

Supporting Information

Counter anions influence the relaxation dynamics of phenoxy- bridged Dy₂ single molecule magnets

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Table S1. Crystallographic Data and Structure Refinement for **1-4**.

Compound	1	2	3	4
Formula	C ₅₃ H ₆₀ Cl ₂ Dy ₂ N ₁₂ O ₁₅	C ₅₅ H ₆₃ Dy ₂ N ₁₄ O ₂₁	C ₅₇ H ₇₀ Cl ₂ Dy ₂ N ₁₂ O ₂₄	C ₁₂₀ H ₁₃₃ Cl ₂ Dy ₄ F ₁₂ N ₂₄ O ₃₉ S ₄
Formula weight	1501.03	1581.19	1703.15	3612.64
Temperature/K	173.15	173.15	173.15	173.15
Crystal system	monoclinic	monoclinic	monoclinic	triclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> $\bar{1}$
<i>a</i> /Å	14.434(5)	14.515(3)	14.0961(9)	15.7602(13)
<i>b</i> /Å	17.950(7)	18.063(4)	18.9669(12)	18.2693(15)
<i>c</i> /Å	26.051(9)	27.276(7)	26.3438(18)	24.804(2)
α /°	90	90	90	95.9670(10)
β /°	93.072(8)	92.250(5)	104.9210(10)	100.081(2)
γ /°	90	90	90	90.9640(10)
Volume/Å ³	6740(4)	7146(3)	6805.8(8)	6989.1(10)
<i>Z</i>	4	4	4	2
ρ_{calc} /g·cm ⁻³	1.479	1.470	1.662	1.717
F(000)	2992	3164	3416	3606
Crystal size/mm ³	0.12×0.11×0.1	0.12×0.11×0.1	0.2×0.15×0.1	0.15×0.12×0.1
Reflns collected	41046	39282	26112	43444
Rint	0.0812	0.1037	0.0447	0.027
GOF on F ²	1.031	0.995	1.107	1.027
R1, wR2 [<i>I</i> ≥2σ(<i>I</i>)]	0.0657, 0.1855	0.0586, 0.1368	0.0582, 0.1517	0.0400, 0.1099
R1, wR2 [all data]	0.0887, 0.2011	0.0932, 0.1544	0.0729, 0.1595	0.0479, 0.1168
CCDC number	2004686	2004687	2004688	2004689

Table S2. CShM Values of **1-4**.

central atom	coordination polyhedron	1	2	3	4
Dy(1)	Square antiprism (SAPR-8, D4d)	4.253	4.009	4.275	4.112
	Triangular dodecahedron (TDD-8, D2d)	3.447	3.499	3.844	3.895
Biaugmented trigonal prism J50 (JBTPR-8, C2v)	Biaugmented trigonal prism J50 (JBTPR-8, C2v)	4.839	4.762	4.793	4.934
	Biaugmented trigonal prism (BTPR-8, C2v)	3.952	3.76	3.943	4.157
	Snub diphenoid J84 (JSD-8, D2d)	5.684	5.775	5.823	5.872
	Snub diphenoid J84 (JSD-8, D2d)	6.262	5.854	6.088	6.346
Dy(2)	Square antiprism (SAPR-8, D4d)	4.335	4.361	4.26	4.592
	Triangular dodecahedron (TDD-8, D2d)	4.455	4.061	4.118	4.556
	Biaugmented trigonal prism J50 (JBTPR-8, C2v)	5.144	5.214	5.221	5.342
	Biaugmented trigonal prism (BTPR-8, C2v)	4.32	4.533	4.451	4.549

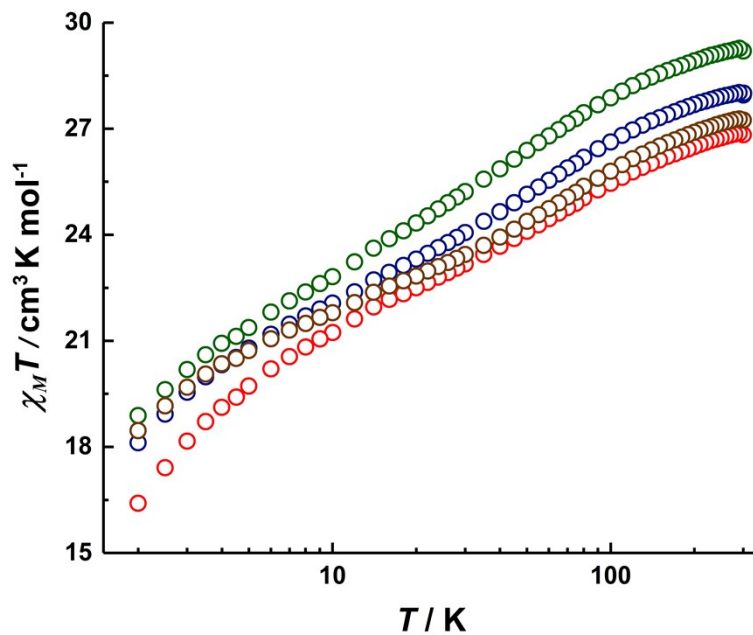


Figure S1. Temperature dependence of the $\chi_M T$ values at 1000 Oe for **1** (red), **2** (blue), **3** (green) and **4** (brown) with the x axis in log scale to highlight the low temperature magnetic properties.

