Supplementary Information

A family of $\{Cr^{III}_2Ln^{III}_2\}$ butterfly complexes: Effect of the lanthanide ion on the single molecule magnet properties

Stuart K. Langley,*,†,‡ Daniel P. Wielechowski,† Nicholas F. Chilton,♯ Boujemaa Moubaraki,† and Keith S. Murray*,†

†Dr. S. K. Langley, Mr. D. P. Wielechowski, Dr. B. Moubaraki, Em. Prof. K. S. Murray, School of Chemistry, Monash University, Clayton, Victoria 3800, Australia

email: keith.murray@monash.edu

‡Dr. S. K. Langley, School of Science and the Environment, Chemistry Division, Manchester Metropolitan University, Manchester, England.

email: s.langley@mmu.ac.uk

♯Dr. N. F. Chilton, School of Chemistry, The University of Manchester, Manchester M13 9PL, U.K.

Table S1. Crystallographic data for compounds **2 - 7**.

	2	**3**	**4**
Formula[a]	$Cr_2Pr_2C_{44}H_{60}O_{24}N_4$	$Cr_2Nd_2C_{44}H_{60}O_{24}N_4$	$Cr_2Gd_2C_{40}H_{48}O_{20}N_4$
M, $gmol^{-1}$	1414.78	1421.44	1323.32
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$
a/Å	8.0730(5)	8.0857(4)	7.9552(3)
b/Å	18.1966(12)	18.2300(8)	17.2589(6)
c/Å	17.9681(12)	17.9342(9)	17.3417(6)
α/deg	90	90	90
β/deg	95.794(2)	95.7520(10)	92.2190(10)
γ/deg	90	90	90
V/$Å^3$	2626.0(3)	2628.8(2)	2379.20(15)
T/K	123(2)	123(2)	123(2)
Z	2	2	2
ρ_{calc} [g cm^{-3}]	1.789	1.796	1.847
λ^b/ Å	0.71073	0.71073	0.71073

Data Measured	20655	27926	14799
Ind. Reflns	5981	8079	6979
R_{int}	0.0295	0.0312	0.0367
Reflns with $I > 2\sigma(I)$	4940	6441	5127
Parameters	350	350	309
Restraints	2	1	0
R_1^d (obs), wR_2^d (all)	0.0563, 0.1493	0.0590, 0.1615	0.0432, 0.1132
goodness of fit	1.046	1.052	1.038
Largest residuals/ e Å $^{-3}$	3.735, -2.034	3.163, -1.958	3.131, -1.058

	5	**6**	**7**
Formula[a]	$Cr_2Tb_2C_{40}H_{48}O_{20}N_4$	$Cr_2Ho_2C_{40}H_{48}O_{20}N_4$	$Cr_2Er_2C_{44}H_{60}O_{22}N_4$
M, $gmol^{-1}$	1326.66	1338.68	1435.48
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$
a/Å	7.9196(4)	7.9823(6)	12.6681(4)
b/Å	17.3124(8)	17.2497(12)	11.6507(4)
c/Å	17.4215(9)	17.3295(13)	19.8972(6)
α/deg	90	90	90
β/deg	92.174(2)	92.336(3)	104.224(2)
γ/deg	90	90	90
V/Å^3	2386.9(2)	2384.2(3)	1220.74(6)
T/K	123(2)	123(2)	123(2)
Z	2	2	2
ρ_{calc} [g cm^{-3}]	1.846	1.865	1.675
λ^b/ Å	0.71073	0.71073	0.71073
Data Measured	11909	25719	14594
Ind. Reflns	5275	7259	6445
R_{int}	0.0435	0.0280	0.0351
Reflns with $I > 2\sigma(I)$	3977	6053	5185
Parameters	328	309	373
Restraints	12	0	35
R_1^d (obs), wR_2^d (all)	0.0406, 0.1027	0.0313, 0.0816	0.0975, 0.0372
goodness of fit	1.021	1.038	1.030
Largest residuals/ e Å $^{-3}$	1.965, -0.990	2.970, -1.032	1.728, -0.578

[a] Including solvate molecules. [b] Graphite monochromator.

