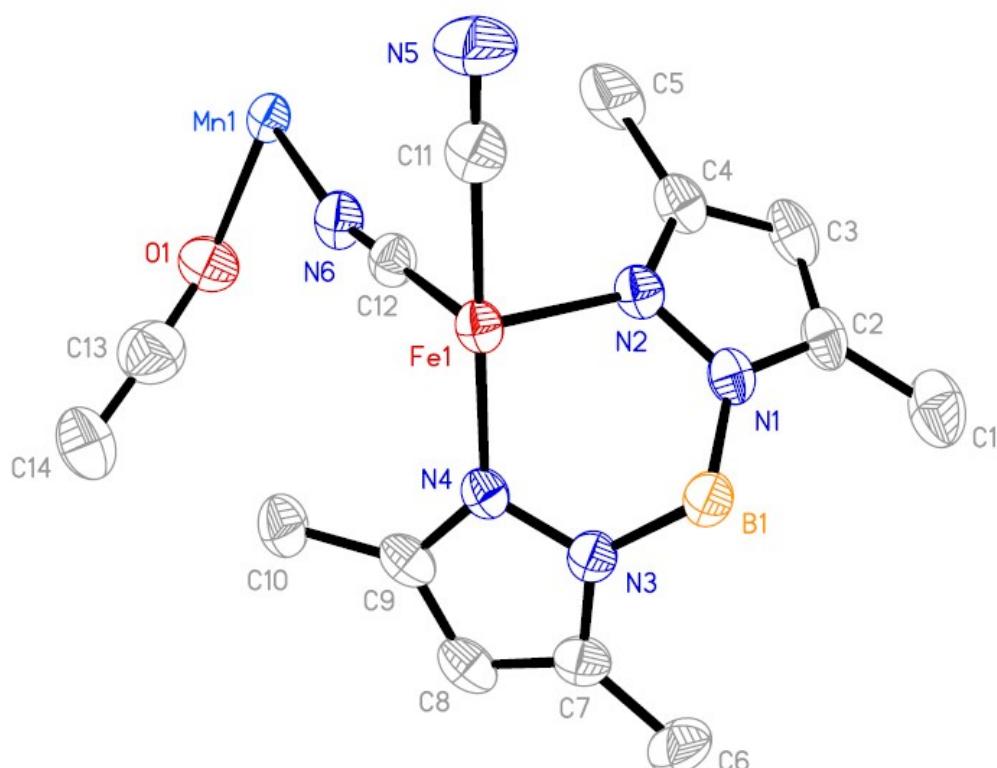


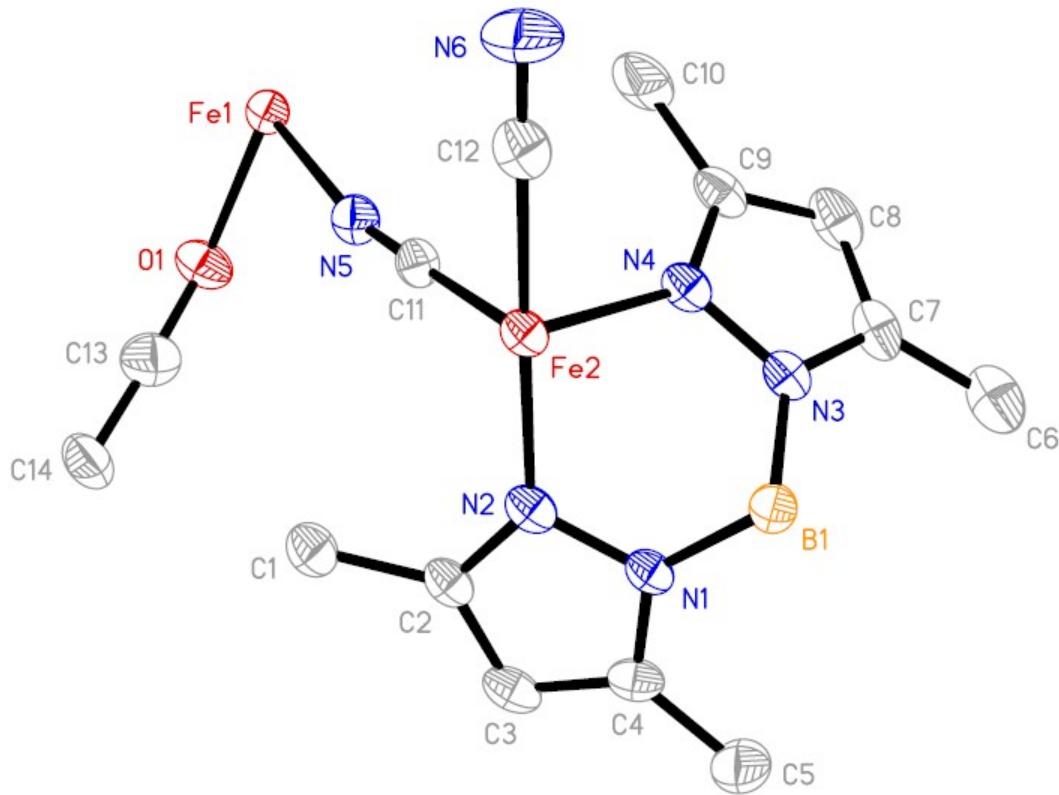
## Syntheses, structures, and magnetic properties of three new cyano-bridged heterobimetallic chains based on $[\text{Fe}(\text{Tp}^*)(\text{CN})_3]^-$