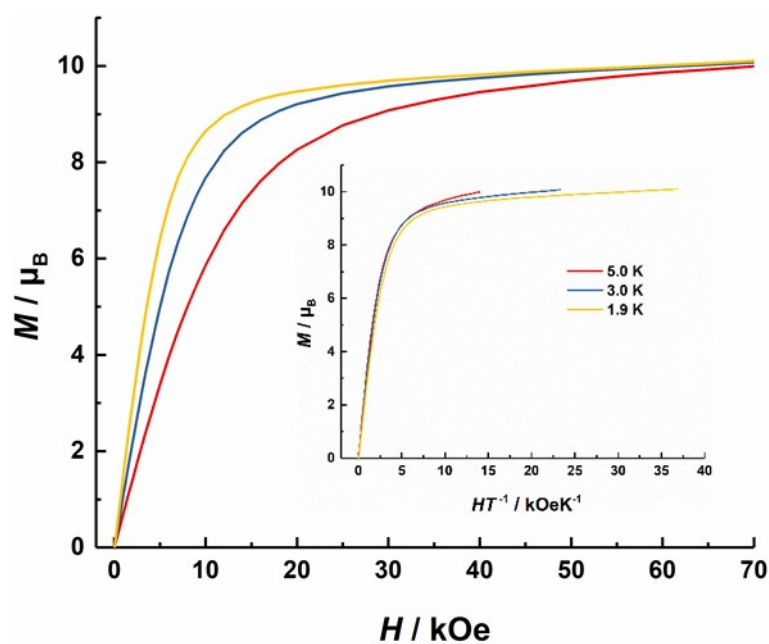


Figure S2. Field dependence of magnetization for **1**. Inset: M versus H/T plot for **1**.

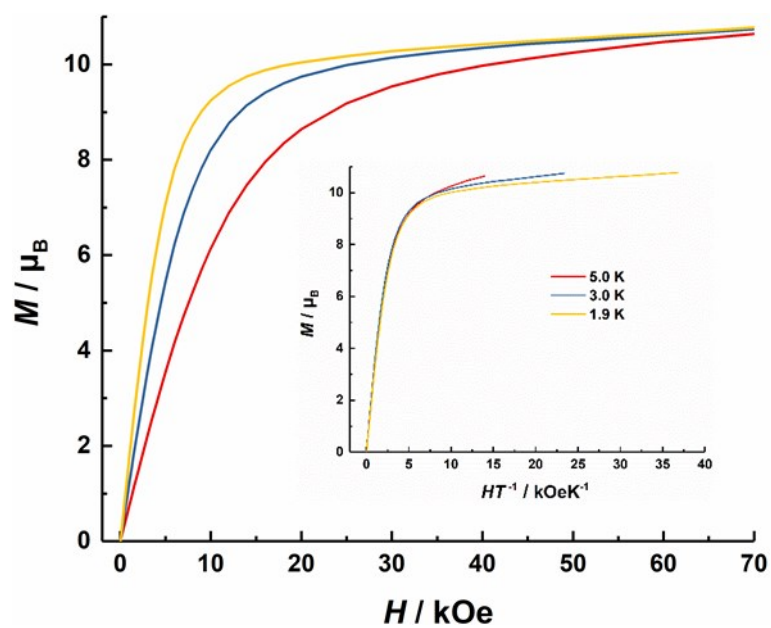


Figure S3. Field dependence of magnetization for **2**. Inset: M versus H/T plot for **2**.

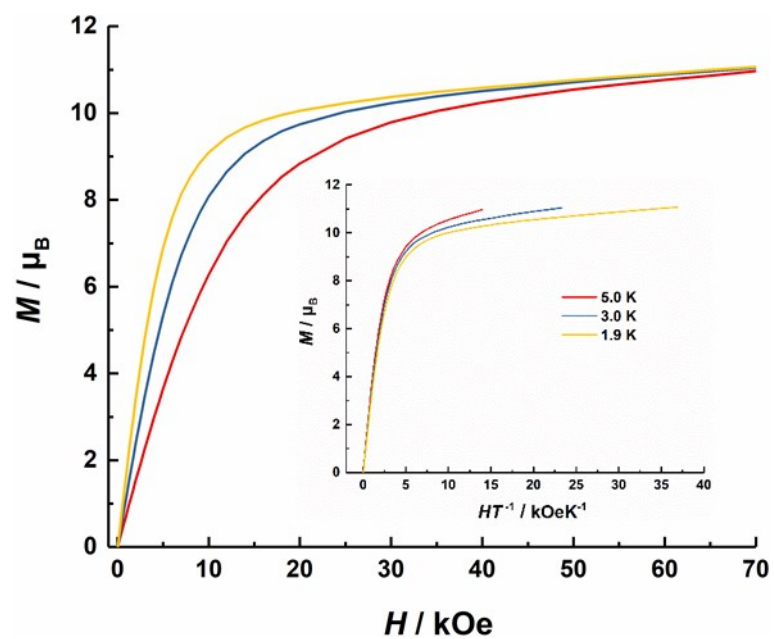


Figure S4. Field dependence of magnetization for **3**. Inset: M versus H/T plot for **3**.

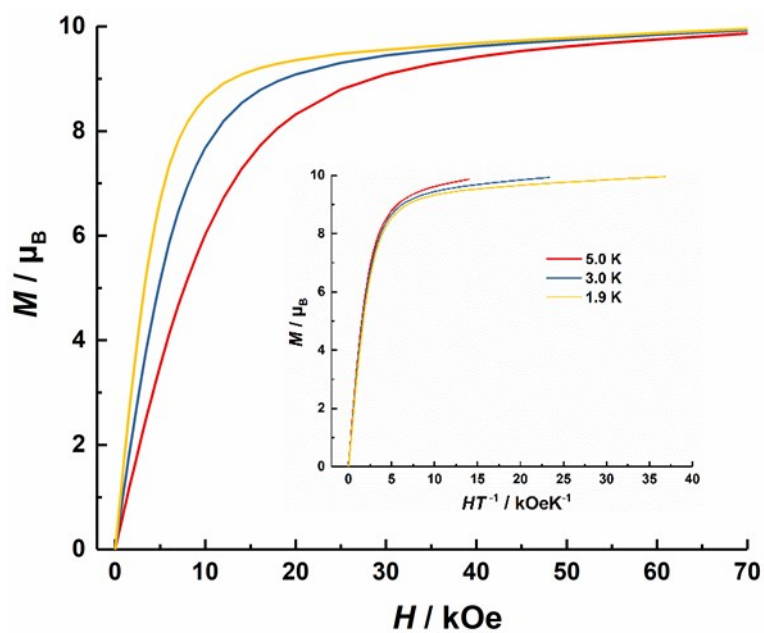


Figure S5. Field dependence of magnetization for **4**. Inset: M versus H/T plot for **4**.