[d] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, $wR2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$.

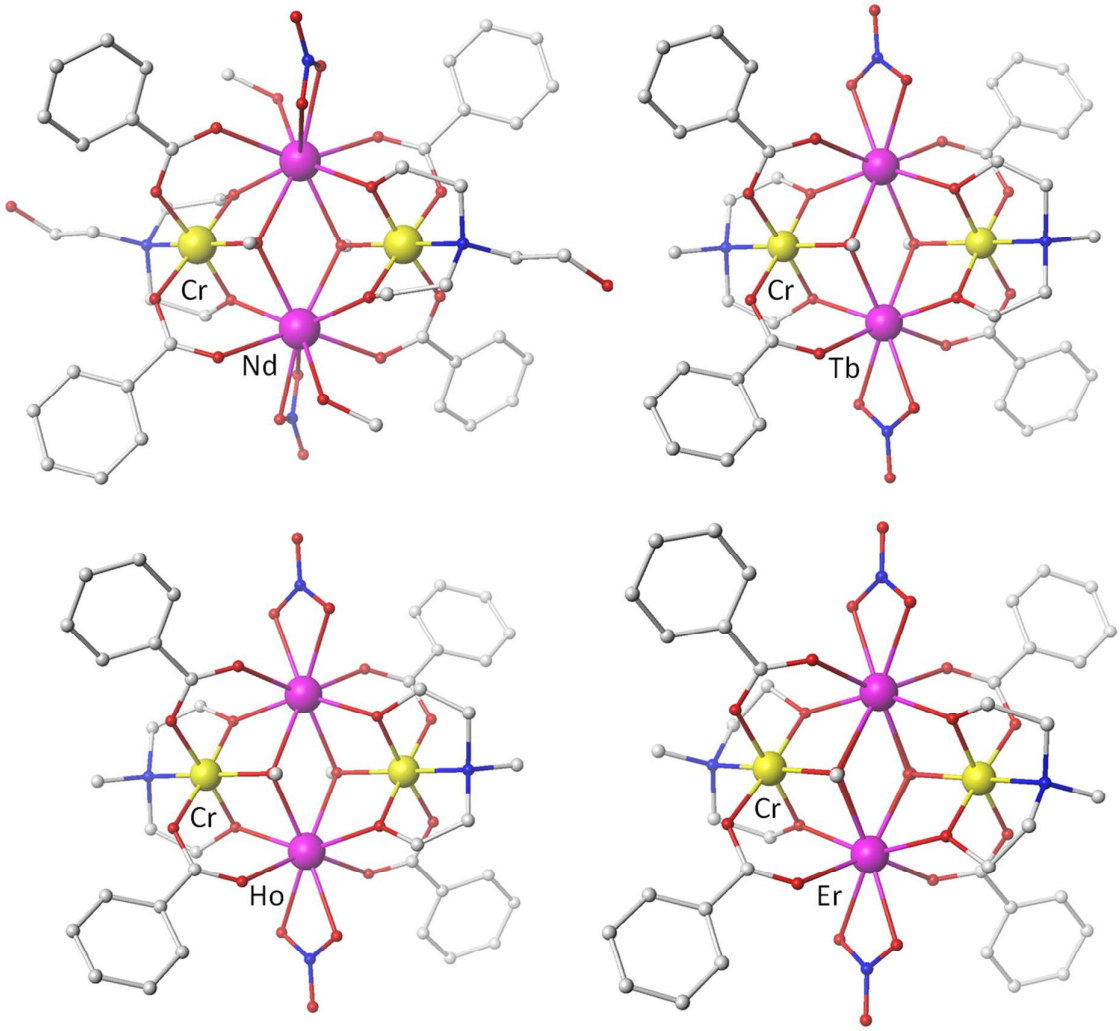

Figure S1. The molecular structure of compounds **3** (top left), **5** (top right), **6** (bottom left) and **7** (bottom right). The H atoms are omitted for clarity. Colour scheme; Cr^{III}, yellow; Ln^{III}, purple; O, red; N, blue; C, light grey.

