Electronic Supplementary Information for

The influence of light on the field-induced magnetization dynamics of two Er(III) coordination polymers with different halogen substituents

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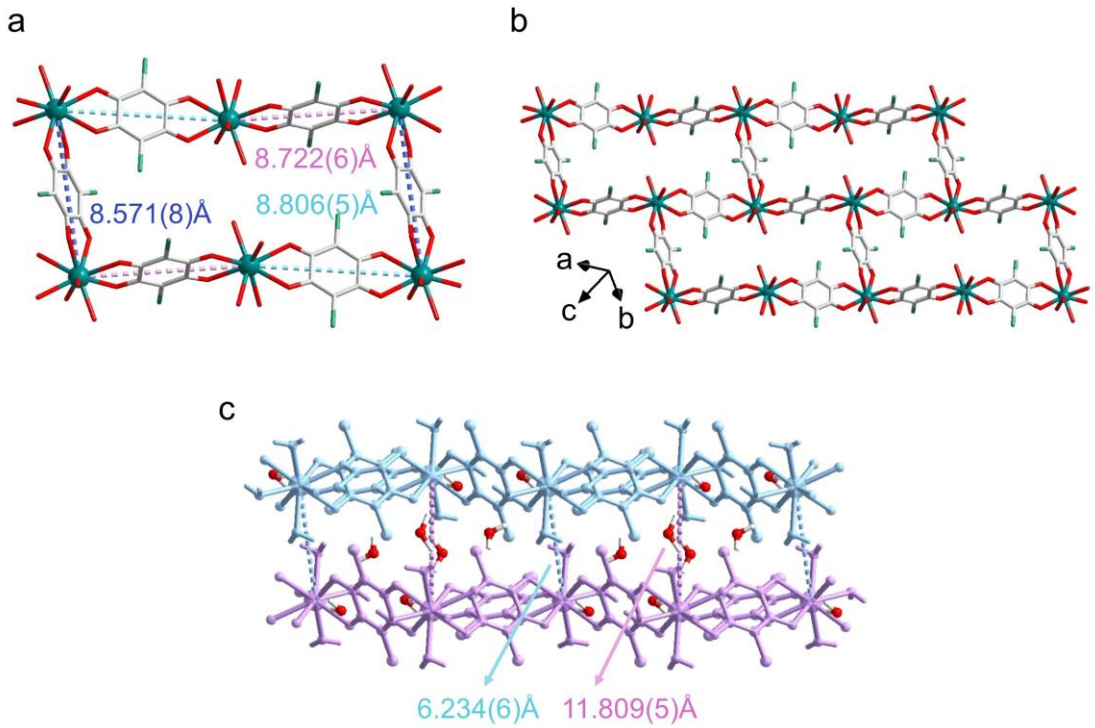


Fig. S1 (a) View of one six-membered ring in **1**. (b) Top view of 2D hexagonal layer in **1**. (c) Side view of the layers in **1**. The closest Er(III) sites in neighboring layers is 6. 234(6) Å in **1**. Cyan, red, green and grey spheres represent Er, O, Cl and C atoms, respectively.