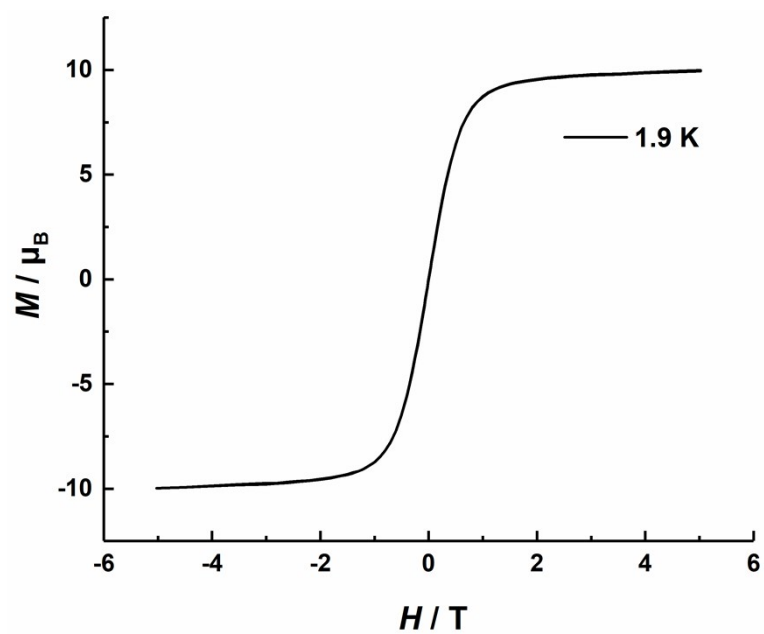


Figure S6. Variable magnetic field magnetization measurement for **1** at 1.9 K.

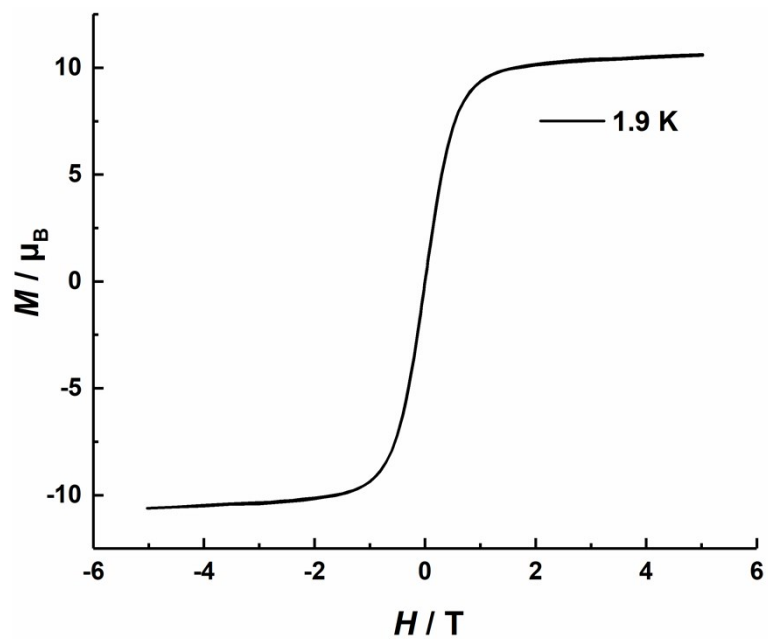


Figure S7. Variable magnetic field magnetization measurement for **2** at 1.9 K.

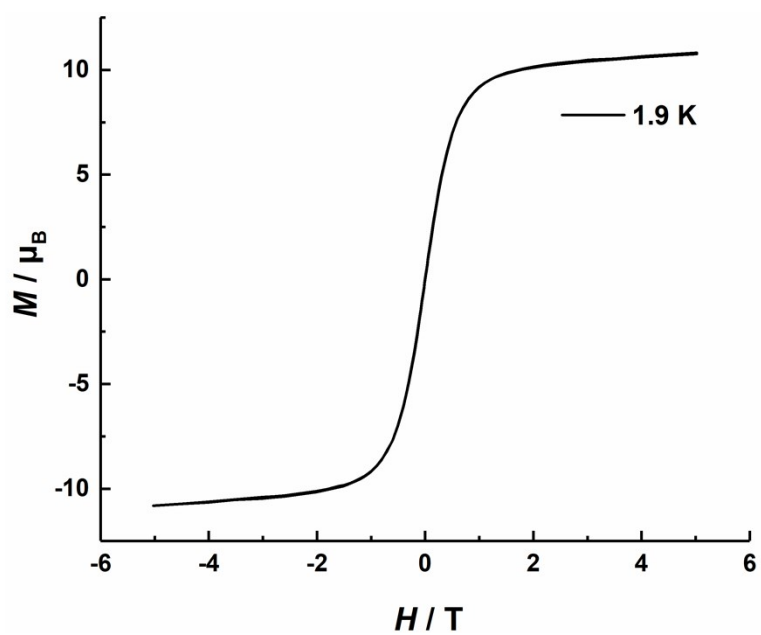


Figure S8. Variable magnetic field magnetization measurement for **3** at 1.9 K.