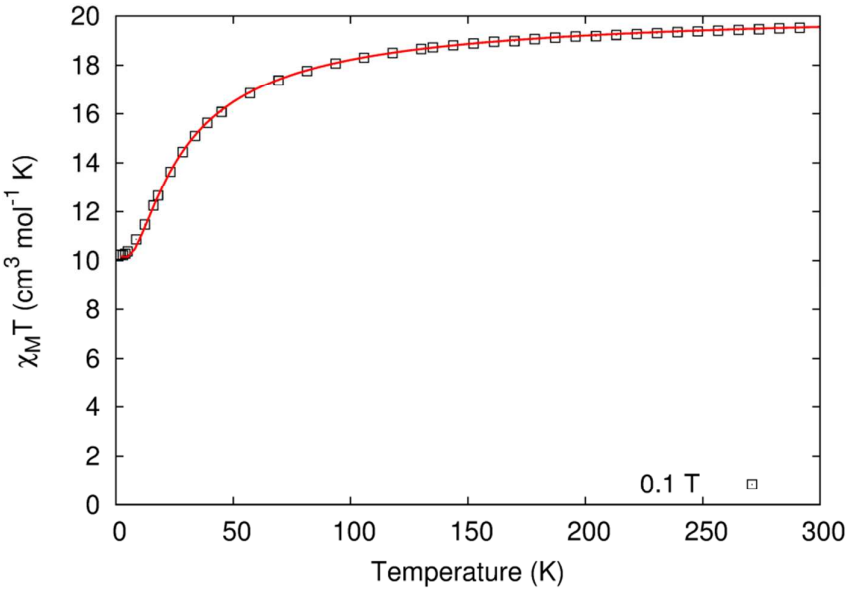

Figure S2. Plot of $\chi_M T$ *versus* T for **4** measured under a 0.1 T magnetic field. Red line is a fit to the data with parameters given in the text.

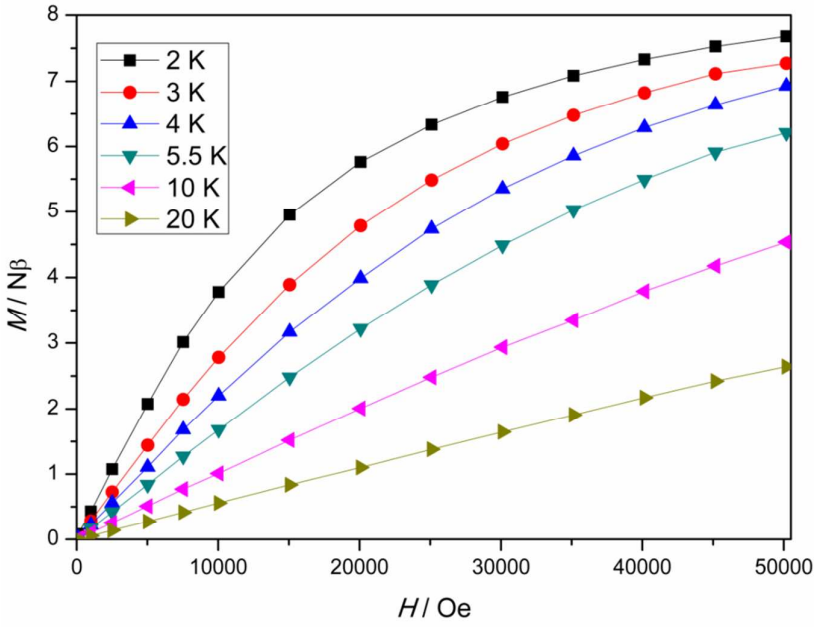

Figure S3. Isothermal magnetization *versus* field plots for **2** (Pr). The solid lines just join the points.

