Supplementary Materials

for

Magnetic Behavior of Luminescent Dinuclear Dysprosium and Terbium Complexes Derived from Phenoxyacetic Acid and 2,2′-Bipyridine

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Table S1. Crystallographic data for **1–3**

	1	**2**	**3**
Empirical formula	$C_{72}H_{70}N_4O_{20}Dy_2$	$C_{72}H_{70}N_4O_{20}Tb_2$	$C_{72}H_{70}N_4O_{20}Y_2$
Formula weight	1636.32	1629.16	1489.14
Crystal system	Triclinic	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a (Å)	10.1675(6)	10.169(4)	10.168(3)
b (Å)	11.7571(4)	11.791(5)	11.788(4)
c (Å)	14.2186(6)	14.295(6)	14.272(5)
α (°)	98.618(3)	98.573(8)	98.459(6)
β (°)	94.315(4)	94.356(6)	94.192(6)
γ (°)	91.681(4)	91.468(5)	91.417(7)
V (Å^3)	1674.32(14)	1688.8(12)	1686.4(10)
Z	1	1	1
ρ_{calcd} (g cm^{-3})	1.623	1.602	1.466
λ (Mo K$_\alpha$) (Å)	0.71073	0.71073	0.71073
μ (mm^{-1})	2.293	2.155	1.791
T (K)	120(2)	120(2)	120(2)
F(000)	822	820	768
2θ range for data collection (°)	4.768—49.978	8.044—54.924	8.044—54.956
Index ranges	$-11 \le h \le 12$	$-13 \le h \le 10$	$-12 \le h \le 13$
	$-13 \le k \le 12$	$-15 \le k \le 15$	$-15 \le k \le 15$
	$-16 \le l \le 16$	$-17 \le l \le 18$	$-15 \le l \le 18$
No. measured reflections	11021	13659	12391
No. independent reflections	5712	7388	7305
R_{int}	0.0614	0.0381	0.0335
No. refined parameters	427	463	463
No. observed reflections, $I > 2\sigma(I)$	5445	6509	5833
Goodness-of-fit on F^2, S	1.053	1.060	0.942
$R_1{}^a$, $wR_2{}^b$ [$I > 2\sigma(I)$]	0.0804, 0.2279	0.0383, 0.0855	0.0505, 0.1292
$R_1{}^a$, $wR_2{}^b$ (all data)	0.0827, 0.2311	0.0460, 0.0972	0.0658, 0.1460

$^aR_1 = [\sum||F_o| - |F_c||/\sum|F_o|]$. $^bwR_2 = [\sum w(F_o{}^2 - F_c{}^2)^2/\sum w(F_o{}^2)^2]^{1/2}$

Table S2. Summary of SHAPE analysis around Ln^{III} centre(s) for **1** and **2** and Y^{III} centre(s) in **3** (Ln = Dy for **1**, Ln = Tb for **2**).

ML_9		**1**	**2**	**3**
Enneagon	D_{9h}	34.683	34.702	34.832
Octagonal pyramid	C_{8v}	22.504	22.542	22.588
Heptagonal bipyramid	D_{7h}	17.284	17.152	17.257
Johnson triangular cupola J3	C_{3v}	15.396	15.479	15.527
Capped cube J8	C_{4v}	10.411	10.367	10.193
Spherical-relaxed capped cube	C_{4v}	10.158	10.074	10.024
Capped square antiprism J10	C_{4v}	1.907	1.996	1.848
Spherical capped square antiprism	C_{4v}	1.620	1.676	1.638
Tricapped trigonal prism J51	D_{3h}	3.448	3.595	3.497
Spherical tricapped trigonal prism	D_{3h}	2.911	2.981	2.954
Tridiminished icosahedron J63	C_{3v}	13.868	13.795	13.953
Hula-hoop	C_{2v}	9.548	9.444	9.641
Muffin	C_s	**1.267**	**1.285**	**1.278**

Table S3. Selected bond angles in ⁰ for Dy^{III} , Tb^{III} and Y^{III} centre(s) in **1, 2** and **3,** respectively. Symmetry: A, –*x*, –*y*, 2–*z* for **1**; A, –*x*, 1–*y*, 2–*z* for **2** and A, –*x*, 1–*y*, –*z* for **3**.