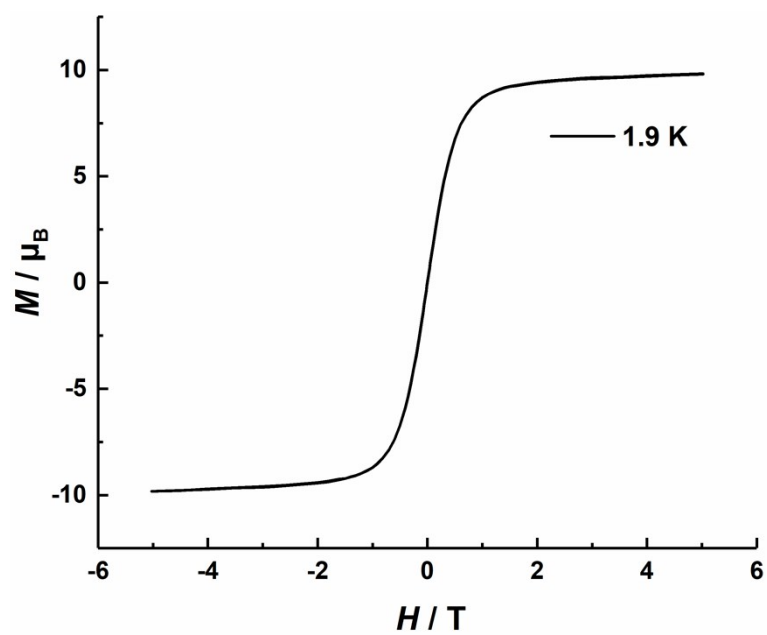


Figure S9. Variable magnetic field magnetization measurement for **4** at 1.9 K.

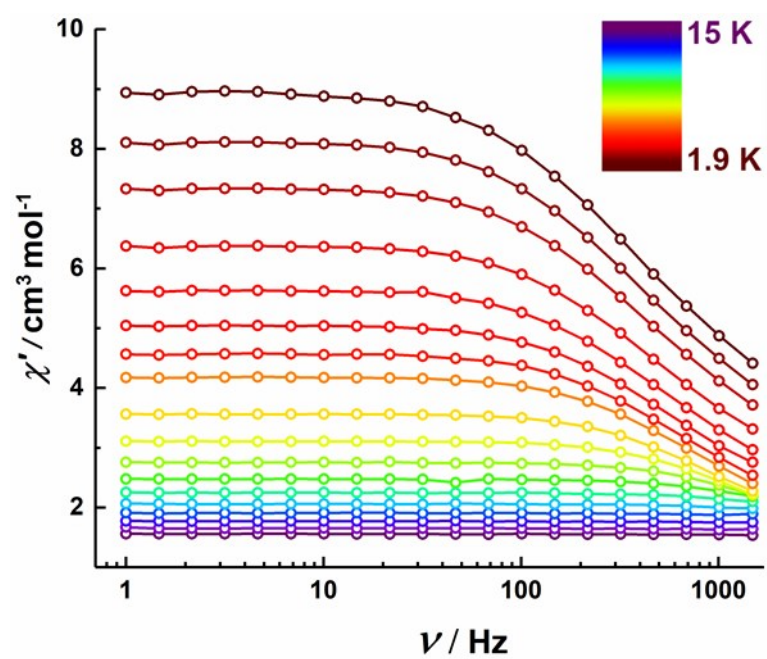


Figure S10. Frequency dependence under zero dc field of the in-phase ac susceptibility component at indicated temperature for **1**.

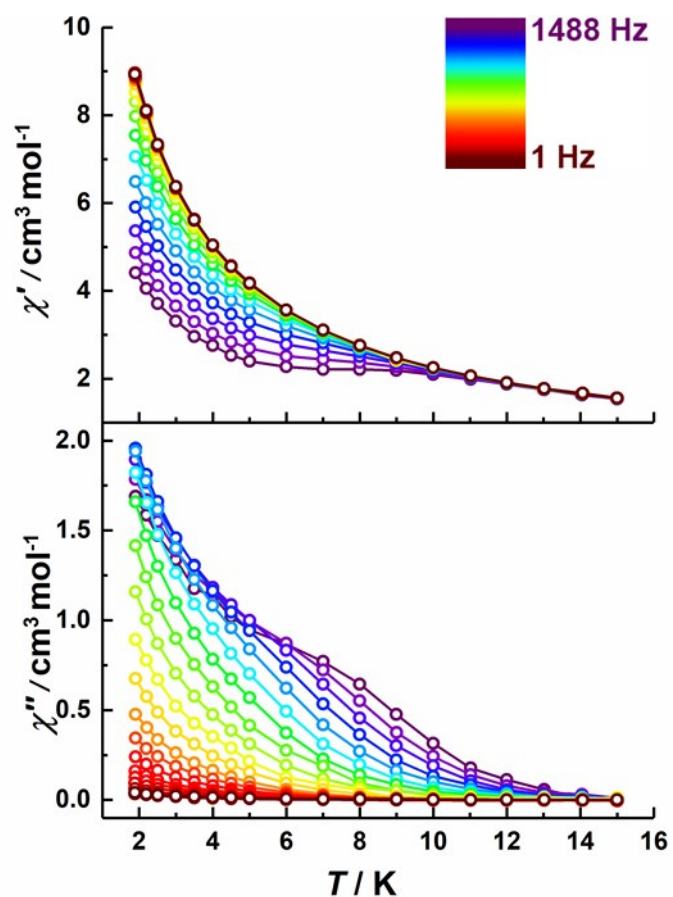


Figure S11. Temperature dependence under zero dc field of the in-phase (top) and the out-of-phase (bottom) ac susceptibility component at indicated ac frequency for **1**.

Table S3. Parameters Gained From the Fitting of Relaxation Time (τ) Versus Temperature (T^{-1}) Plots for **1**, **2** and **4**. For **3**, Parameters Gained From the e.q. (3).

<i>compound</i>	U_{eff}/K	τ_0/s	τ_{OTM}/s	$A/\text{s}^{-1}\text{K}^{-1}$	$C/\text{s}^{-1}\text{K}^{-n}$	n
1	45.1	4.97×10^{-7}	6.1×10^{-4}	/	7.8×10^{-6}	9.0
2	44.2	4.14×10^{-6}	1.4×10^{-3}	258	0.34	5.4
3	1.3	2.79×10^{-5}	/	/	/	/
4	56.2	6.15×10^{-6}	2.0×10^{-3}	49	0.3	4.8