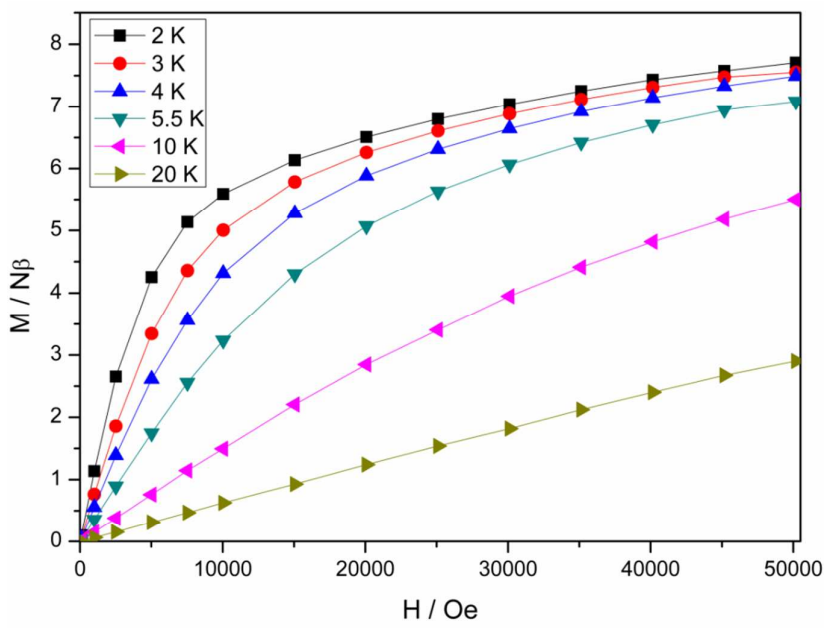

Figure S4. Isothermal magnetization *versus* field plots for **3** (Nd). The solid lines just join the points.

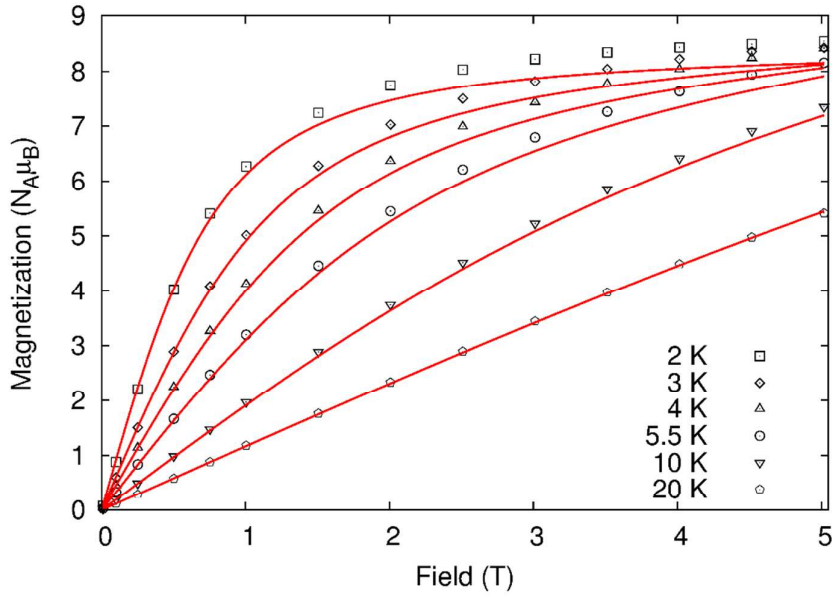

Figure S5. Isothermal magnetization *versus* field plots for **4** (Gd). The solid red lines are fits of the experimental data using the parameters given in the text.