Dapeng Dong,<sup>a</sup> Yanjuan Zhang,<sup>b</sup> Chengqi Jiao,<sup>b</sup> Liang Zhao,<sup>b</sup> Tao Liu<sup>\*b</sup> Dedi Liu,<sup>a</sup> Zhenghua Li,<sup>a</sup> Jia Liu<sup>a</sup> and Dongping Liu<sup>\*a</sup>

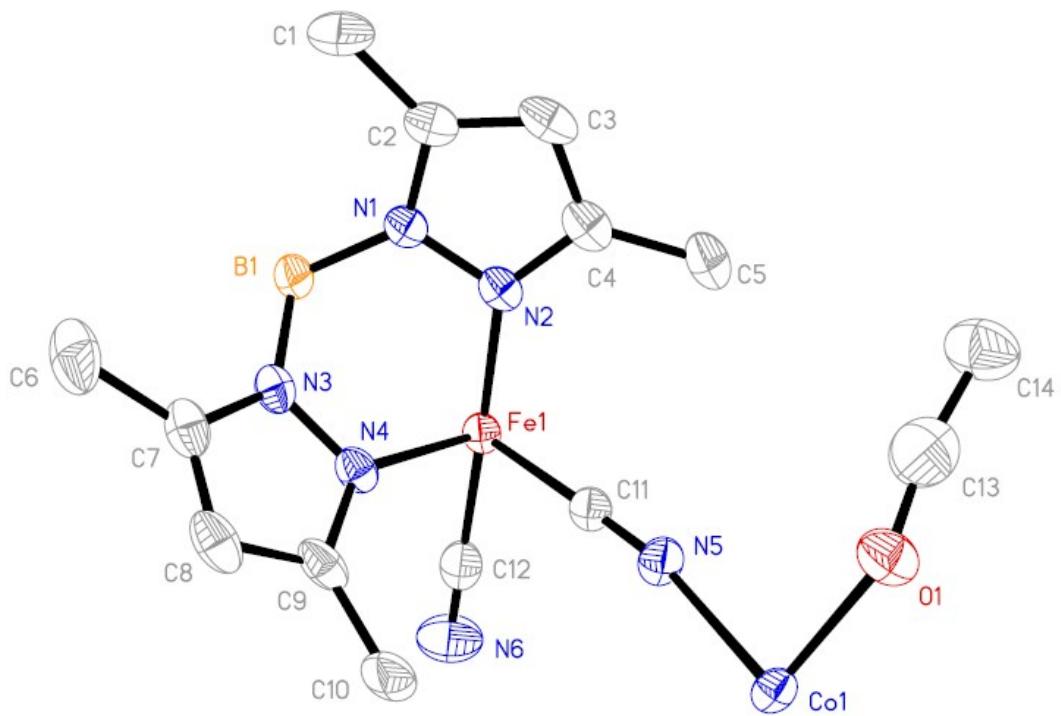
### Supporting Information



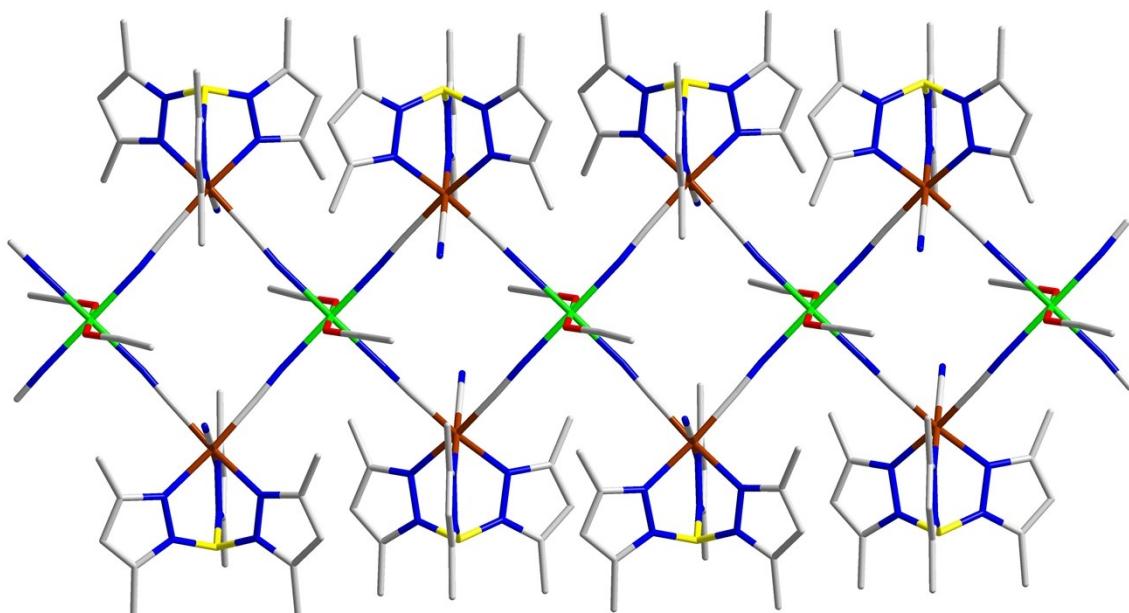
**Fig S1.** Asymmetric unit of compound **1** showing the atom labeling. Thermal ellipsoids are shown at the 30% probability level. All H atoms and water molecules are omitted for clarity.