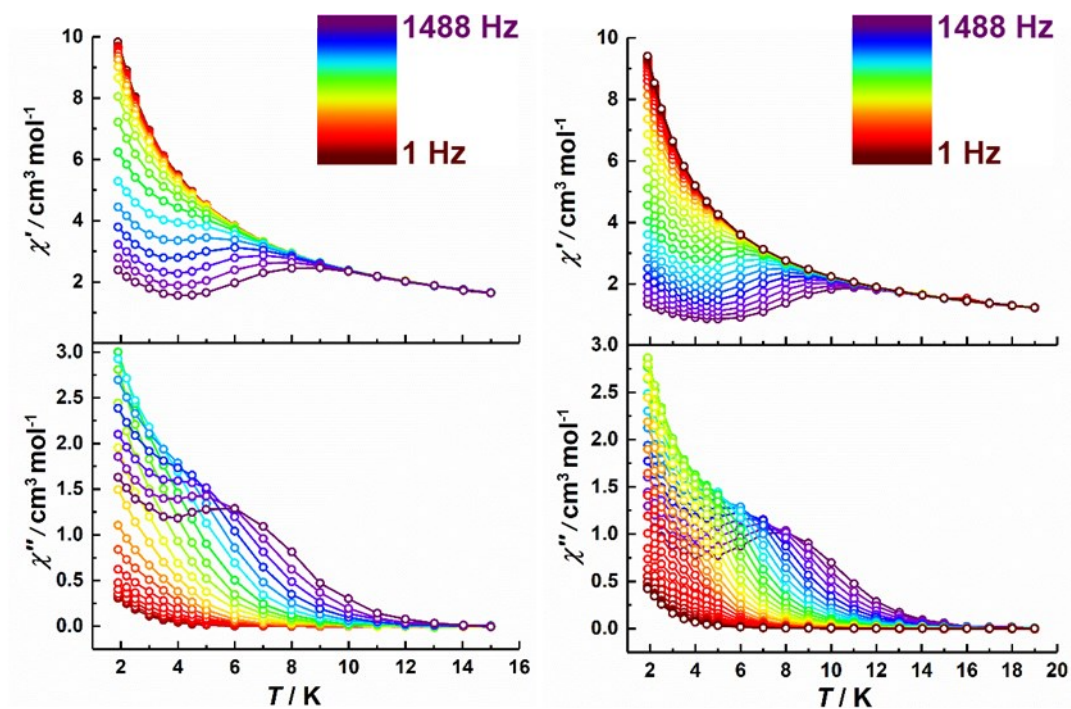


Figure S12. Temperature dependence under 500 (left) and 600 (right) Oe dc field of the in-phase (top) and the out-of-phase (bottom) ac susceptibility component at indicated ac frequency for **2** (left) and **4** (right).

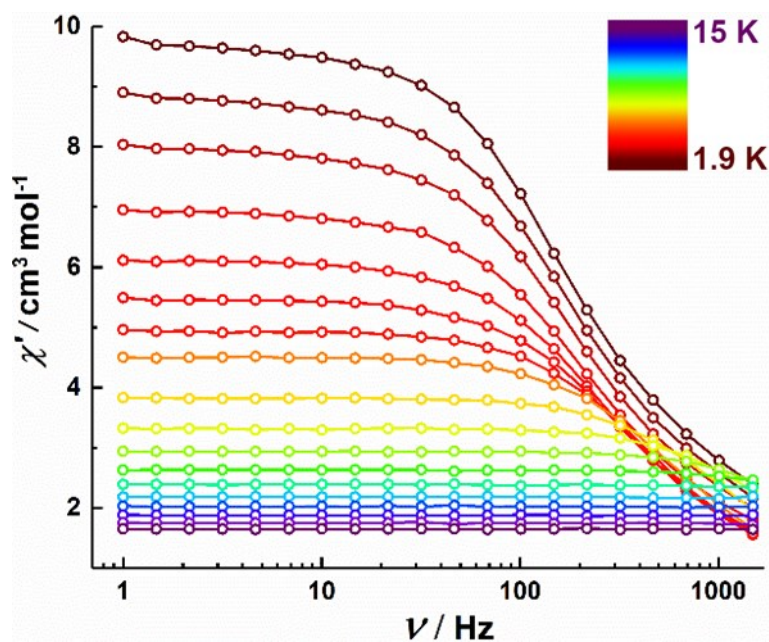


Figure S13. Frequency dependence under 600 Oe dc field of the in-phase ac susceptibility component at indicated temperature for **2**.

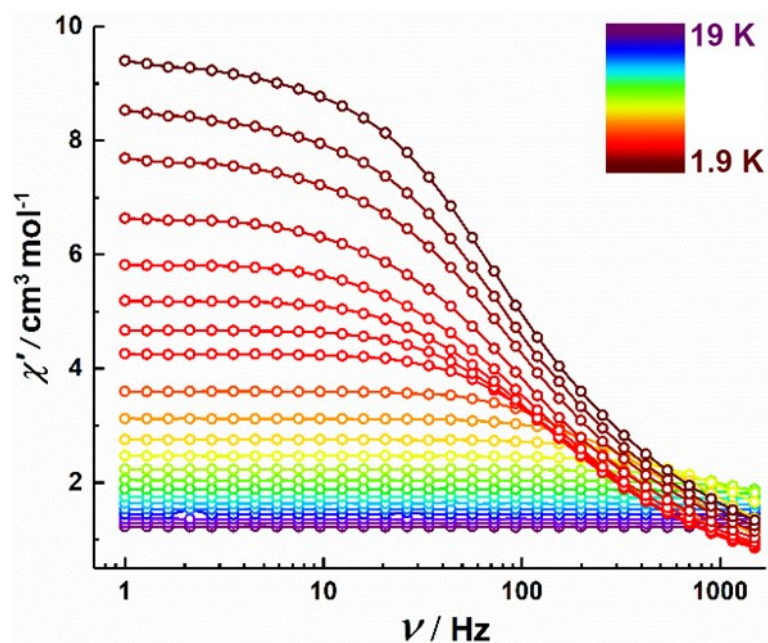


Figure S14. Frequency dependence under 500 Oe dc field of the in-phase ac susceptibility component at indicated temperature for 4.

