

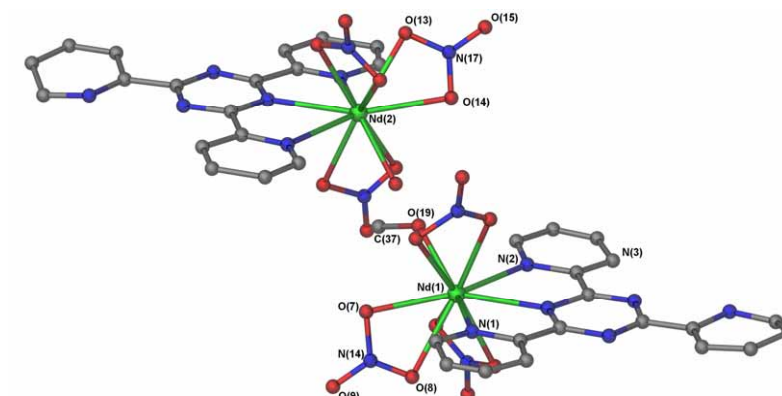
## **Supplementary Material**

### **Lanthanide-3d Cyanometalate Chains Ln(III)-M(III) (Ln = Pr, Nd, Sm, Eu, Gd, Tb; M = Fe) with the Tridentate Ligand 2,4,6-tri(2-pyridyl)-1,3,5-triazine (tptz): Evidence of Ferromagnetic Interactions for the Sm(III)-M(III) compounds (M = Fe, Cr)**

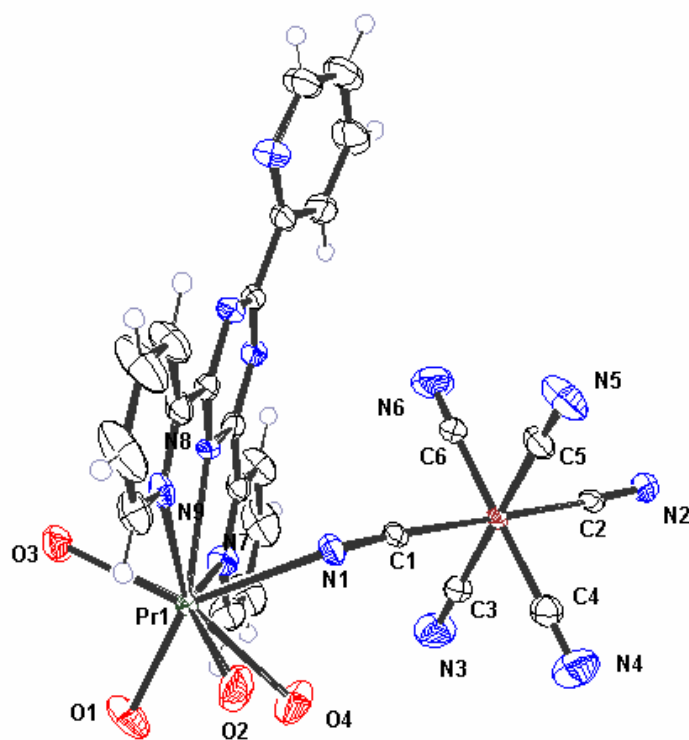
Hanhua Zhao, Nazario Lopez, Andrey Prosvirin, Helen T. Chifotides, and Kim R. Dunbar\*

Figures S1-S13.

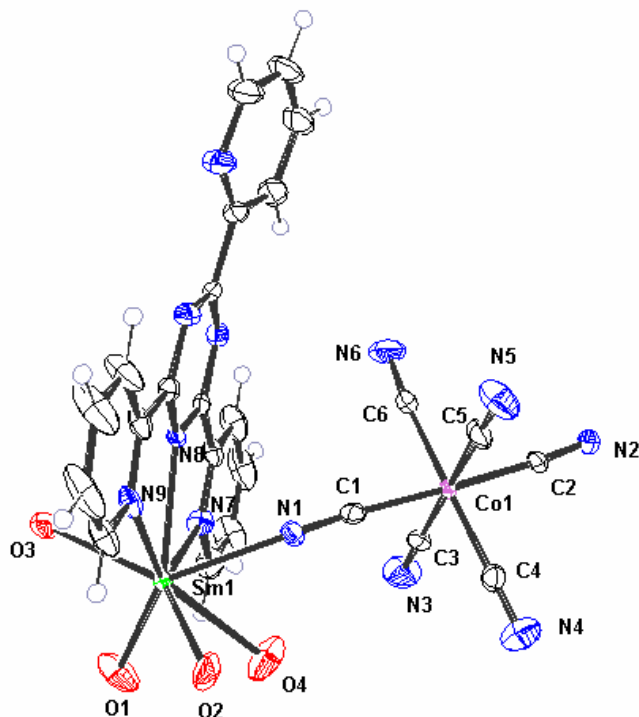
Tables S1-S5.