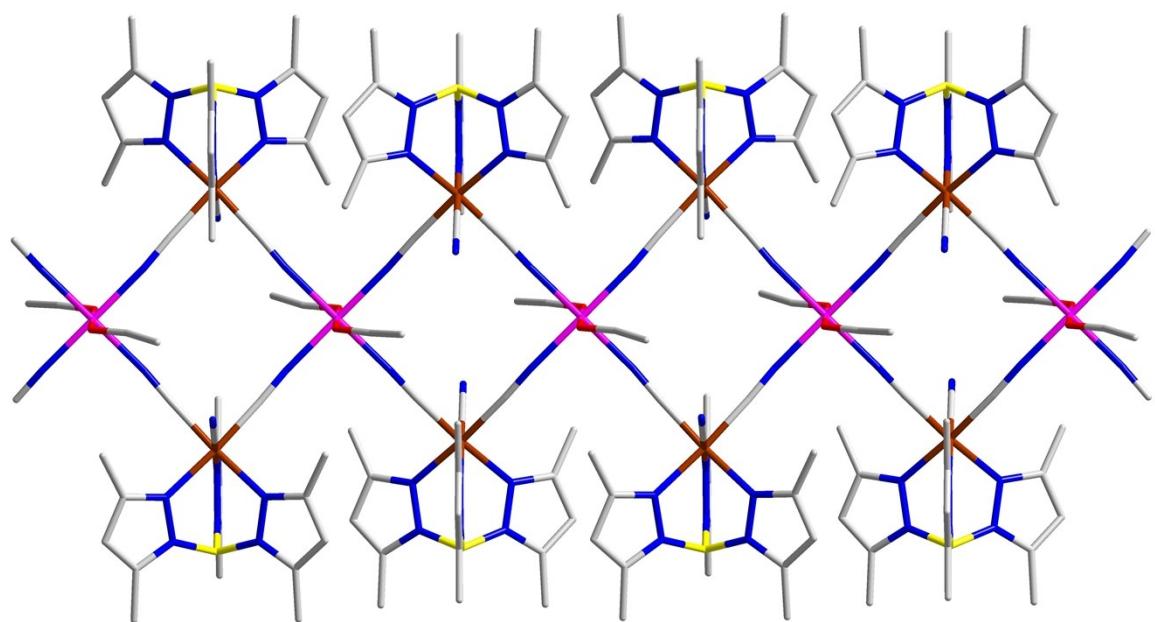
**Fig S2.** Asymmetric unit of compound **2** showing the atom labeling. Thermal ellipsoids are shown at the 30% probability level. All H atoms and water molecules are omitted for clarity.



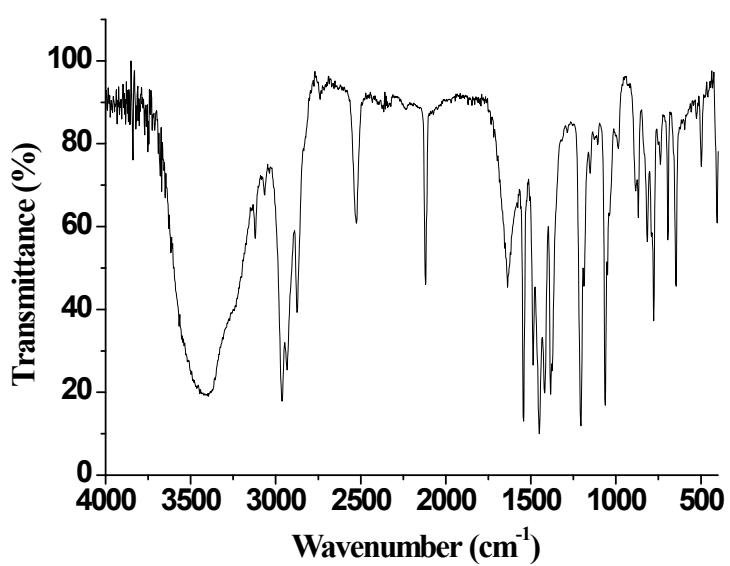
**Fig S3.** Asymmetric unit of compound 3 showing the atom labeling. Thermal ellipsoids are shown at the 30% probability level. All H atoms and water molecules are omitted for clarity.