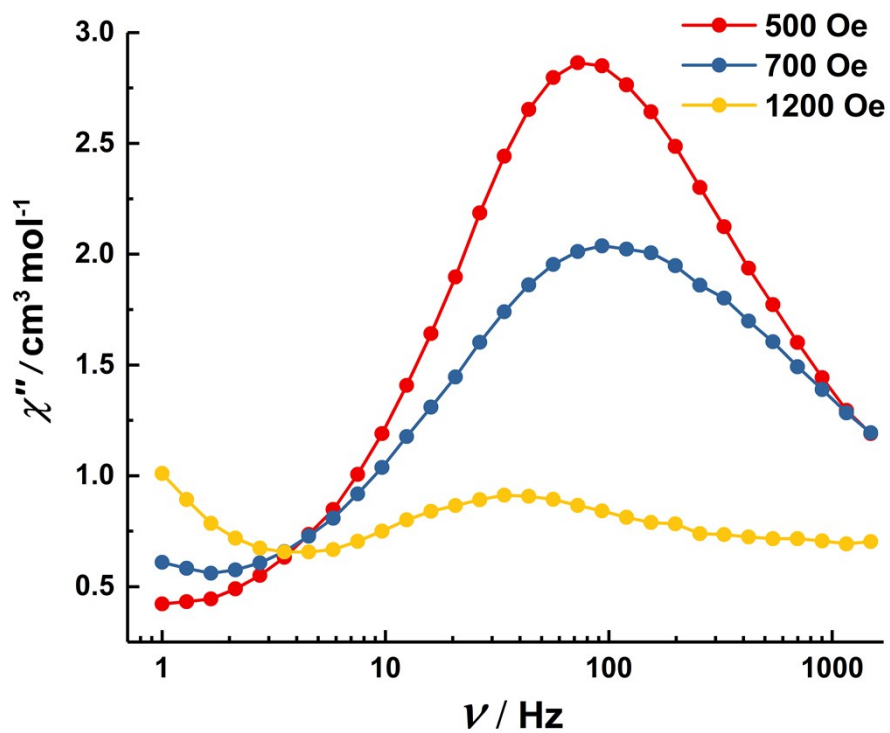


Figure S15. χ'' versus ν plot at 1.9 K under various applied dc field for 4.

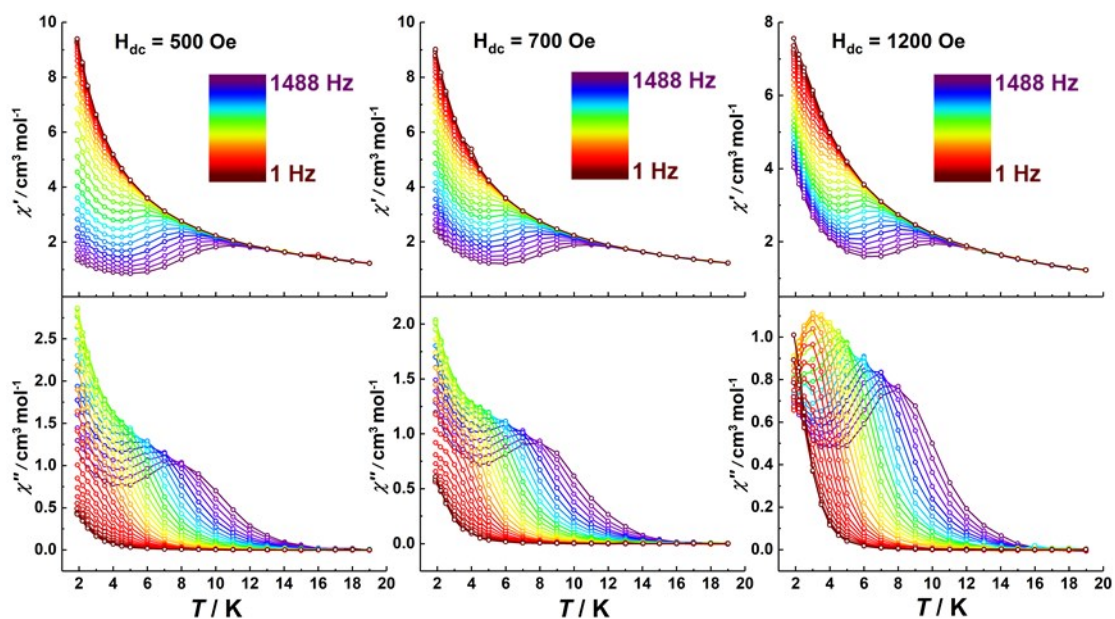


Figure S16. Temperature dependence under 500 (left), 700 (middle) and 1200 (right) Oe dc field of the in-phase (top) and the out-of-phase (bottom) ac susceptibility component at indicated ac frequency for **4**.

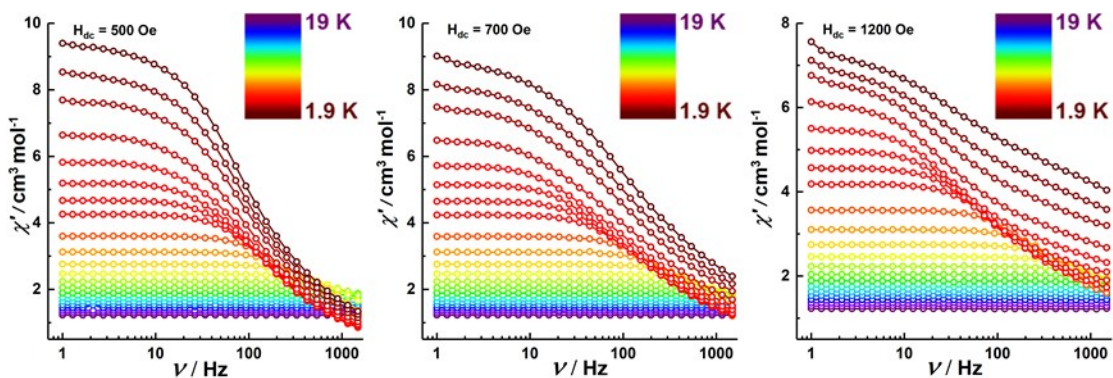


Figure S17. Frequency dependence under 500 (left), 700 (middle) and 1200 (right) Oe dc field of the in-phase ac susceptibility component at indicated temperature for **4**.