1		**2**		**3**	
O1–Dy1–O2	53.6(2)	O1–Tb1–O2	53.52(10)	O1–Y1–O2	53.95(8)
O1–Dy1–O3	143.7(2)	O1–Tb1–O3A	143.08(10)	O1–Y1–O3	143.39(8)
O1–Dy1–O4	81.6(2)	O1–Tb1–O4	82.15(11)	O1–Y1–O4A	81.96(8)
O1–Dy1–O4A	146.1(2)	O1–Tb1–O4A	146.68(10)	O1–Y1–O4	145.82(8)
O1–Dy1–O5	80.9(2)	O1–Tb1–O5A	80.66(10)	O1–Y1–O5A	80.62(8)
O1–Dy1–O6	128.8(2)	O1–Tb1–O6	129.08(10)	O1–Y1–O6	129.74(8)
O1–Dy1–N1	73.7(2)	O1–Tb1–N1	73.56(10)	O1–Y1–N1	73.41(8)
O1–Dy1–N2	98.7(2)	O1–Tb1–N2	98.54(11)	O1–Y1–N2	98.96(9)
O2–Dy1–O3	144.0(2)	O2–Tb1–O3A	144.12(10)	O2–Y1–O3	143.81(8)
O2–Dy1–O4	79.6(2)	O2–Tb1–O4	79.80(11)	O2–Y1–O4A	80.27(9)
O2–Dy1–O4A	141.0(2)	O2–Tb1–O4A	141.55(10)	O2–Y1–O4	141.43(7)
O2–Dy1–O5	131.3(2)	O2–Tb1–O5A	130.88(10)	O2–Y1–O5A	131.38(8)
O2–Dy1–O6	77.3(2)	O2–Tb1–O6	77.52(11)	O2–Y1–O6	77.98(8)
O2–Dy1–N1	102.5(2)	O2–Tb1–N1	102.14(11)	O2–Y1–N1	101.86(8)
O2–Dy1–N2	72.2(2)	O2–Tb1–N2	72.42(11)	O2–Y1–N2	71.81(9)
O3–Dy1–O4	125.7(2)	O3A–Tb1–O4	125.77(10)	O3–Y1–O4A	125.40(8)
O3–Dy1–O4A	50.85(19)	O3A–Tb1–O4A	50.55(9)	O3–Y1–O4	50.82(7)
O3–Dy1–O5	83.0(2)	O3A–Tb1–O5A	83.02(10)	O3–Y1–O5A	82.94(8)
O3–Dy1–O6	84.6(2)	O3A–Tb1–O6	84.87(11)	O3–Y1–O6	84.18(8)
O3–Dy1–N1	71.1(2)	O3A–Tb1–N1	70.63(10)	O3–Y1–N1	71.18(8)
O3–Dy1–N2	73.4(2)	O3A–Tb1–N2	73.18(10)	O3–Y1–N2	73.49(8)
O4–Dy1–O4A	74.9(2)	O4–Tb1–O4A	75.24(11)	O4A–Y1–O4	74.59(8)
O4–Dy1–O5	77.0(2)	O4–Tb1–O5A	77.05(10)	O4A–Y1–O5A	76.76(8)
O4–Dy1–O6	75.7(2)	O4–Tb1–O6	75.66(11)	O4A–Y1–O6	75.75(8)
O4–Dy1–N1	146.4(2)	O4–Tb1–N1	147.07(11)	O4A–Y1–N1	146.72(9)
O4–Dy1–N2	143.9(2)	O4–Tb1–N2	144.06(10)	O4A–Y1–N2	143.82(8)
O4A–Dy1–O5	70.3(2)	O4A–Tb1–O5A	70.71(10)	O4–Y1–O5A	70.14(8)
O4A–Dy1–O6	68.2(2)	O4A–Tb1–O6	68.31(10)	O4–Y1–O6	67.84(8)
O4A–Dy1–N1	115.1(2)	O4A–Tb1–N1	114.72(10)	O4–Y1–N1	115.23(7)
O4A–Dy1–N2	114.6(2)	O4A–Tb1–N2	114.15(10)	O4–Y1–N2	114.67(8)
O5–Dy1–O6	134.8(2)	O5A–Tb1–O6	135.15(10)	O5A–Y1–O6	134.37(8)
O5–Dy1–N1	77.0(2)	O5A–Tb1–N1	77.33(10)	O5A–Y1–N1	77.43(8)
O5–Dy1–N2	139.0(2)	O5A–Tb1–N2	138.75(11)	O5A–Y1–N2	139.32(8)
O6–Dy1–N1	137.8(2)	O6–Tb1–N1	137.17(11)	O6–Y1–N1	137.46(9)
O6–Dy1–N2	76.4(2)	O6–Tb1–N2	76.42(11)	O6–Y1–N2	76.29(8)
N1–Dy1–N2	63.9(3)	N1–Tb1–N2	63.29(11)	N1–Y1–N2	63.87(9)

Table S4. Parameters obtained from Cole-Cole fitting for **1'**

Temperature (K)	χ_{Iso}	α	τ
1.85	1.65685	0.39319	0.00158
2	1.52722	0.39129	0.00104
2.14	1.42086	0.39499	6.47199×10^{-4}
2.28	1.34858	0.4047	4.31688×10^{-4}
2.42	1.26468	0.41444	2.64278×10^{-4}
2.56	1.19661	0.4215	1.68696×10^{-4}
2.71	1.1338	0.41602	1.13535×10^{-4}
2.85	1.07559	0.40023	7.95908×10^{-5}
3	1.0228	0.37676	5.77927×10^{-5}
3.25	0.94568	0.33286	3.39518×10^{-5}
3.5	0.88112	0.29911	1.97928×10^{-5}
3.75	0.82689	0.27736	1.1478×10^{-5}
4	0.78035	0.272	6.34172×10^{-6}

Table S5: List of parameters related to the magnetic properties of **1'**

Parameter (Unit)	Value	Standard Error
A ($s^{-1} H^{-4} K^{-n}$)	2.39×10^{-27}	0
H (Oe)	1000	0
n	2	0
C ($s^{-1} K^{-m}$)	78.834	0.22677
m	3	0
ΔE (cm^{-1})	16.261	0.49221
τ_0 (s)	2.425×10^{-8}	7.80855×10^{-9}
QTM (s^{-1})	7.897×10^{26}	0

Table S6. Spectral parameters of the absorption spectra for complexes **1**, **2** and HL^1 and L^2 in acetonitrile

Complex 1		**Complex 2**	
λ_{max} (nm)	ε (M^{-1} cm^{-1})	λ_{max} (nm)	ε (M^{-1} cm^{-1})
220	39,792	220	43,354
236	23,001	236	25,914
243(shoulder)	20,180	243(shoulder)	22,609
271(shoulder)	29,837	271(shoulder)	32,158
277	31,776	277	34,031
Phenoxyacetic acid (HL^1)		**2,2′-bipyridine (L^2)**	
218	7,608	236	11,613
263(shoulder)	1,078	243(shoulder)	10,197
270	1,522	281	14,785
276	1,224		