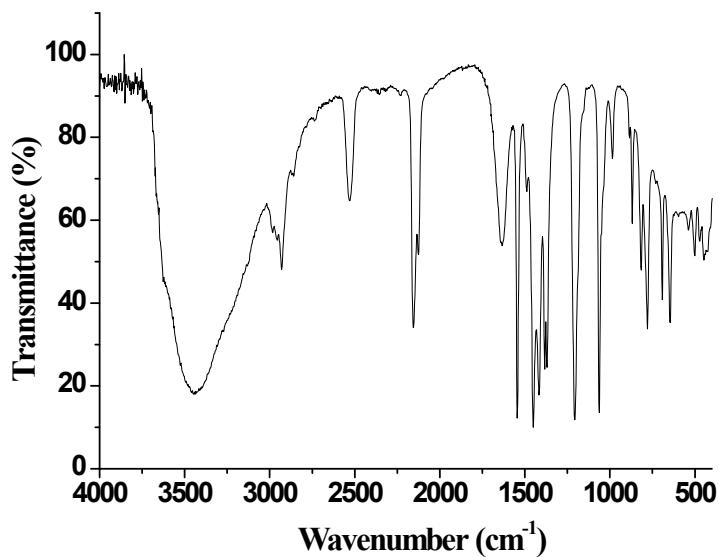
**Fig. S4.** Side view of a 1-D double-zigzag chain along the c-axis for compound 2. H atoms and water molecules have been omitted for clarity. Atomic scheme: Fe(II), bright green; Fe(III), brown; C, gray; N, blue; B, yellow; O, red.



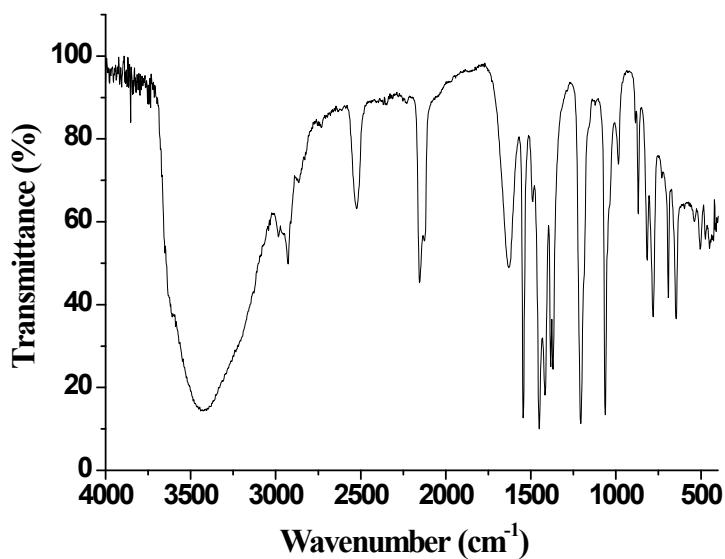
**Fig. S5.** Side view of a 1-D double-zigzag chain along the c-axis for compound 3. H atoms and water molecules have been omitted for clarity. Atomic scheme: Co(II), pink; Fe(III), brown; C, gray; N, blue; B, yellow; O, red.



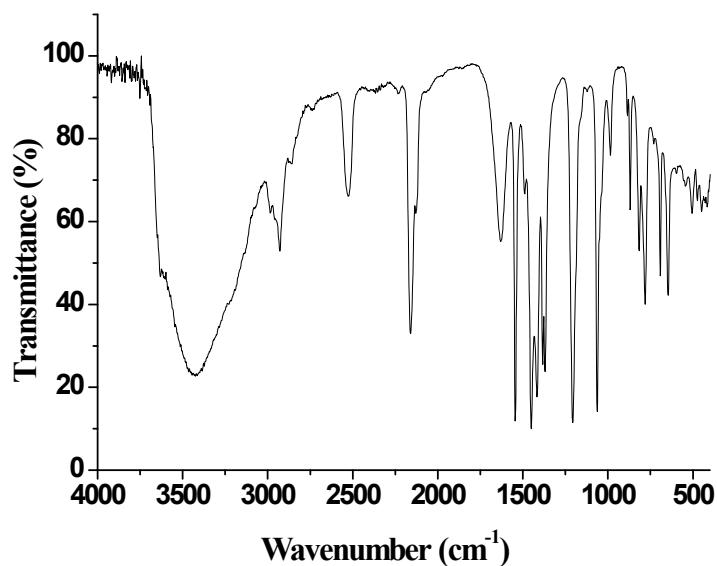
**Fig S6.** The IR spectrum of compound  $[\text{Bu}_4\text{N}][\text{Fe}(\text{Tp}^*)(\text{CN})_3]$ .