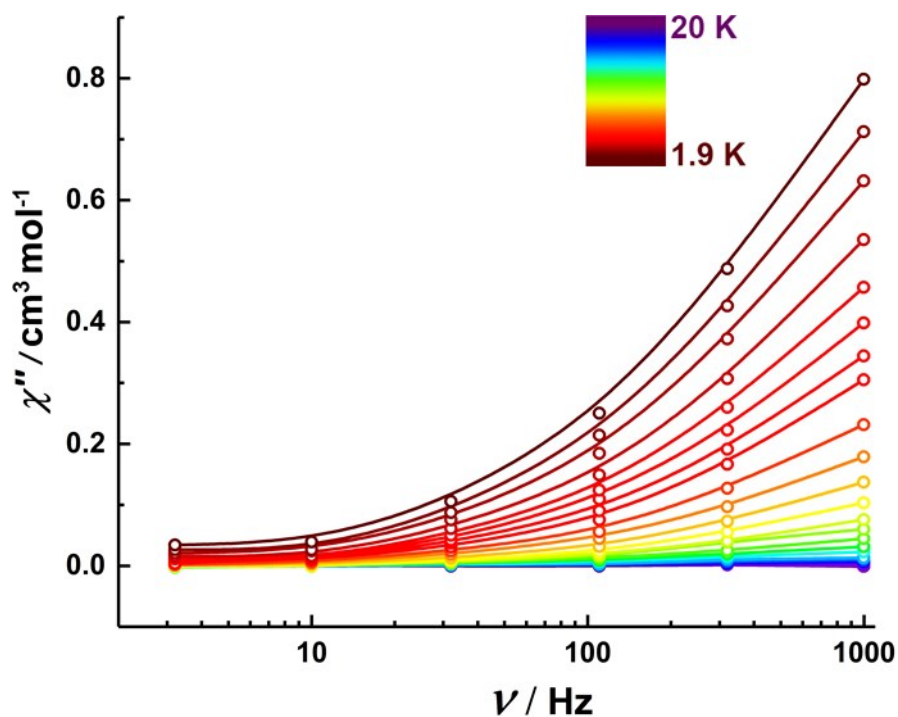


Figure S18. Frequency dependence under zero dc field of the out-of-phase ac susceptibility component at indicated temperature for **3**.

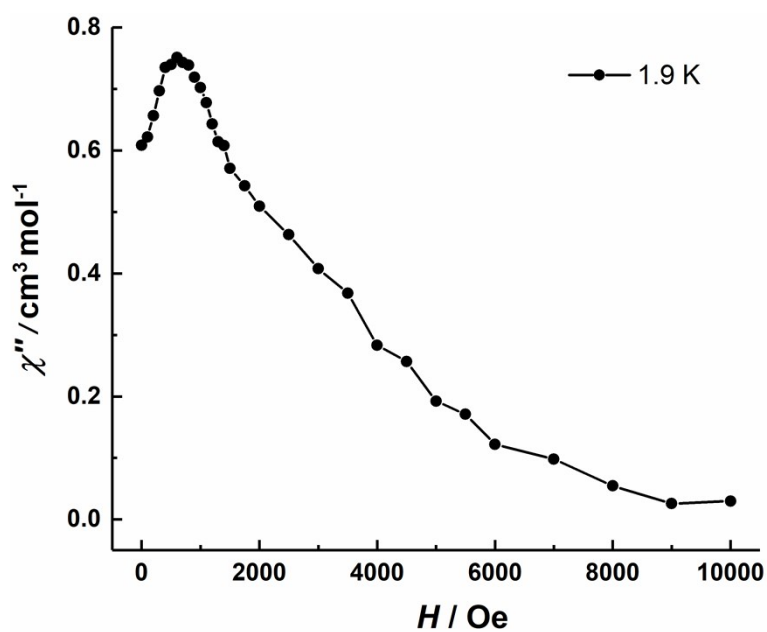


Figure S19. Field dependence of out-of-phase ac susceptibilities for **3** at 1.9 K, 997 Hz.

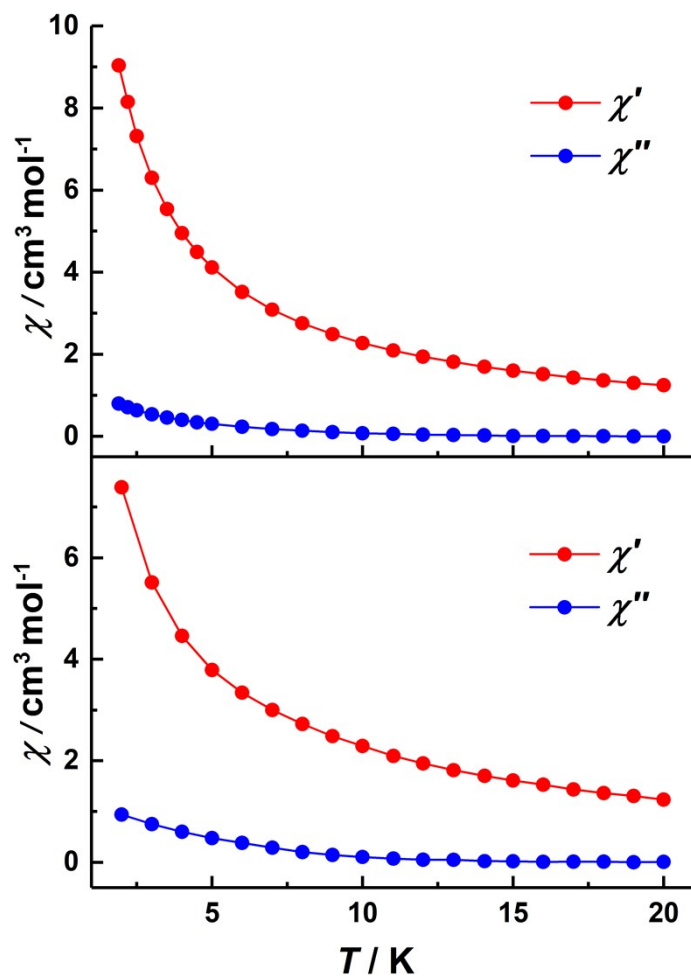


Figure S20. Temperature dependence under 0 (top) and 600 (bottom) Oe dc field of the in-phase (red) and the out-of-phase (blue) ac susceptibility component at 997 Hz for **3**.