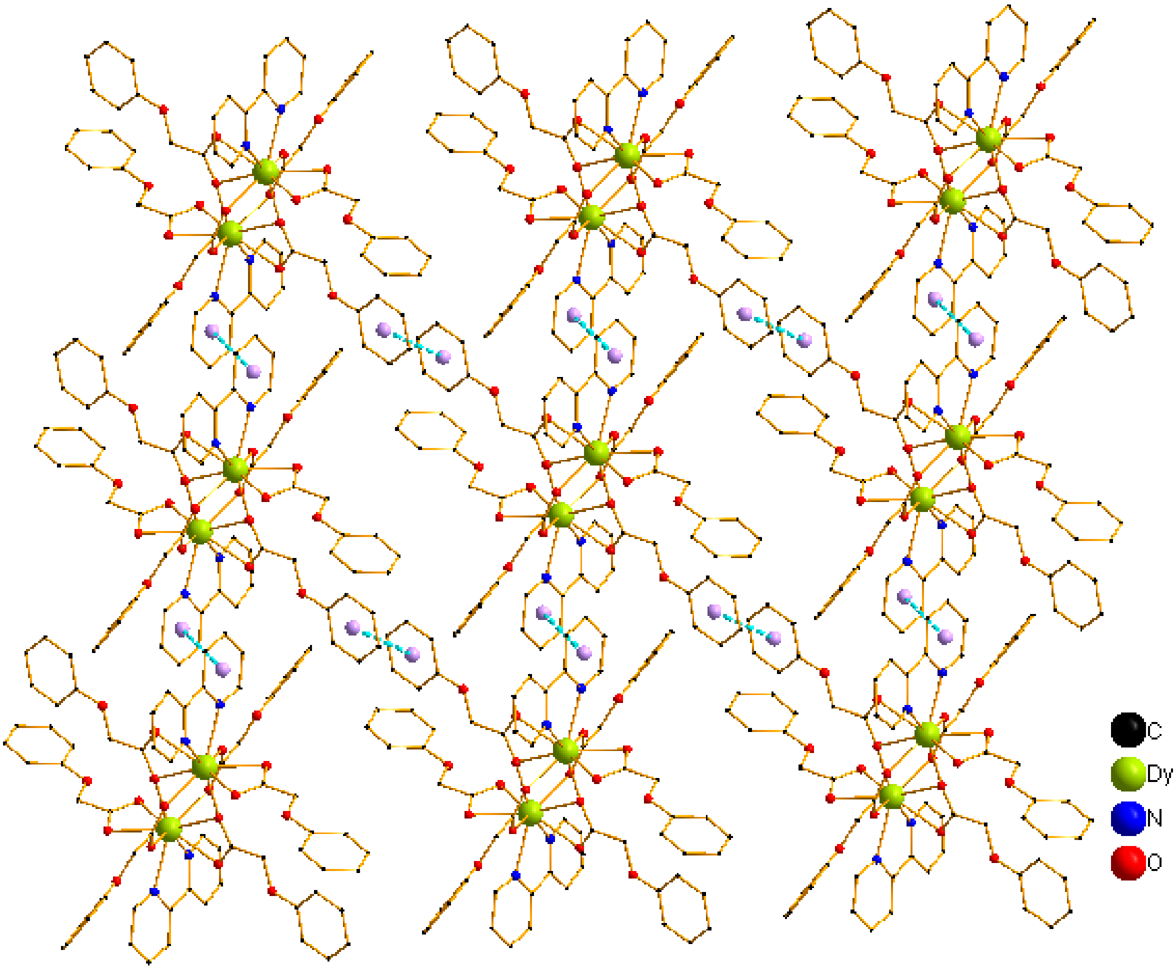


Figure S1. Perspective view of two dimensional sheet caused by intermolecular π···π stacking interactions in crystallographic *bc* plane for complex **1**. Hydrogen atoms are omitted for clarity.

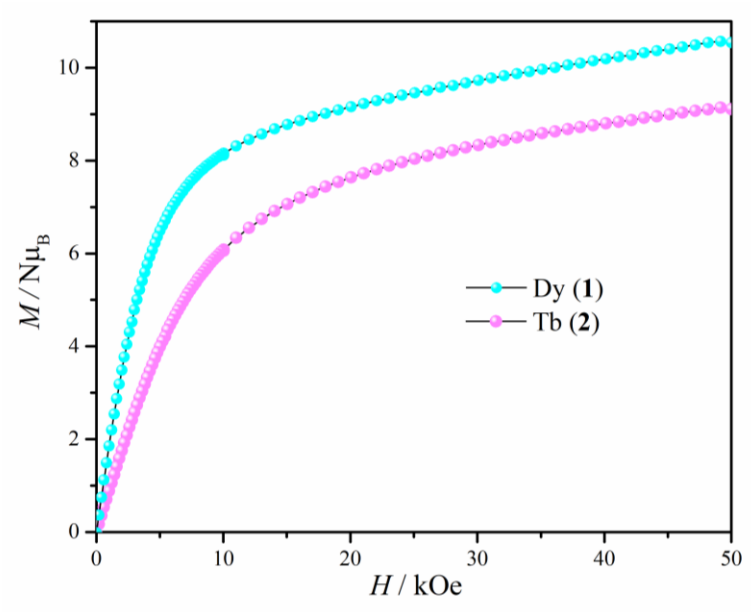


Figure S2. Magnetization (M) vs. Field (H) plots at 1.8 K.