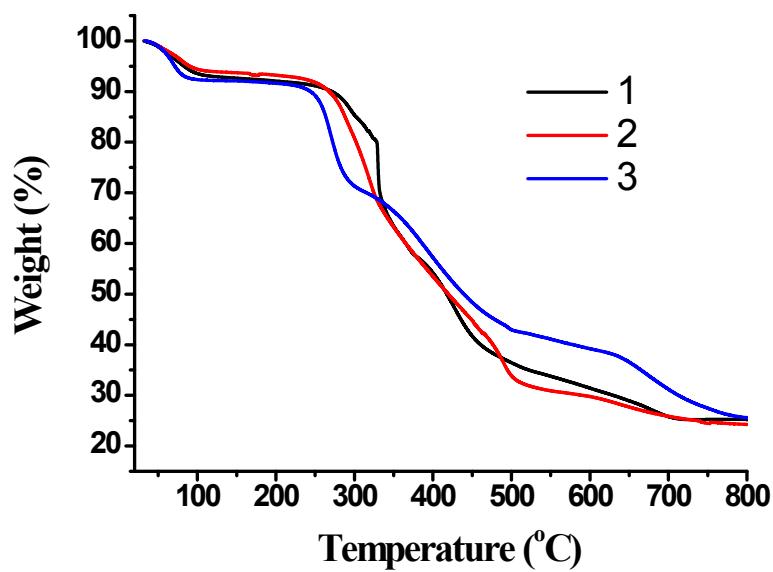
**Fig S7.** The IR spectra of compounds 1.



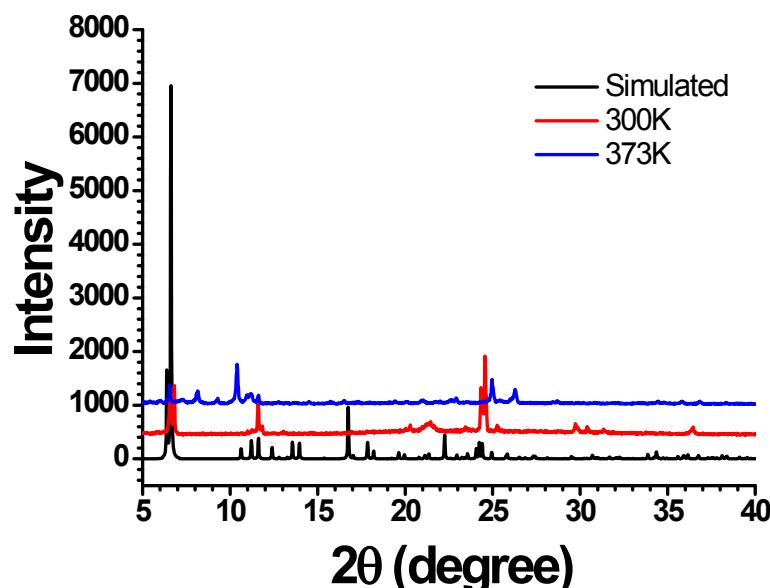
**Fig S8.** The IR spectra of compounds 2.



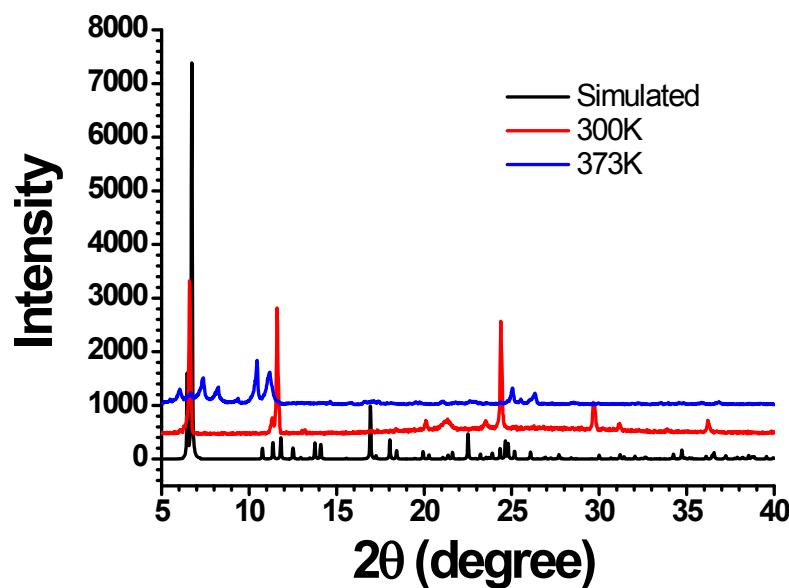
**Fig S9.** The IR spectra of compounds 3.