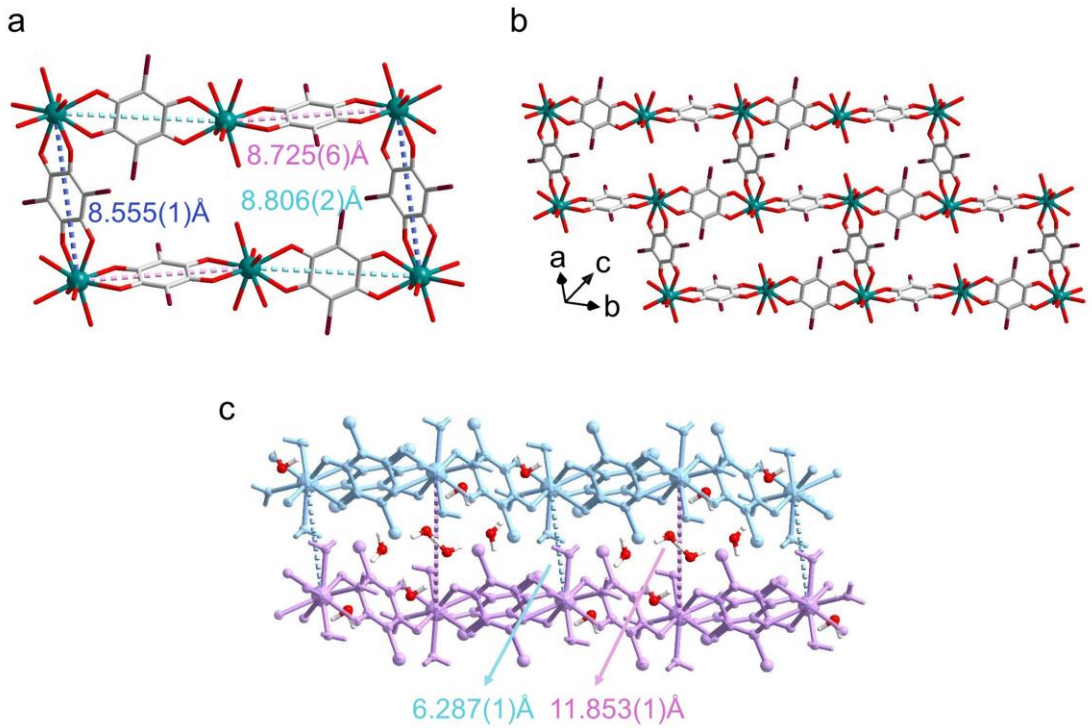


Fig. S2 View of one six-membered ring in **2**. (b) Top view of 2D hexagonal layer in **2**. (c) Side view of the layers in **2**. The closest Er(III) sites in neighboring layers is 6. 287(1) Å in **2**. Cyan, red, wine and grey spheres represent Er, O, Br and C atoms, respectively.

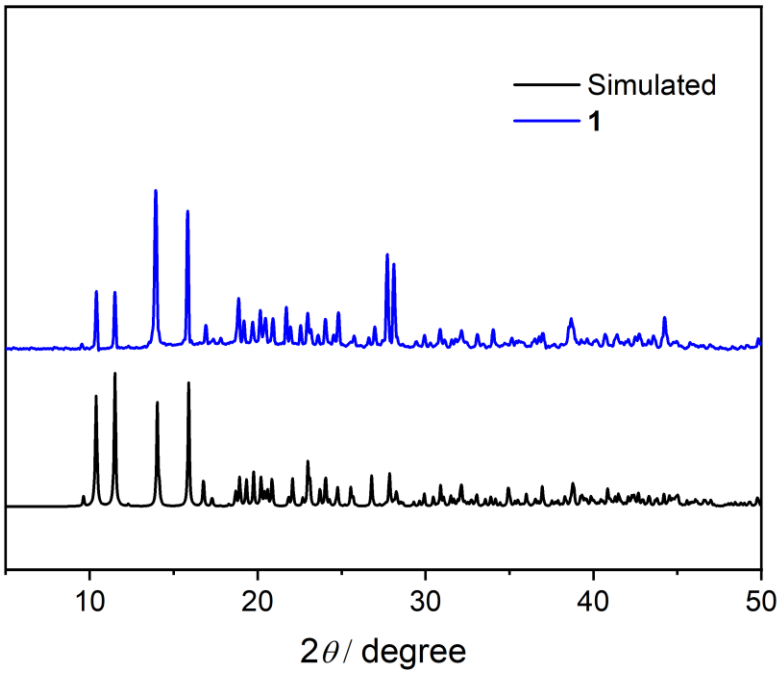
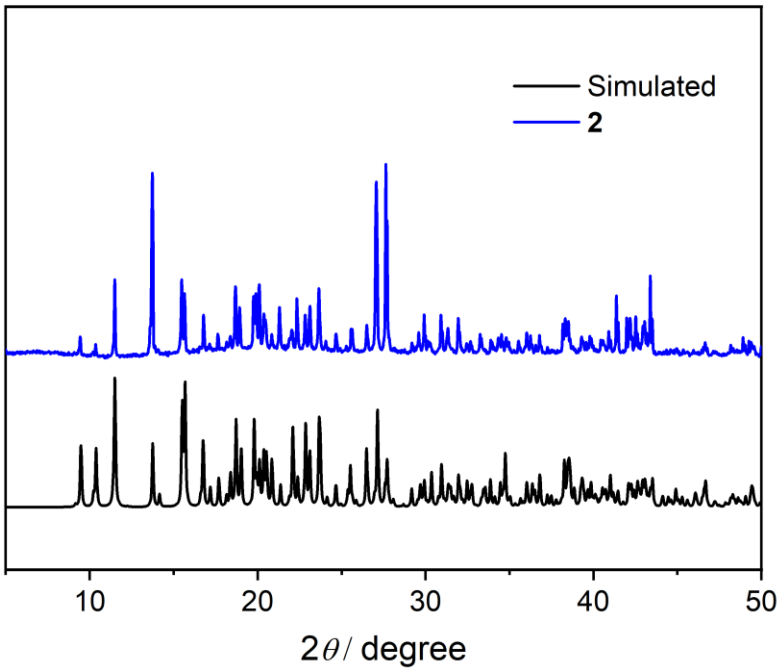


Fig. S3 Experimental and simulated PXRD patterns for **1**.