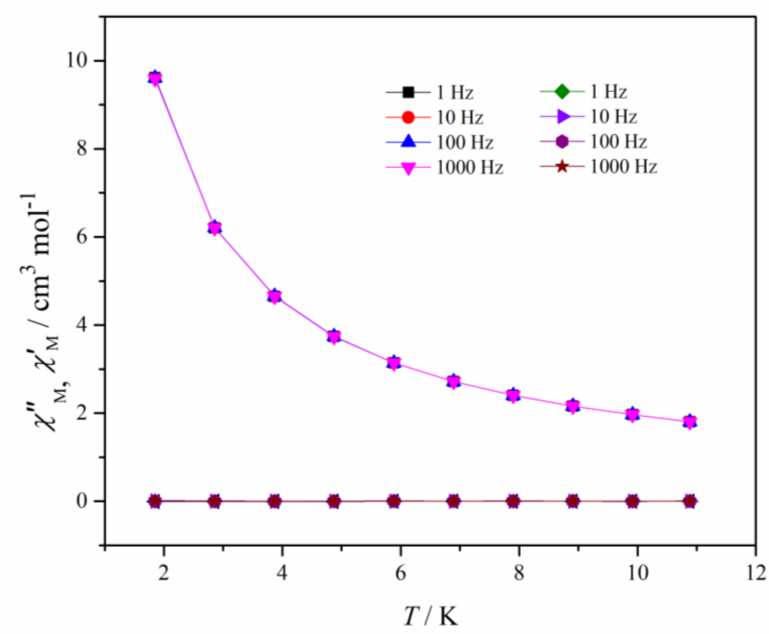
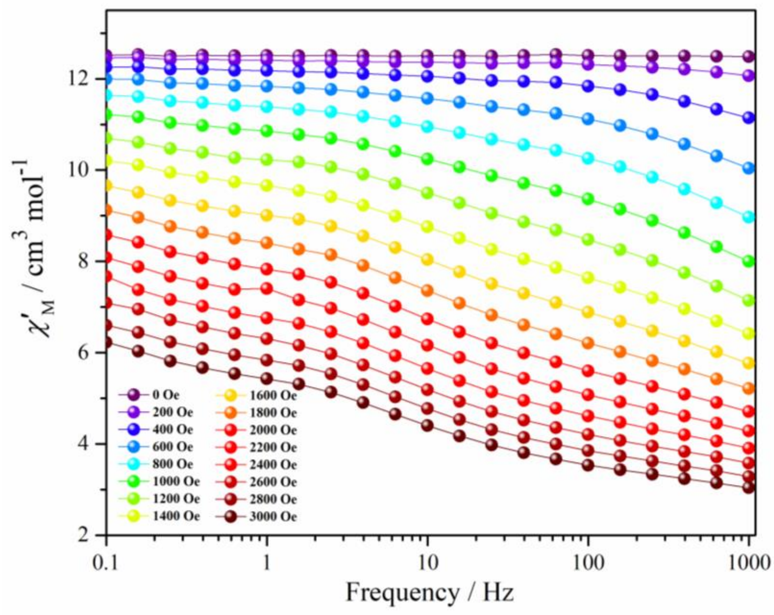
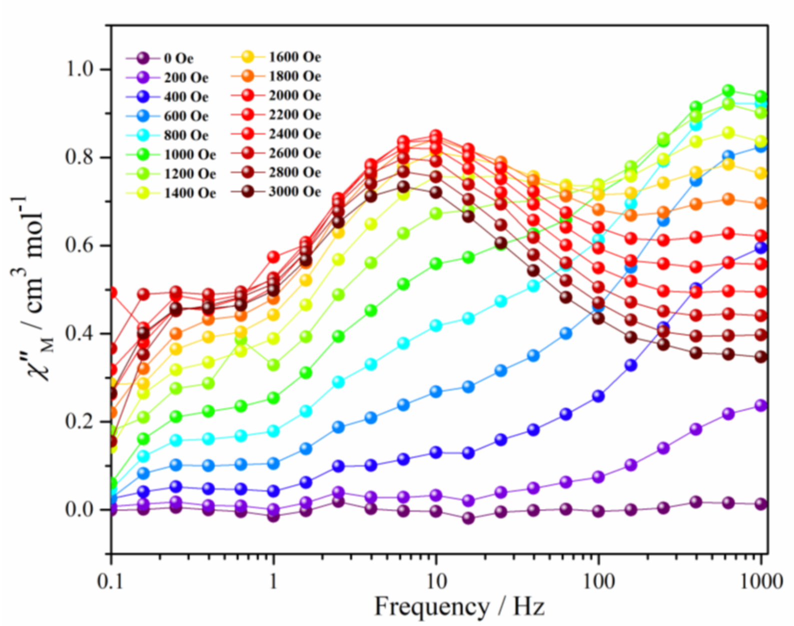


Figure S3. Frequency and temperature dependency without dc field for complex **1**.



(a)



(b)

Figure S4. Frequency dependency of the (a) in phase and (b) out of phase ac susceptibility under indicated dc fields at 1.85 K for **1**.