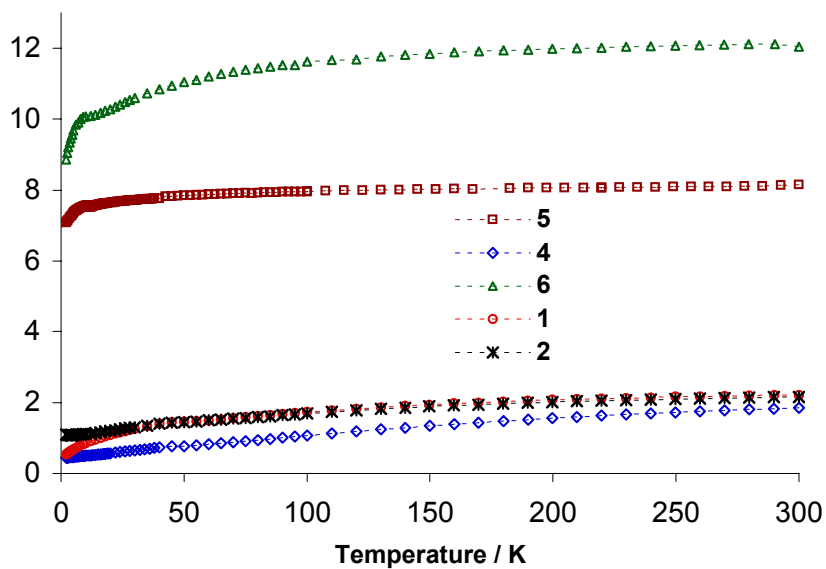
**Figure S1.** Structure of  $[\text{Nd}(\text{tptz})(\text{NO}_3)_3(\text{H}_2\text{O})][\text{Nd}(\text{tptz})(\text{NO}_3)_3(\text{CH}_3\text{OH})]$ .



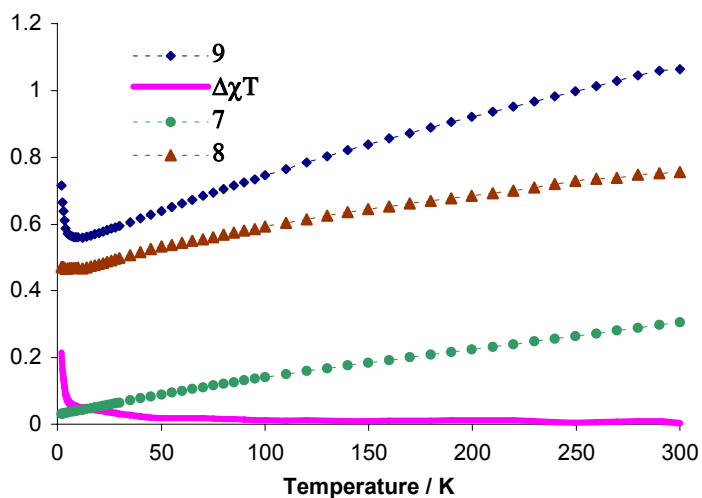
**Figure S2.** Thermal ellipsoid plot for  $\{[\text{Pr}(\text{tptz})(\text{H}_2\text{O})_4\text{Fe}(\text{CN})_6] \cdot 8\text{H}_2\text{O}\}_\infty$  (**1**) drawn at the 50% probability level; water crystallization molecules in the lattice have been omitted for the sake of clarity.