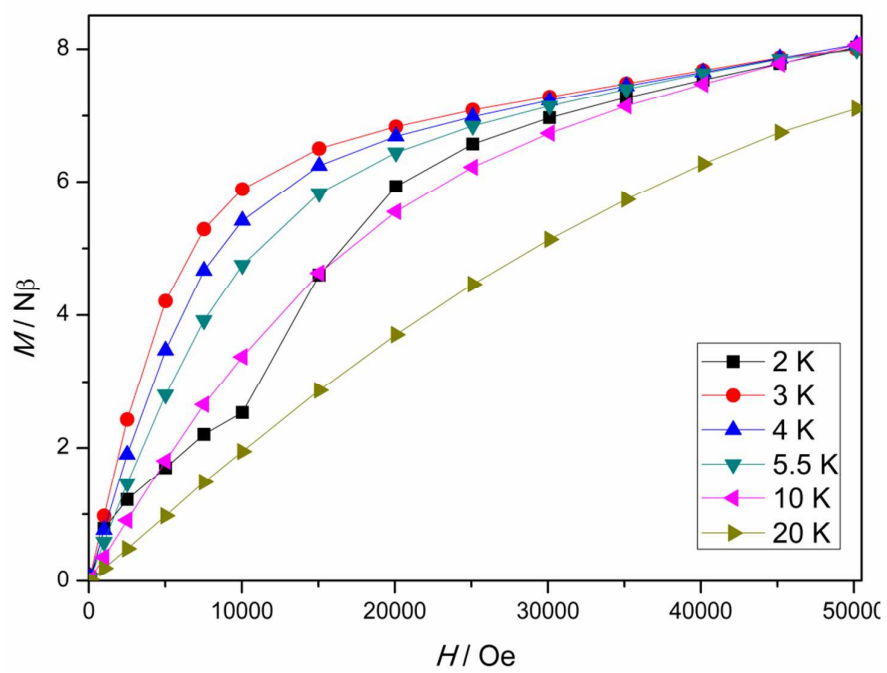

Figure S6. Isothermal magnetization *versus* field plots for **5** (Tb). The solid lines just join the points.

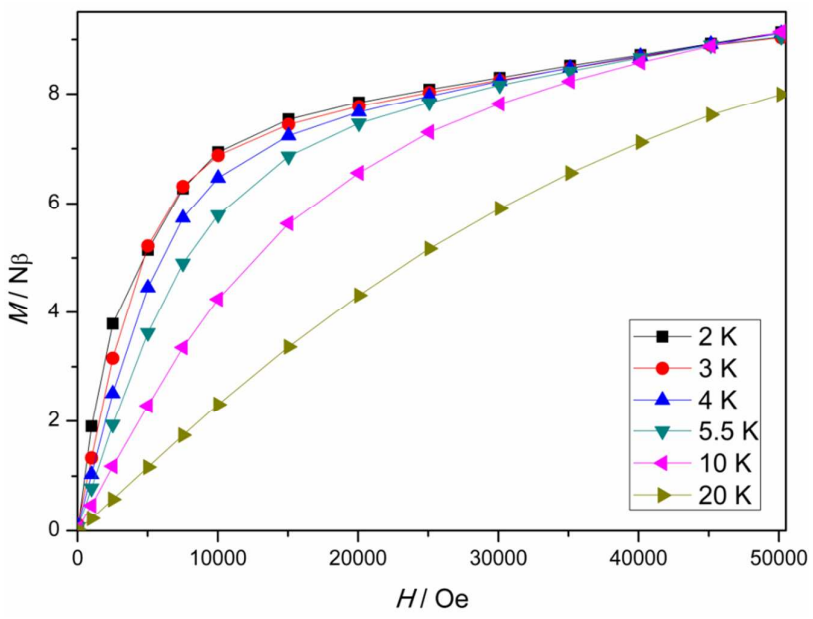

Figure S7. Isothermal magnetization *versus* field plots for **6** (Ho). The solid lines just join the points.