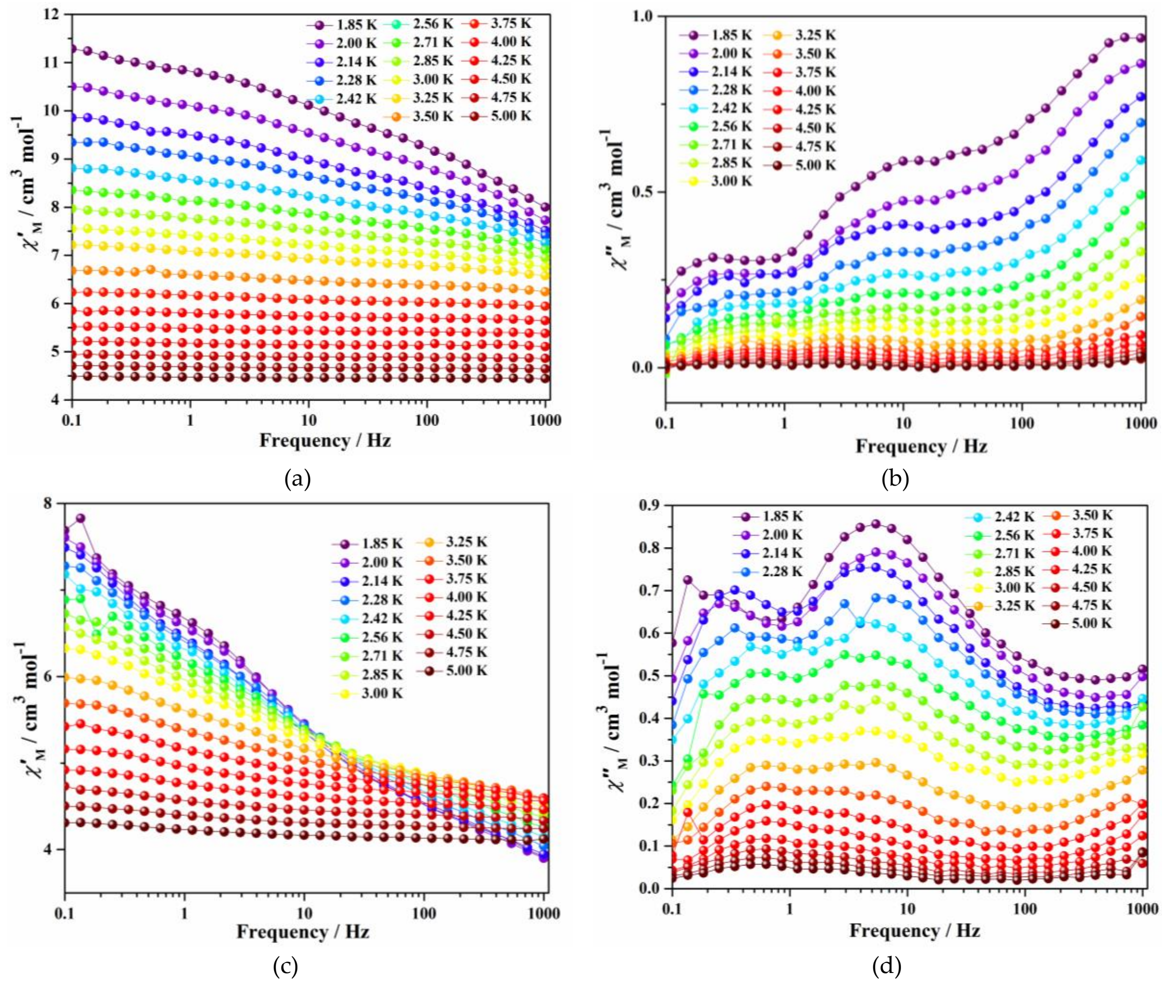


Figure S5. Frequency dependence of the (a) in phase and (b) out of phase components of the ac magnetic susceptibility for **1** under 1000 Oe dc field and frequency dependence of the (c) in phase and (d) out of phase components of the ac magnetic susceptibility for **1** under 2400 Oe dc field.

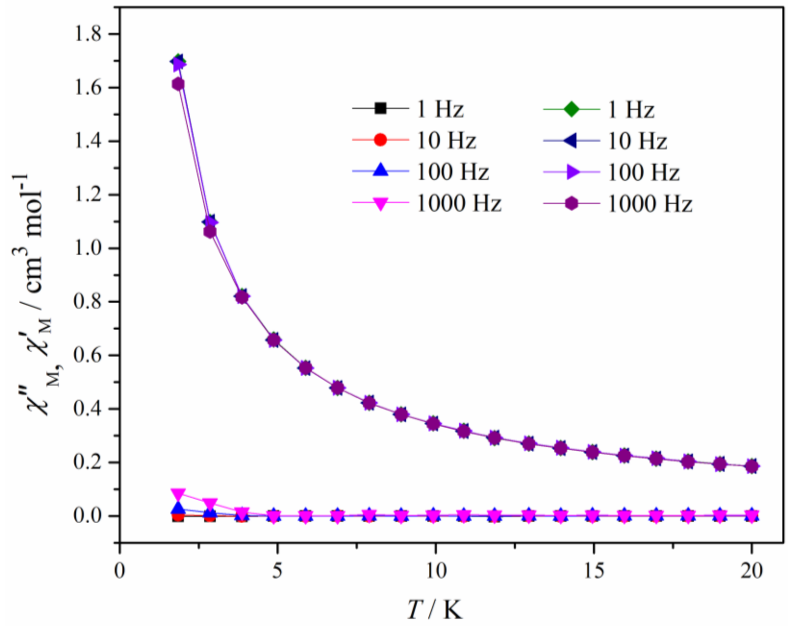
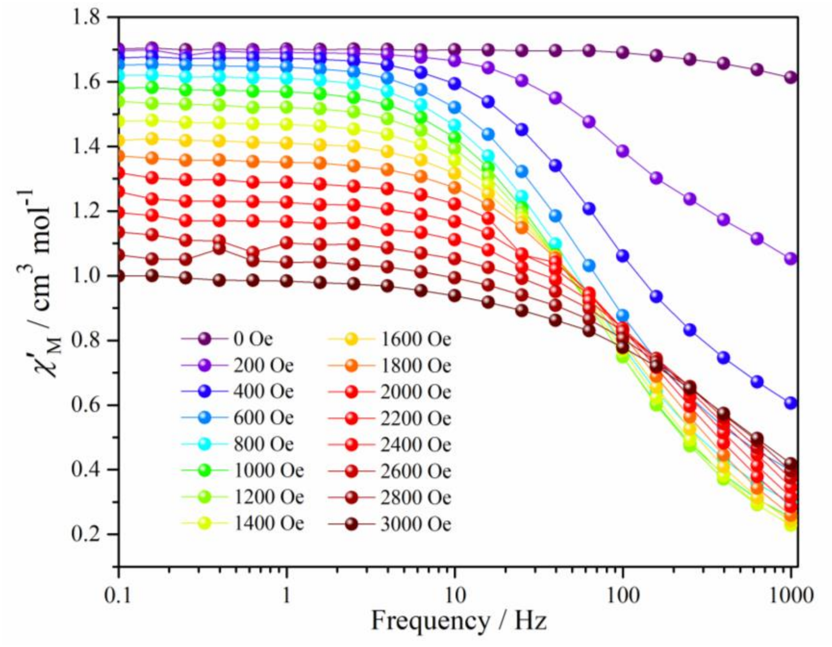
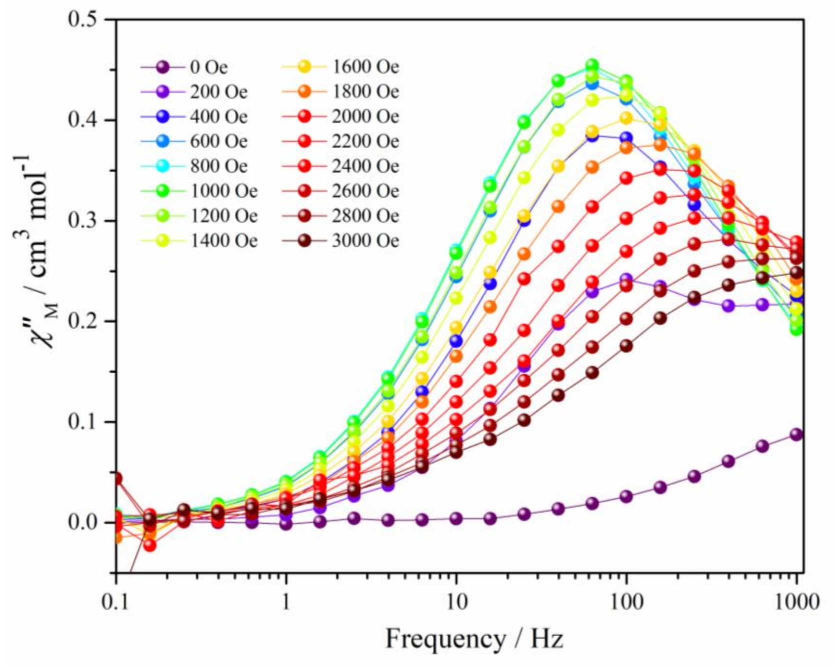