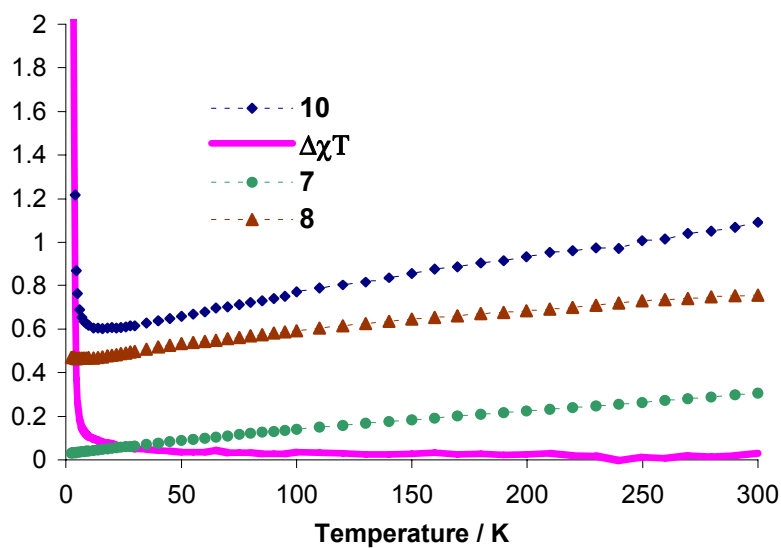
**Figure S3.** Thermal ellipsoid plot for  $\{[\text{Sm}(\text{tpz})(\text{H}_2\text{O})_4\text{Co}(\text{CN})_6]\cdot 8\text{H}_2\text{O}\}_\infty$  (**7**) drawn at the 50% probability level; water molecules of crystallization in the lattice have been omitted for the sake of clarity.



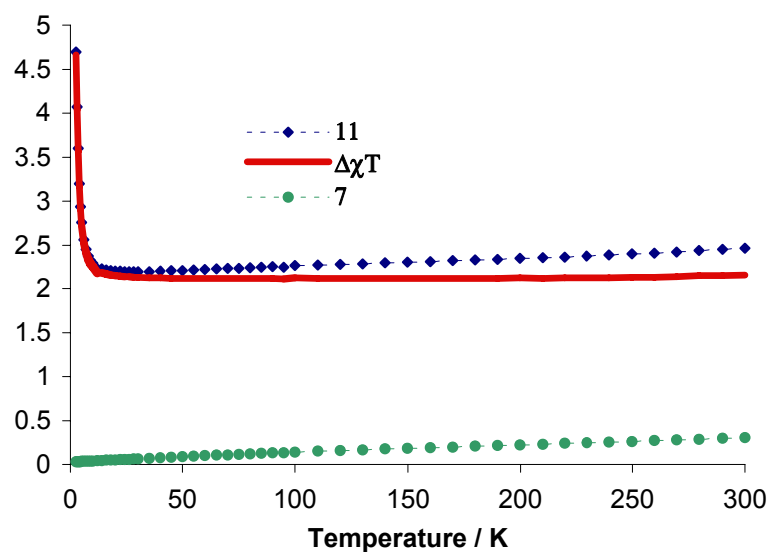
**Figure S4.** Temperature dependence of the  $\chi T$  product for compounds **1** (o), **2** (\*), **4** (◇), **5** (□), **6** (Δ).



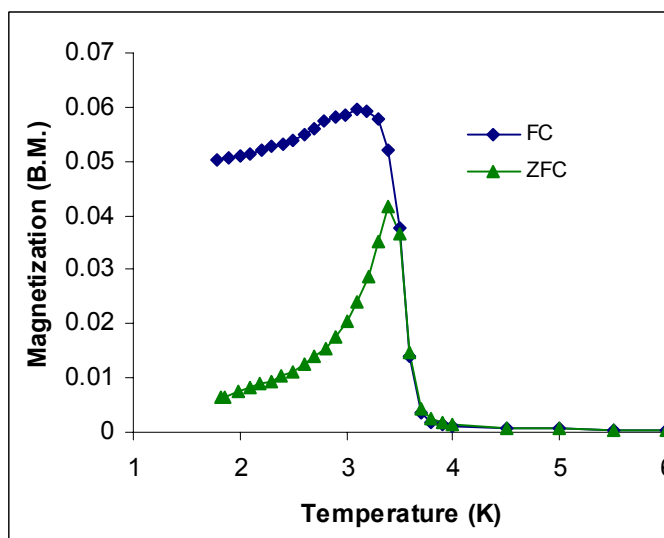
**Figure S5.** Temperature dependence of the  $\chi T$  product for compounds **9** ( $\diamond$ ), **7** ( $\circ$ ), **8** ( $\Delta$ ). The solid line represents the difference  $\Delta\chi T = \chi T$  (**9**) -  $\chi T$  (**7**) -  $\chi T$  (**8**).