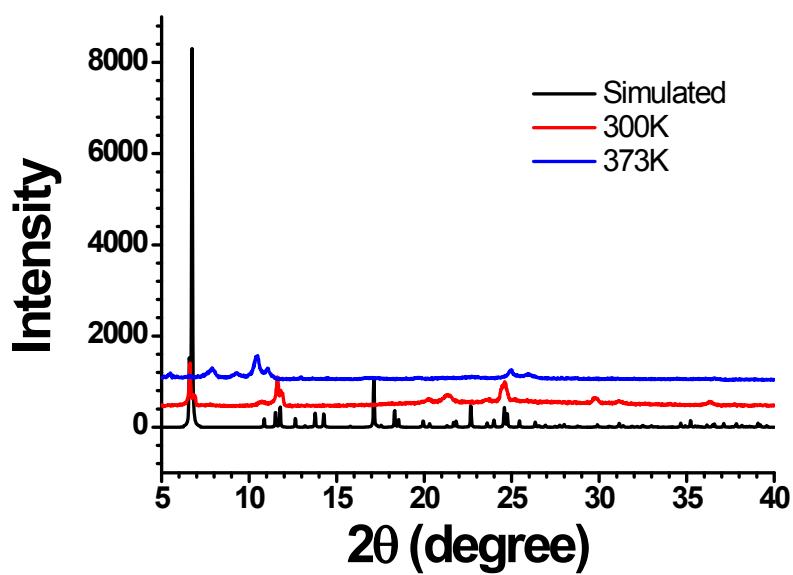
**Fig S10.** The TG curve of compound 1-3.



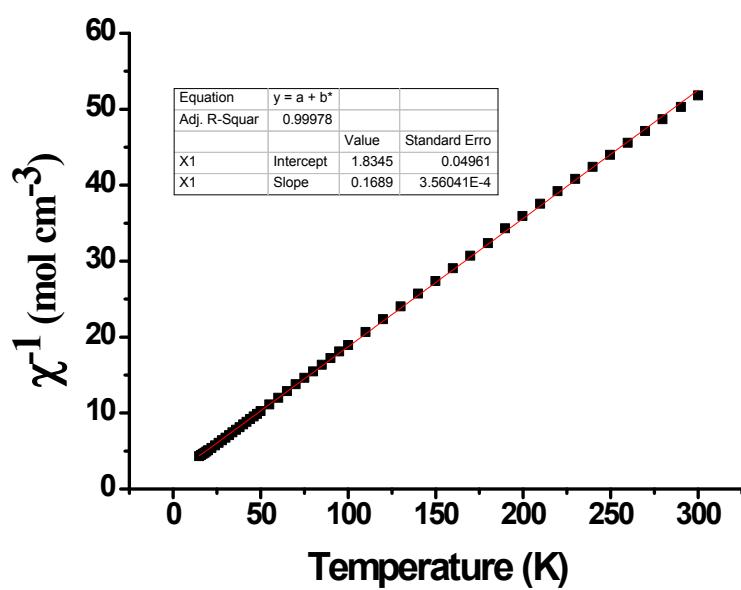
**Fig S11.** The simulated XRD pattern of compound 1 (up) and experimental powder XRD patterns at 300K (middle), 373K (down) of compounds 1.



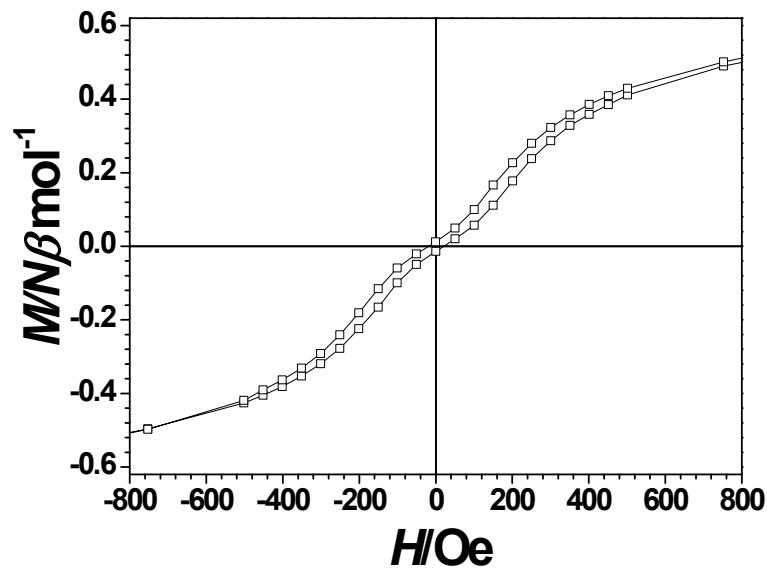
**Fig S12.** The simulated XRD pattern of compound 2 (up) and experimental powder XRD patterns at 300K (middle), 373K (down) of compounds 2.