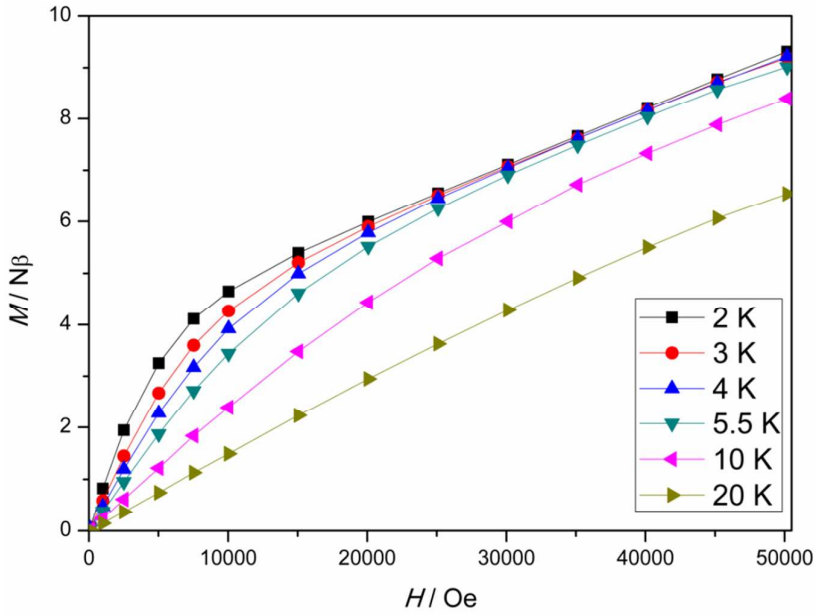

Figure S8. Isothermal magnetization *versus* field plots for **7** (Er). The solid lines just join the points.

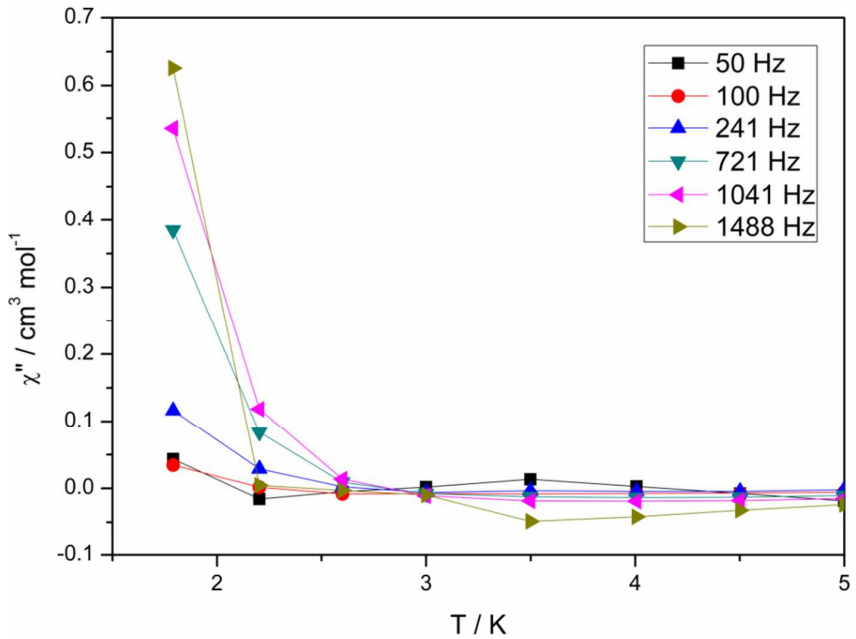

Figure S9. Out-of-phase susceptibility *versus* temperature for **3** (Nd), with $H_{dc} = 0$.