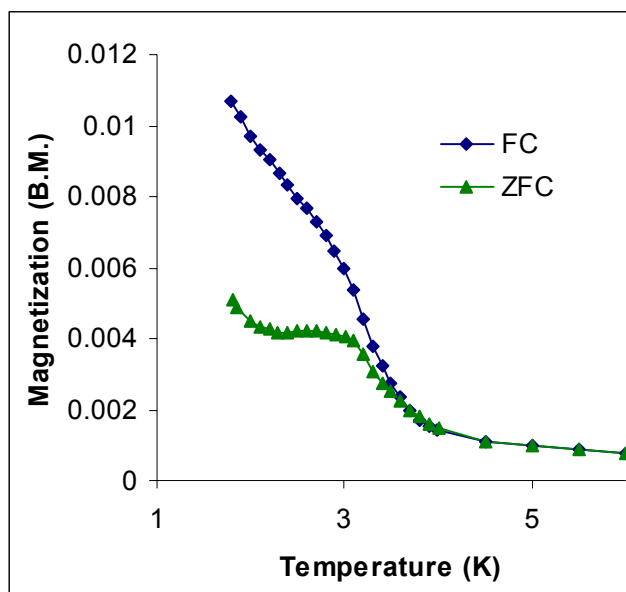
**Figure S6.** Temperature dependence of the  $\chi T$  product for compounds **10** ( $\diamond$ ), **7** ( $\circ$ ), **8** ( $\Delta$ ). The solid line represents the difference  $\Delta\chi T = \chi T$  (**10**) -  $\chi T$  (**7**) -  $\chi T$  (**8**).



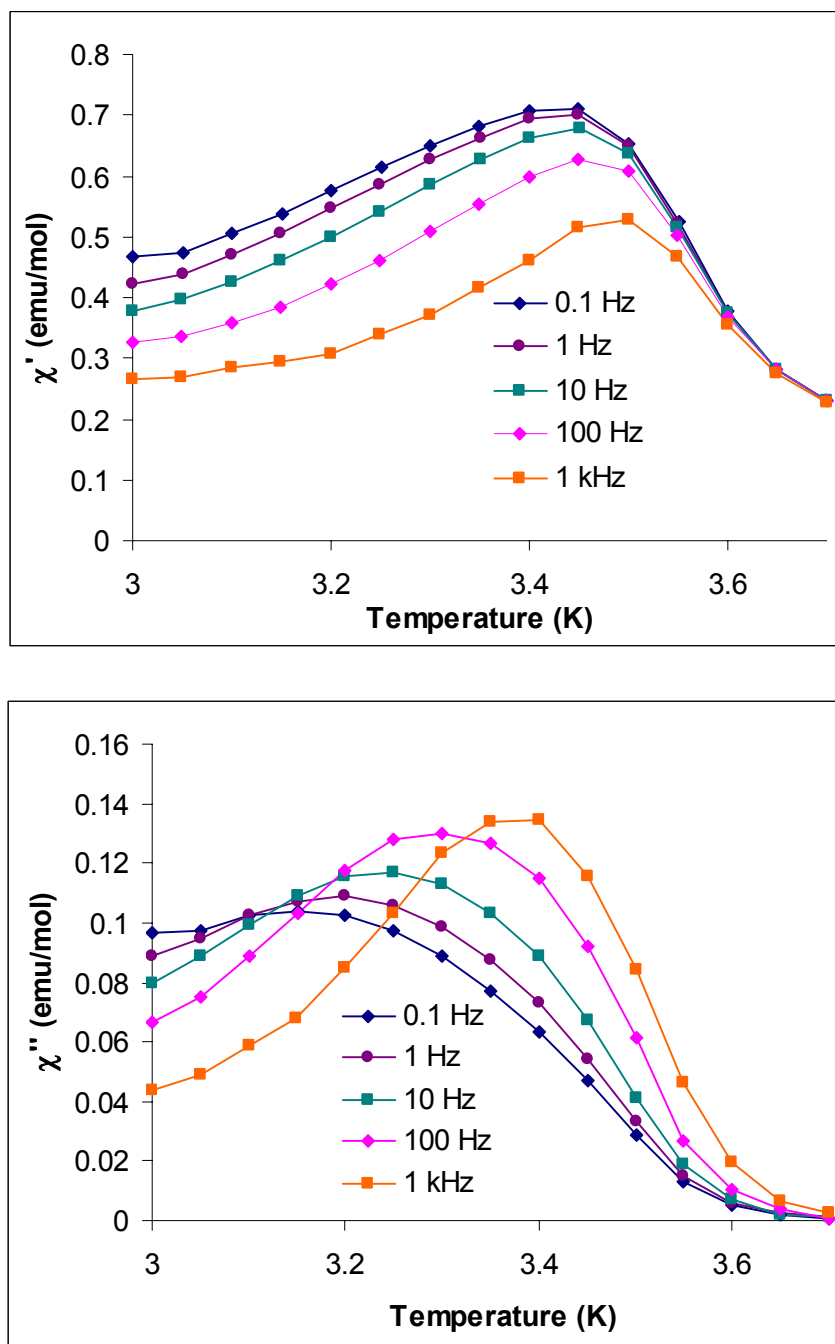
**Figure S7.** Temperature dependence of the  $\chi T$  product for compounds **11** ( $\diamond$ ), **7** ( $\circ$ ). The solid line represents the difference  $\Delta\chi T = \chi T$  (**11**) -  $\chi T$  (**7**).