Figure S6. Frequency and temperature dependency without dc field for complex **1'**.



(a)



(b)

Figure S7. Frequency dependency of the (a) in phase and (b) out of phase ac susceptibility under indicated dc fields at 1.85 K for **1'**.

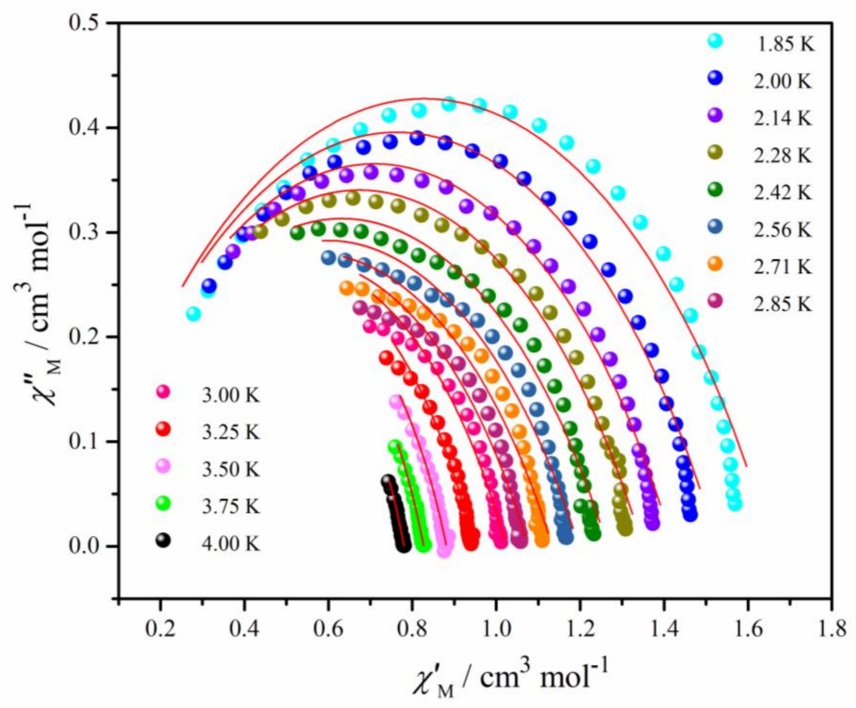
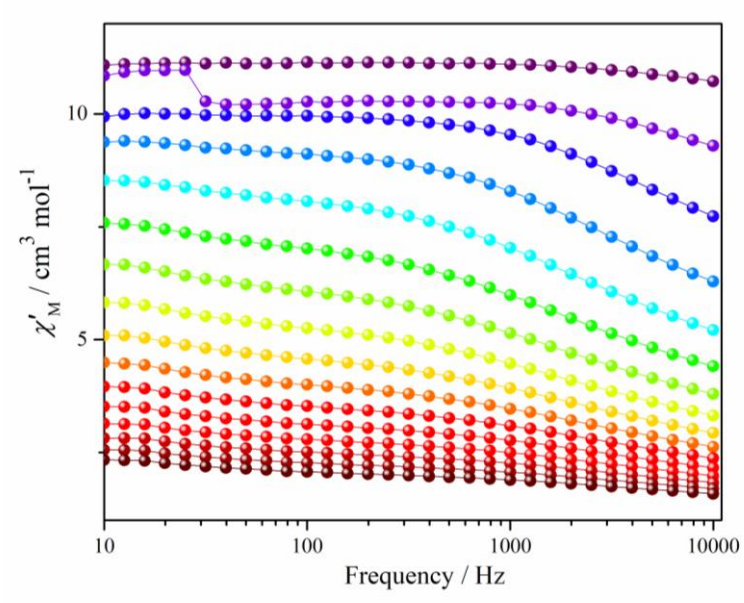
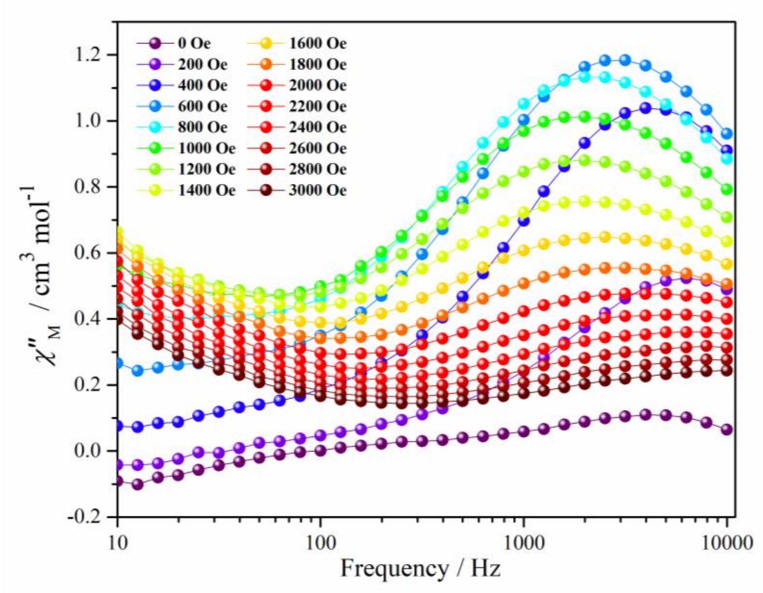


Figure S8. Cole-Cole plots for **1'** at different temperatures.