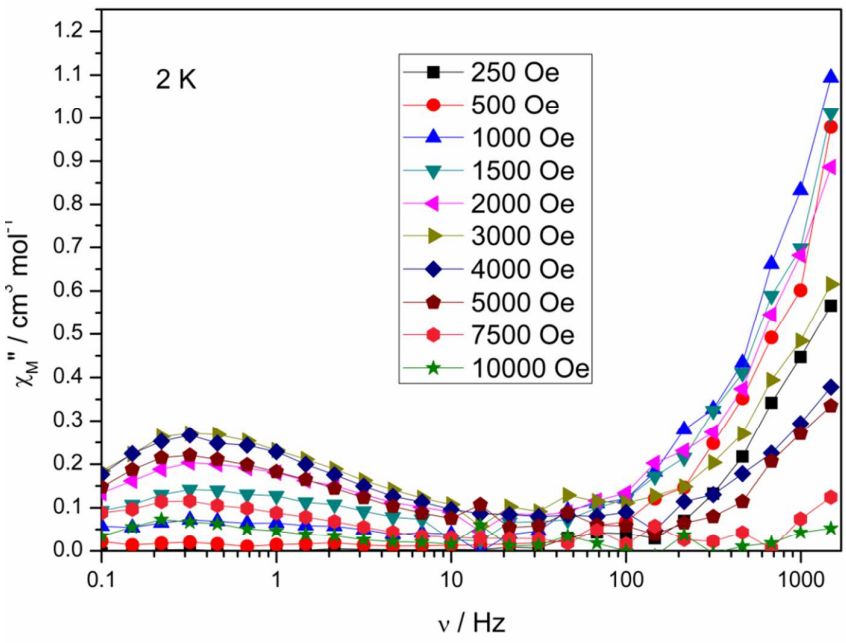

Figure S10. Field dependence of the relaxation time for **3** (Nd).

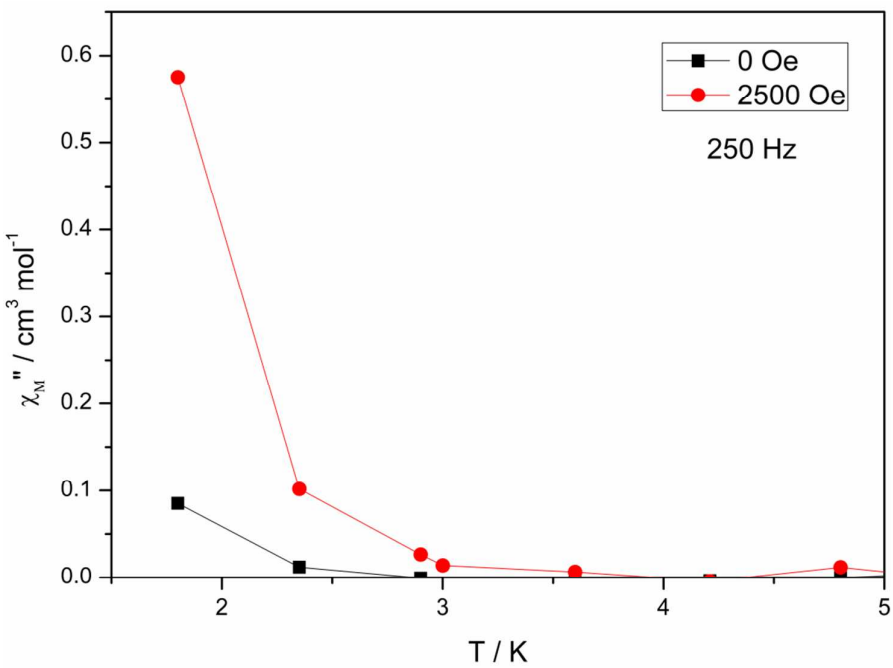

Figure S11. Out-of-phase susceptibility *versus* temperature for **7** (Er) at zero and a 2500 Oe dc magnetic field.