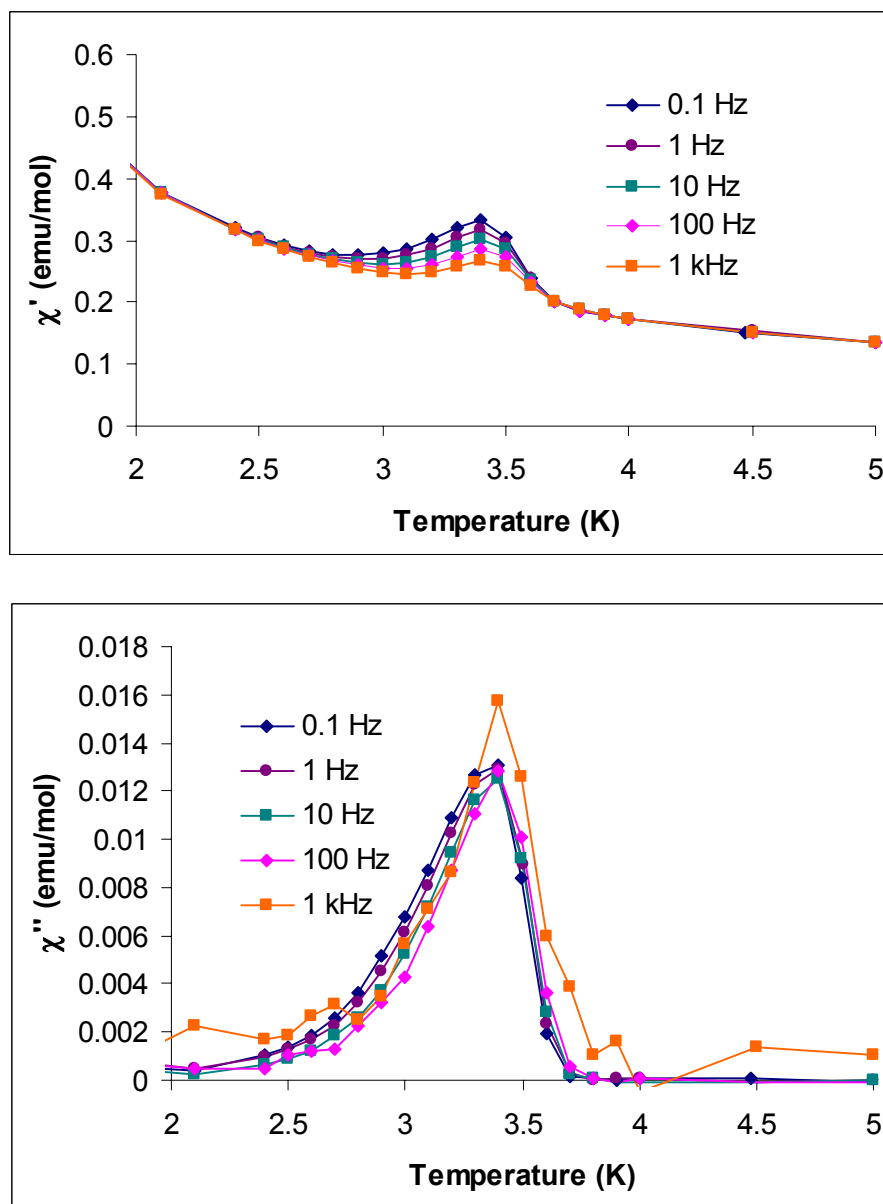
**Figure S8.** Temperature dependence of magnetization in the zero-field-cooling (ZFC) and field-cooling (FC) regime for **10** at magnetic field of 10 Oe.



**Figure S9.** Temperature dependence of magnetization in the zero-field-cooling (ZFC) and field-cooling (FC) regime for **11** at magnetic field of 10 Oe.