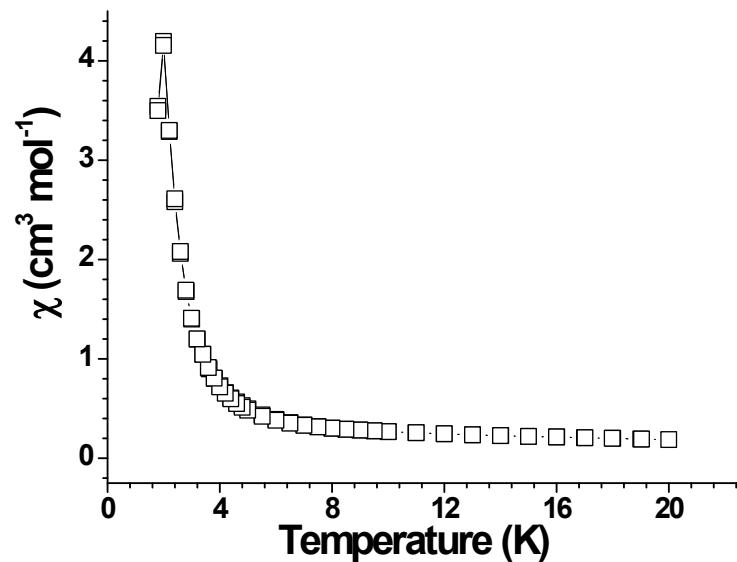
**Fig S13.** The simulated XRD pattern of compound 3 (up) and experimental powder XRD patterns at 300K (middle), 373K (down) of compounds 3.



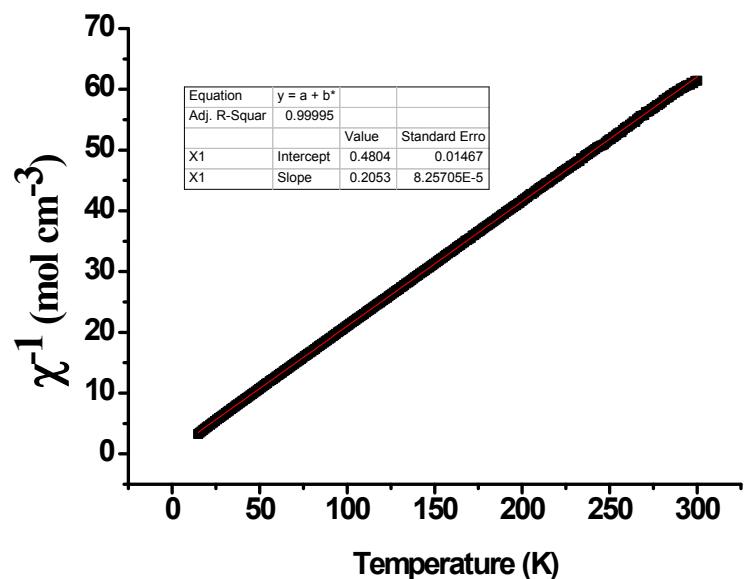
**Fig. S14** Thermal variation of magnetic susceptibility,  $\chi^{-1}$  vs T of compound 1 under an applied field of 1 kOe in the temperature range of 1.8–300 K.



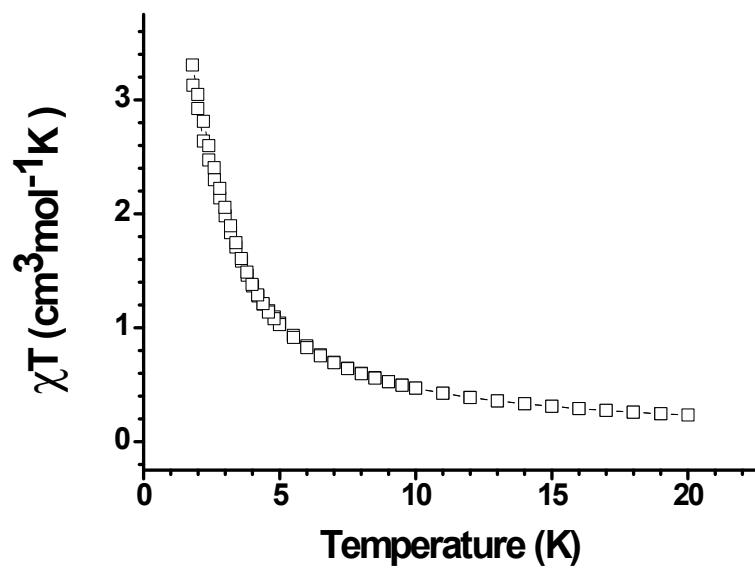
**Fig S15.** Field dependence of the magnetization showing the hysteresis loop for **1** at 1.8 K.