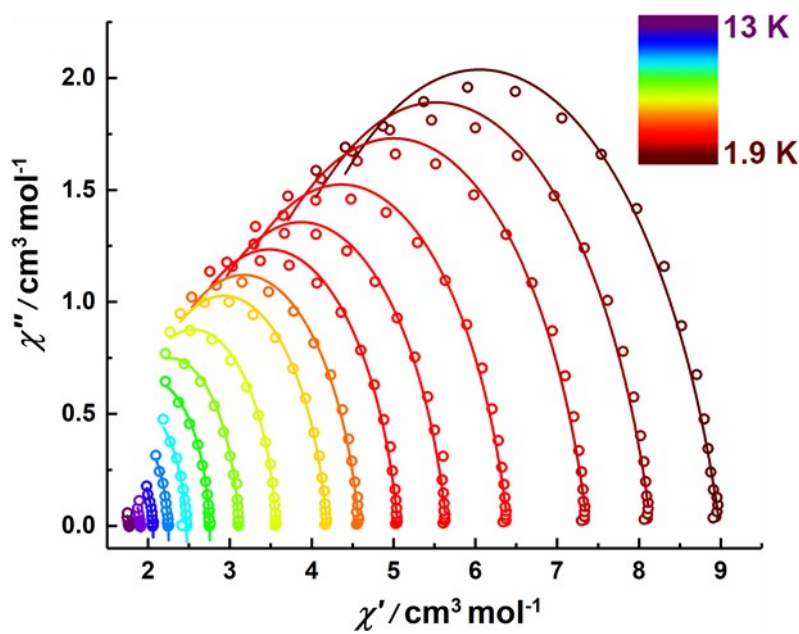


Figure S21. Cole-Cole plot for **1** at 1.9-13 K under zero dc field. The solid lines stand

for the best fit using a generalized Debye model.

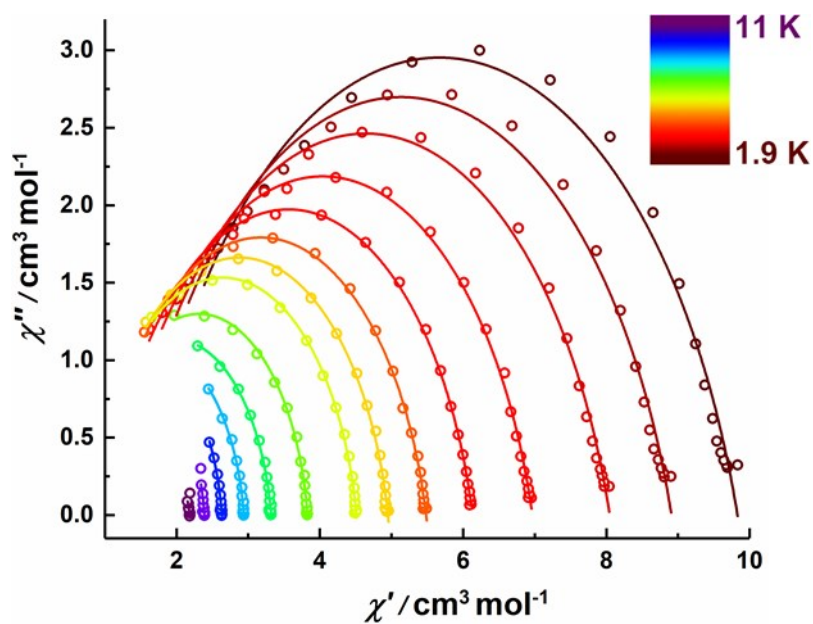


Figure S22. Cole-Cole plot for **2** at 1.9-11 K under 600 Oe applied dc field. The solid lines stand for the best fit using a generalized Debye model.

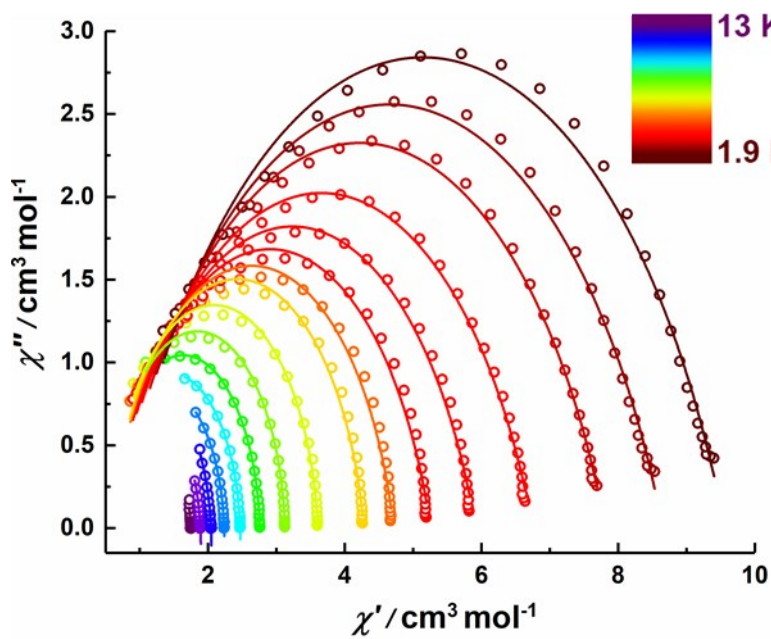


Figure S23. Cole-Cole plot for **4** at 1.9-13 K under 500 Oe applied dc field. The solid lines stand for the best fit using a generalized Debye model.