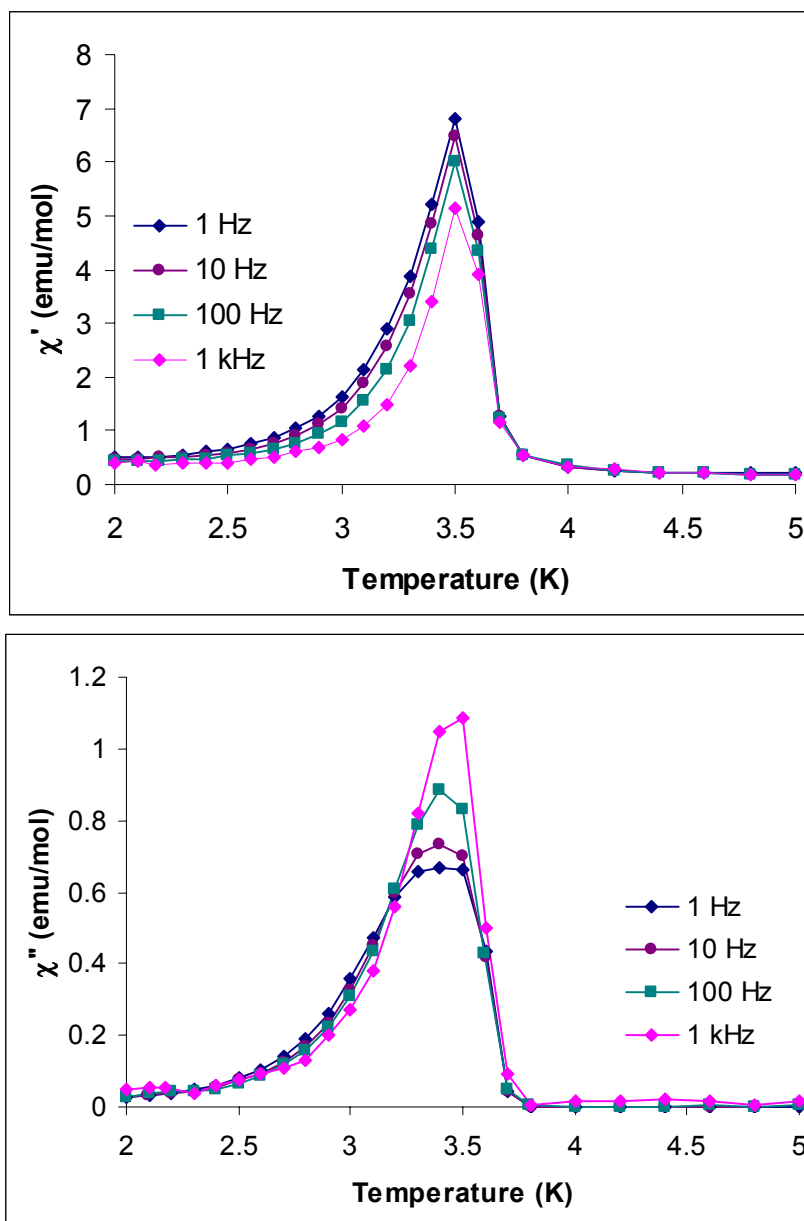


**Figure S10.** Temperature dependence of the real  $\chi'$  (top) and imaginary  $\chi''$  (bottom) components of the ac susceptibility for **3** in vicinity of the phase transition.