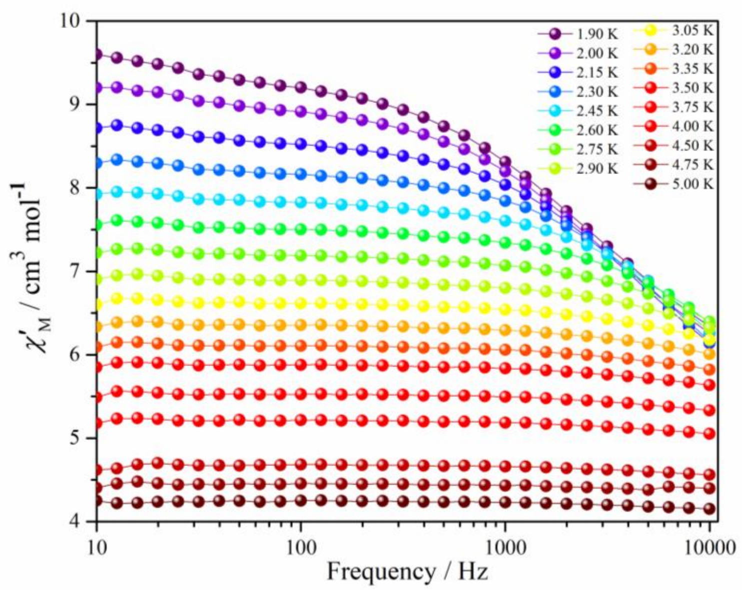


(a)

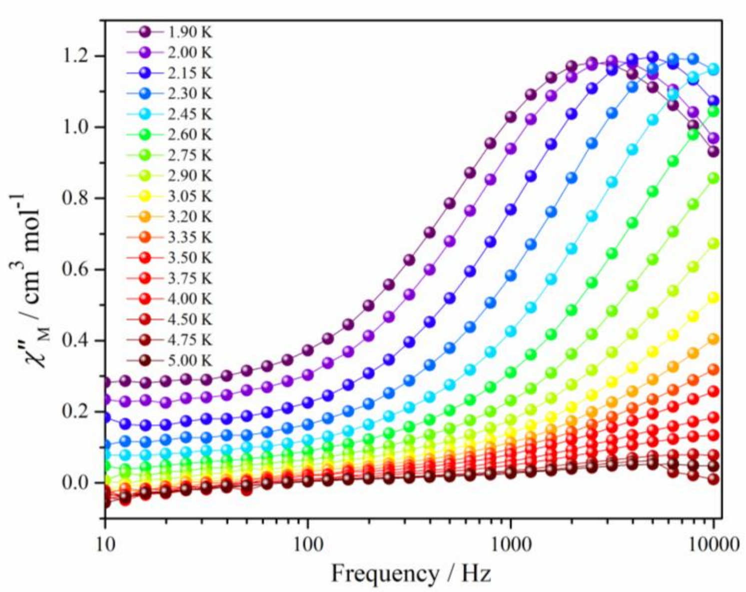


(b)

Figure S9. Frequency dependency of the (a) in phase and (b) out of phase ac susceptibility under indicated dc fields at 1.9 K (the indication for the fields for both plots are shown only in (b) for clarity) for **1** in the high frequency region.



(a)



(b)

Figure S10. Frequency dependency of the (a) in-phase and (b) out-of-phase components of the ac magnetic susceptibility under 600 Oe dc field for **1** in the high frequency region.