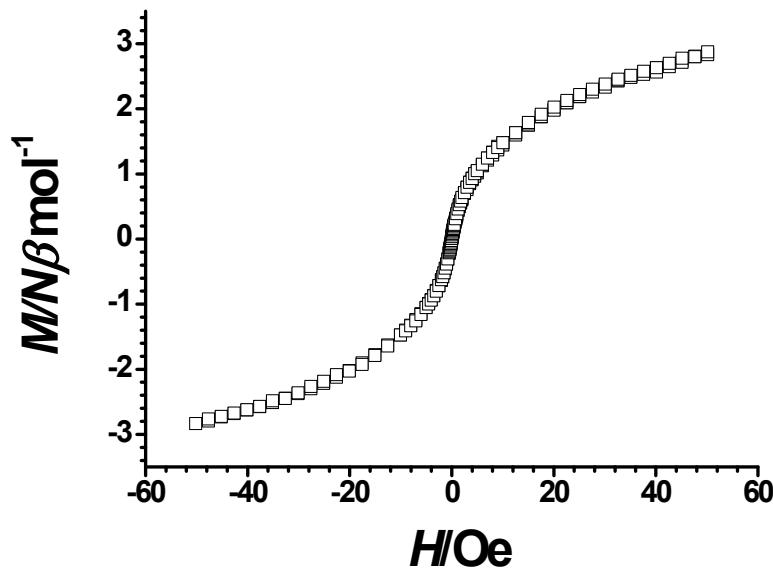
**Fig. S16** The coincident ZFC and FC magnetization curves of **1** at 100 Oe.



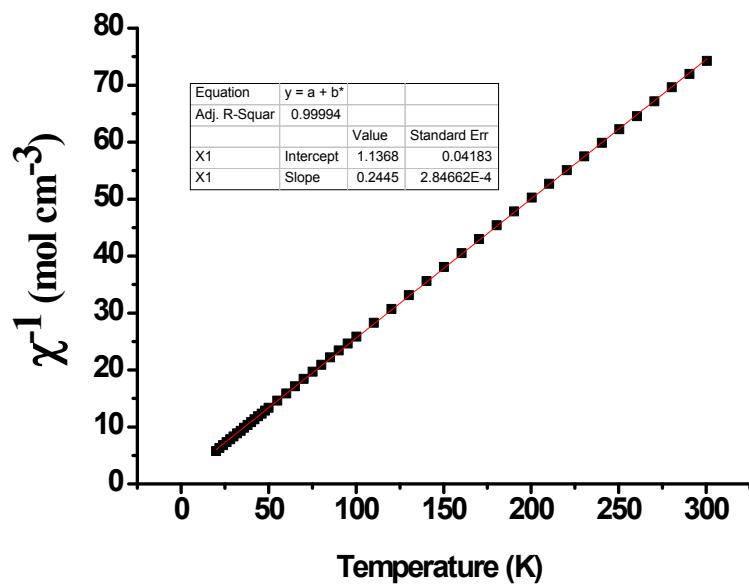
**Fig. S17** Thermal variation of magnetic susceptibility,  $\chi^{-1}$  vs T of compound **2** under an applied field of 1 kOe in the temperature range of 1.8–300 K.



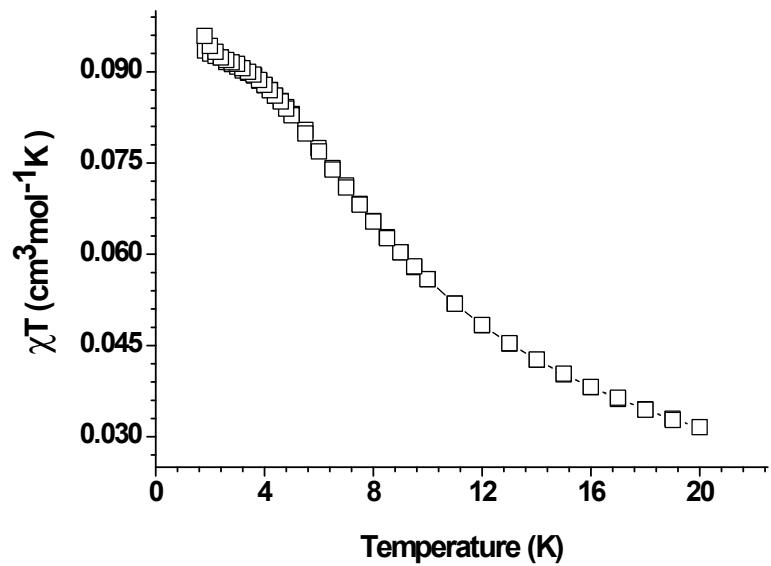
**Fig. S18** The coincident ZFC and FC magnetization curves of **2** at 100 Oe.



**Fig S19.** Field dependence of the magnetization showing the hysteresis loop for **2** at 1.8 K.



**Fig. S20** Thermal variation of magnetic susceptibility,  $\chi^{-1}$  vs T of compound **3** under an applied field of 1 kOe in the temperature range of 1.8–300 K.



**Fig. S21** The coincident ZFC and FC magnetization curves of **3** at 100 Oe.