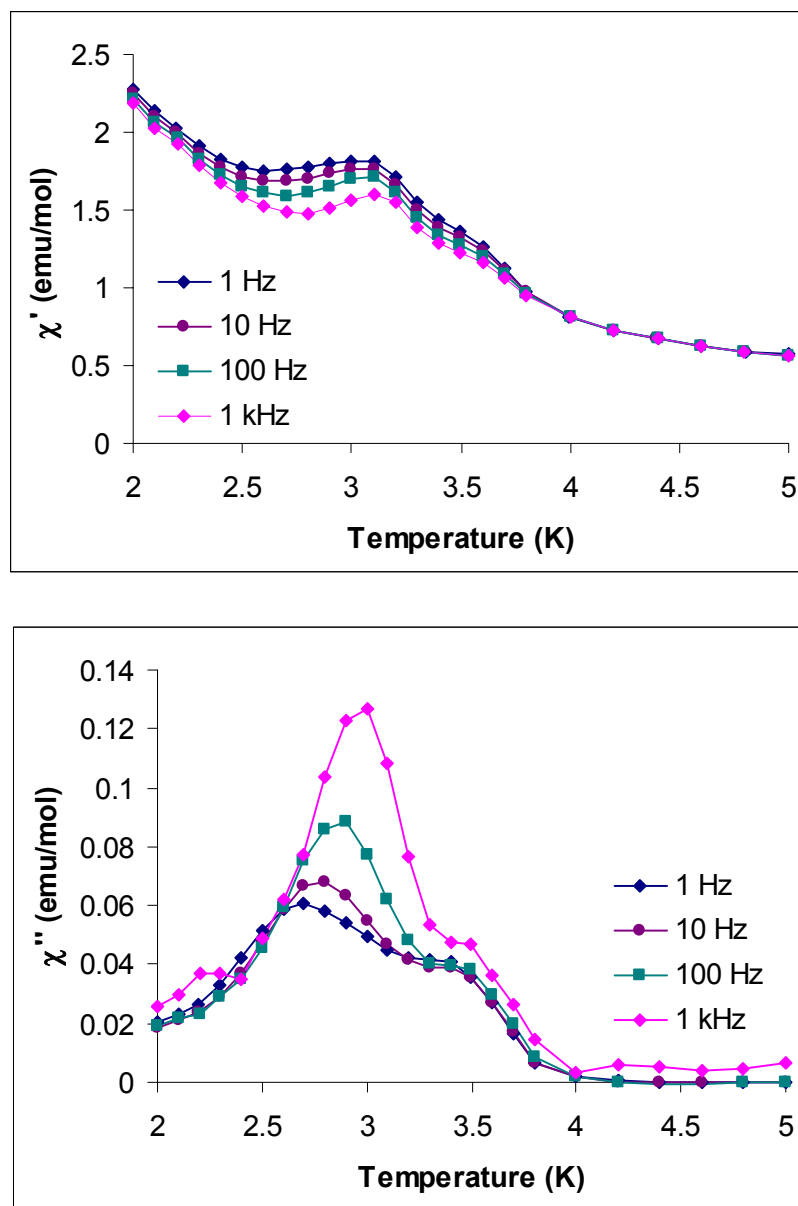


**Figure S11.** Temperature dependence of the real  $\chi'$  (top) and imaginary  $\chi''$  (bottom) components of the ac susceptibility for **9**.





**Figure S12.** Temperature dependence of the real  $\chi'$  (top) and imaginary  $\chi''$  (bottom) components of the ac susceptibility for **10**.



**Figure S13.** Temperature dependence of the real  $\chi'$  (top) and imaginary  $\chi''$  (bottom) components of the ac susceptibility for **11**.

**Table S1.** Selected bond lengths (Å) and angles (°) for compound **1**.

Pr1-O(1)	2.492(5)	Fe(1)-C(3)	1.935(6)
Pr1-O(2)	2.484(5)	Fe(1)-C(4)	1.938(7)
Pr1-O(3)	2.512(4)	Fe(1)-C(5)	1.941(6)
Pr1-O(4)	2.533(5)	Fe(1)-C(6)	1.939(7)
Pr(1)-N(1)	2.566(5)	C(1)-N(1)	1.151(7)
Pr(1)-N(2)	2.535(5)	C(2)-N(2)	1.151(7)
Pr(1)-N(7)	2.683(5)	C(3)-N(3)	1.143(8)
Pr(1)-N(8)	2.640(4)	C(4)-N(4)	1.144(9)
Fe(1)-C(1)	1.923(6)	C(5)-N(5)	1.142(8)
Fe(1)-C(2)	1.917(6)	C(6)-N(6)	1.154(9)
N1-Pr1-N2	135.37(18)	C1-Fe1-C2	177.1(3)
N1-Pr1-N7	84.68(16)	C1-Fe1-C3	87.6(2)
N1-Pr1-N8	65.99(15)	C1-Fe1-C4	90.3(3)
N1-Pr1-N9	75.09(15)	N1-C1-Fe1	174.8(5)
N2-Pr1-N7	139.80(17)	N2-C2-Fe1	176.0(5)
C1-N1-Pr1	147.1(4)	C2-N2-Pr1	169.9(5)