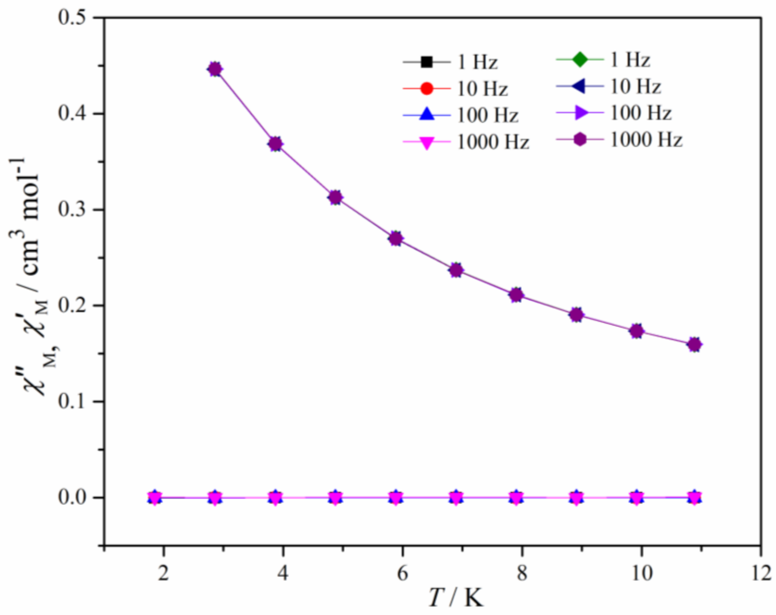
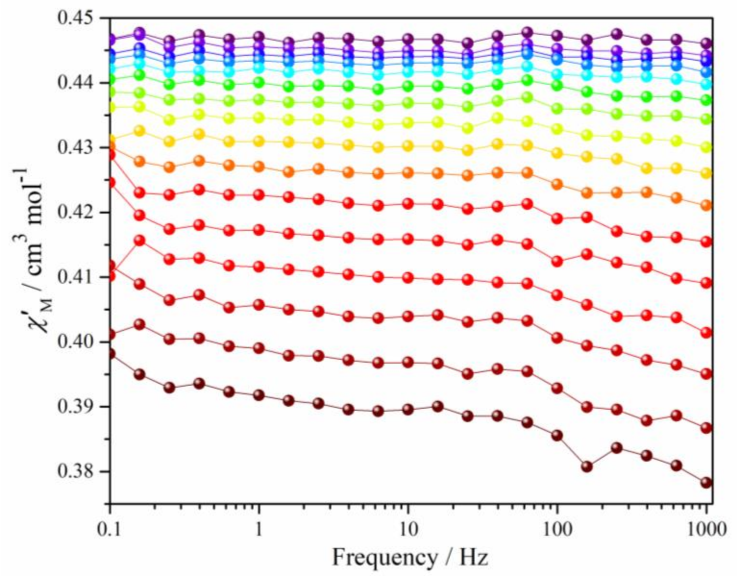
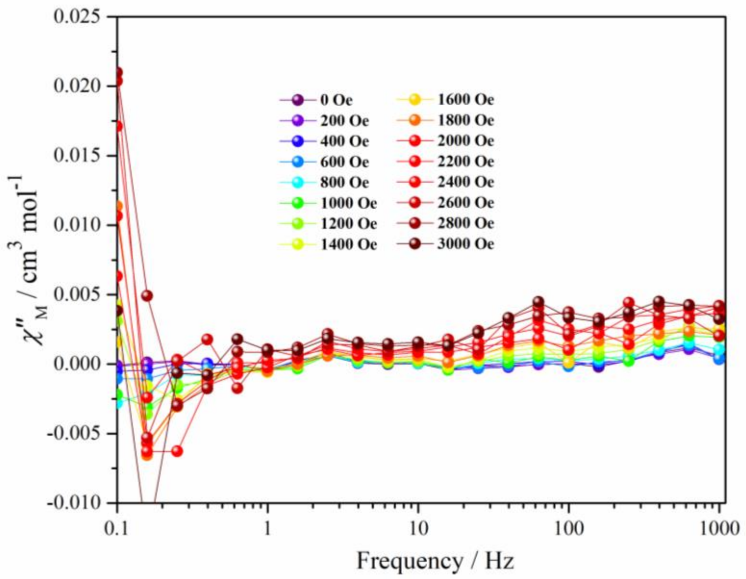


Figure S11. Frequency and temperature dependency without dc field for complex **2**.



(a)



(b)

Figure S12. Frequency dependency of the (a) in phase and (b) out of phase ac susceptibility under indicated dc fields at 1.85 K for **2** (the indication for the fields for both plots are shown only in (b) for clarity).

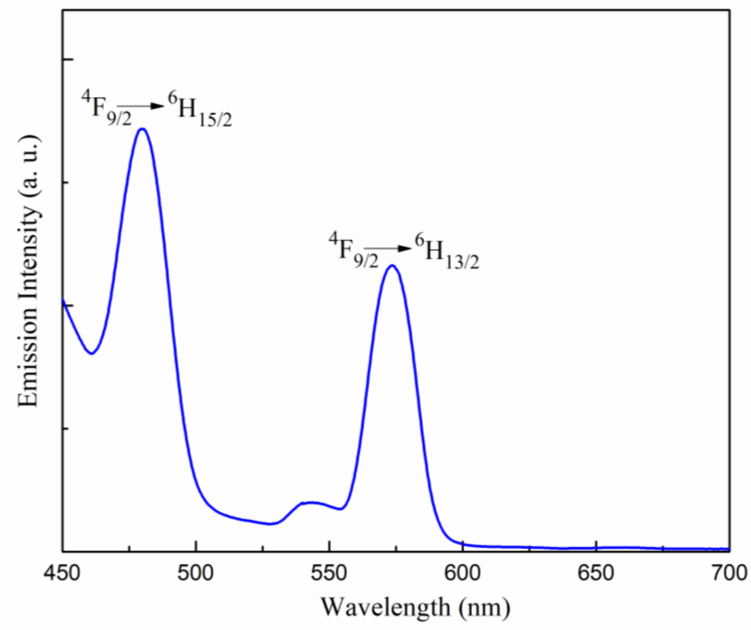


Figure S13. Emission spectrum of complex **1** in acetonitrile at room temperature.

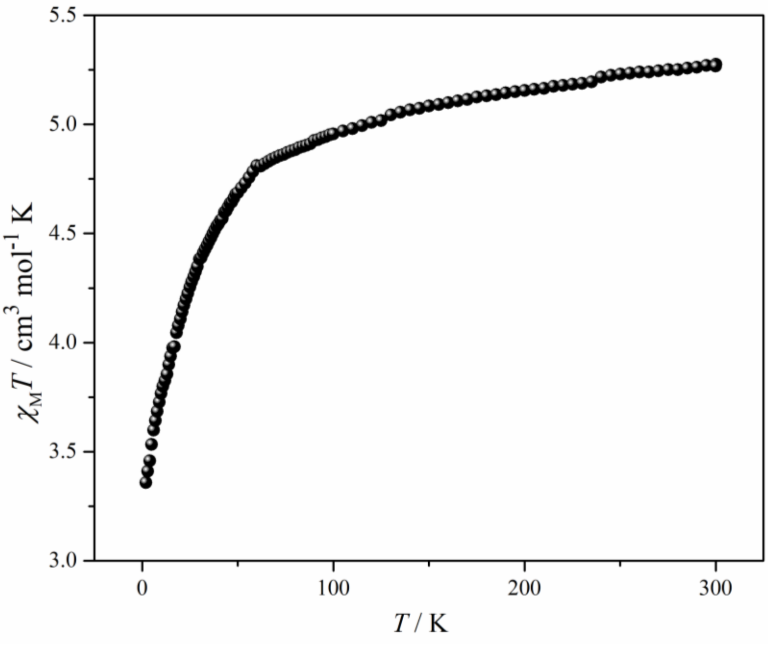


Figure S14. Temperature dependence of the $\chi_M T$ products in 1000 Oe for **1'**.