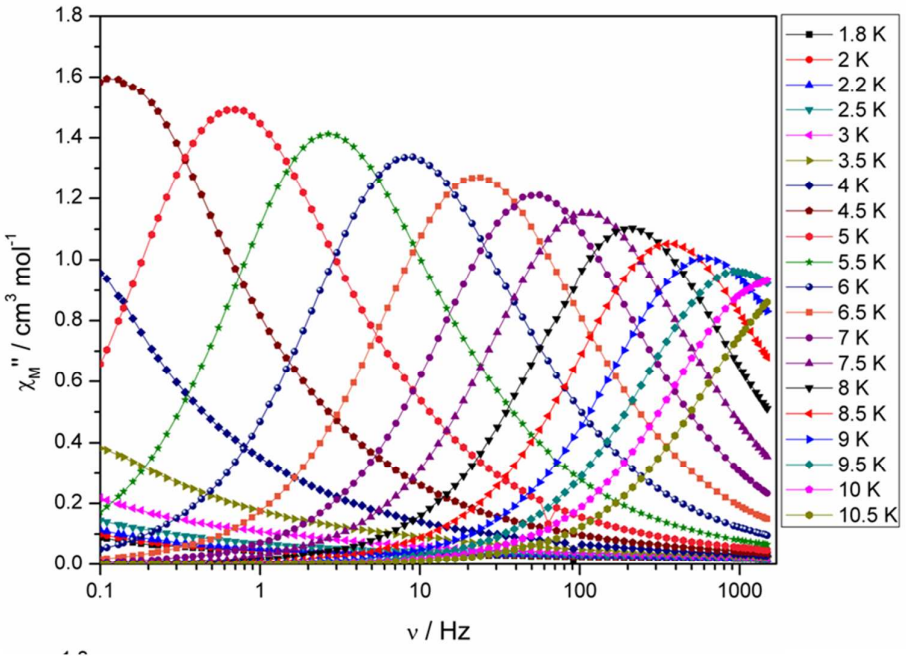

Figure S12. Frequency dependence of χ_M'' for **1** in a zero applied dc field, with an ac field of 3.5 Oe. (see ref 9 in script)

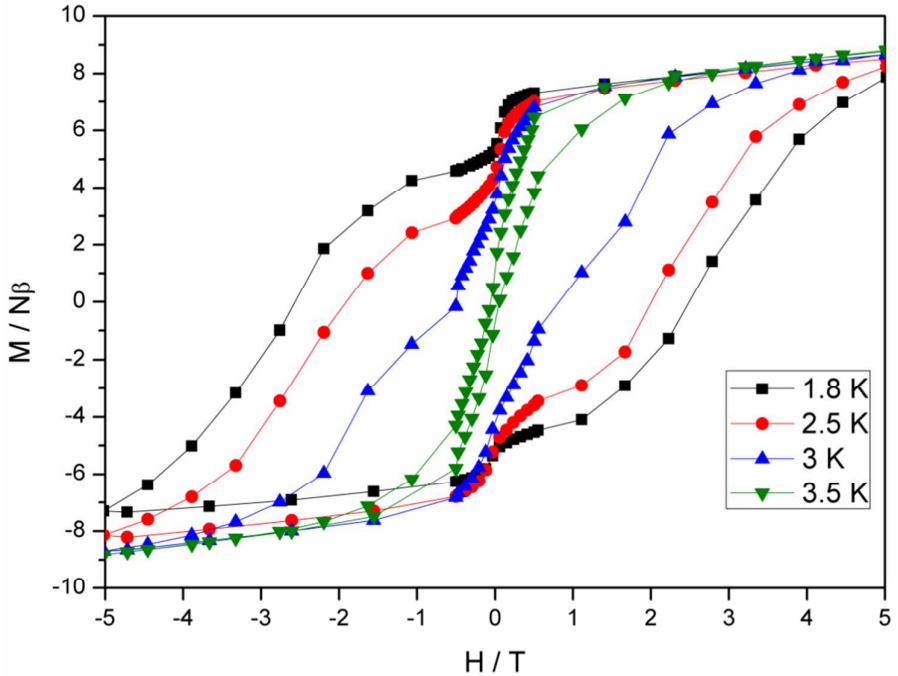

Figure S13. Plot of magnetization (*M*) *versus* field (*H*) for **1**, sweeping the field with an average sweep rate of 0.003 T/s, at the temperatures indicated. (see ref 9 in script)