**Table S2.** Selected bond lengths (Å) and angles (°) for compound **3**.

Sm1-O(1)	2.453(5)	Fe(1)-C(3)	1.942(7)
Sm1-O(2)	2.428(5)	Fe(1)-C(4)	1.945(7)
Sm1-O(3)	2.454(5)	Fe(1)-C(5)	1.942(7)
Sm1-O(4)	2.503(6)	Fe(1)-C(6)	1.940(8)
Sm(1)-N(1)	2.519(5)	C(1)-N(1)	1.148(8)
Sm(1)-N(2)	2.501(5)	C(2)-N(2)	1.142(8)
Sm(1)-N(7)	2.637(6)	C(3)-N(3)	1.144(9)
Sm(1)-N(8)	2.587(5)	C(4)-N(4)	1.147(9)
Fe(1)-C(1)	1.929(6)	C(5)-N(5)	1.141(9)
Fe(1)-C(2)	1.921(7)	C(6)-N(6)	1.157(10)
N1-Sm1-N2	135.61(19)	C1-Fe1-C2	177.1(3)
N1-Sm1-N7	84.60(18)	C1-Fe1-C3	87.9(2)
N1-Sm1-N8	66.17(18)	C1-Fe1-C4	90.1(3)
N1-Sm1-N9	75.79(17)	N1-C1-Fe1	173.9(5)
N2-Sm1-N7	139.74(19)	N2-C2-Fe1	175.9(6)
C1-N1-Sm1	148.1(5)	C2-N2-Sm1	169.6(5)

**Table S3.** Selected bond lengths (Å) and angles (°) for compound **7**.

Sm1-O(3)	2.461(5)	Co(1)-C(5)	1.889(7)
Sm1-O(4)	2.498(6)	Co(1)-C(6)	1.896(7)
Sm(1)-N(1)	2.517(5)	C(1)-N(1)	1.157(8)
Sm(1)-N(2)	2.496(6)	C(2)-N(2)	1.150(8)
Sm(1)-N(7)	2.627(6)	C(3)-N(3)	1.143(8)
Sm(1)-N(8)	2.580(5)	C(4)-N(4)	1.146(9)
Co(1)-C(1)	1.882(6)	C(5)-N(5)	1.149(9)
Co(1)-C(2)	1.881(6)	C(6)-N(6)	1.148(9)
N1-Sm1-N2	136.37(19)	C1-Co1-C2	176.8(3)
N1-Sm1-N7	84.04(17)	C1-Co1-C3	88.1(3)
N1-Sm1-N8	66.48(16)	C1-Co1-C4	91.1(3)
N1-Sm1-N9	76.33(16)	N1-C1-Co1	174.6(5)
N2-Sm1-N7	139.56(18)	N2-C2-Co1	175.4(6)
C1-N1-Sm1	148.3(5)	C2-N2-Sm1	170.3(5)

**Table S4.** Selected bond lengths (Å) and angles (°) for compound **10**.

Sm(1)-N(1)	2.457(5)	Fe(1)-C(4)	1.938(6)
Sm(1)-N(2)	2.456(5)	Fe(2)-C(2)	1.907(6)
Sm(1)-N(7)	2.573(4)	C(1)-N(1)	1.158(7)
Sm(1)-N(8)	2.579(4)	C(2)-N(2)	1.154(7)
Fe(1)-C(1)	1.906(6)	C(3)-N(3)	1.159(7)
Fe(1)-C(3)	1.948(6)	C(4)-N(4)	1.162(7)
N1-Sm1-N2	145.04(15)	N2-C2-Fe2	177.6(5)
N1-Sm1-O1	76.14(15)	C1-Fe1-C3	88.3(2)
N1-Sm1-O2	72.44(15)	C1-Fe1-C4	89.7(2)
C1-N1-Sm1	164.5(4)	C3-Fe1-C4	88.9(2)
C2-N2-Sm1	168.8(4)	O1-Sm1-O2	83.77(13)
N1-C1-Fe1	176.8(5)		

**Table S5.** Selected bond lengths (Å) and angles (°) for compound **11**.

Sm(1)-N(1)	2.525(10)	Cr(1)-C(4)	2.069(13)
Sm(1)-N(2)	2.509(10)	Cr(2)-C(2)	2.071(12)
Sm(1)-N(7)	2.555(10)	C(1)-N(1)	1.153(15)
Sm(1)-N(8)	2.580(9)	C(2)-N(2)	1.154(14)
Cr(1)-C(1)	2.082(13)	C(3)-N(3)	1.166(18)
Cr(1)-C(3)	2.051(15)	C(4)-N(4)	1.138(17)
N1-Sm1-N2	146.3(3)	N2-C2-Cr2	177.0(10)
N1-Sm1-O1	75.6(3)	C1-Cr1-C3	91.2(5)
N1-Sm1-O2	79.2(3)	C1-Cr1-C4	88.6(5)
C1-N1-Sm1	164.9(9)	C3-Cr1-C4	90.1(5)
C2-N2-Sm1	163.9(8)	O1-Sm1-O2	84.0(3)
N1-C1-Cr1	175.6(10)		