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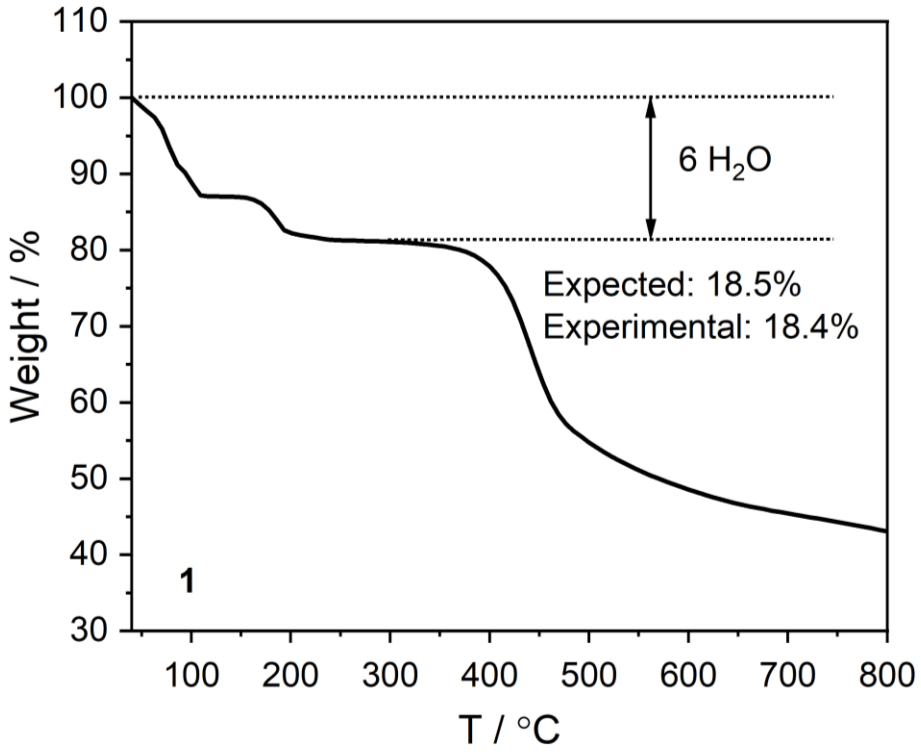


Fig. S5 Thermogravimetric analysis for **1** under N_2 atmosphere (heating rate = 5 °C/min).

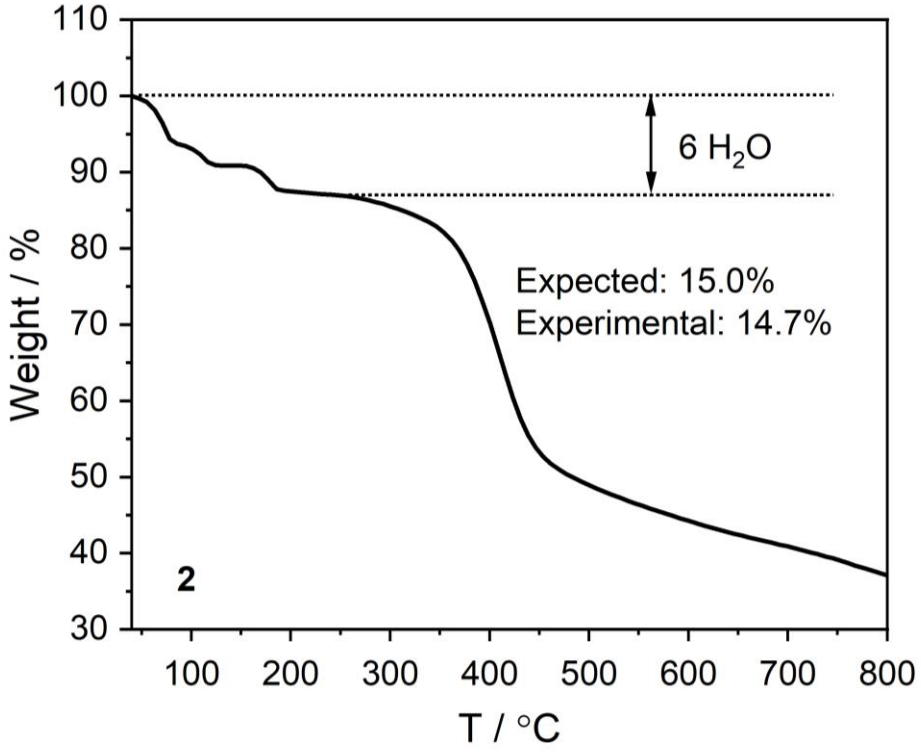
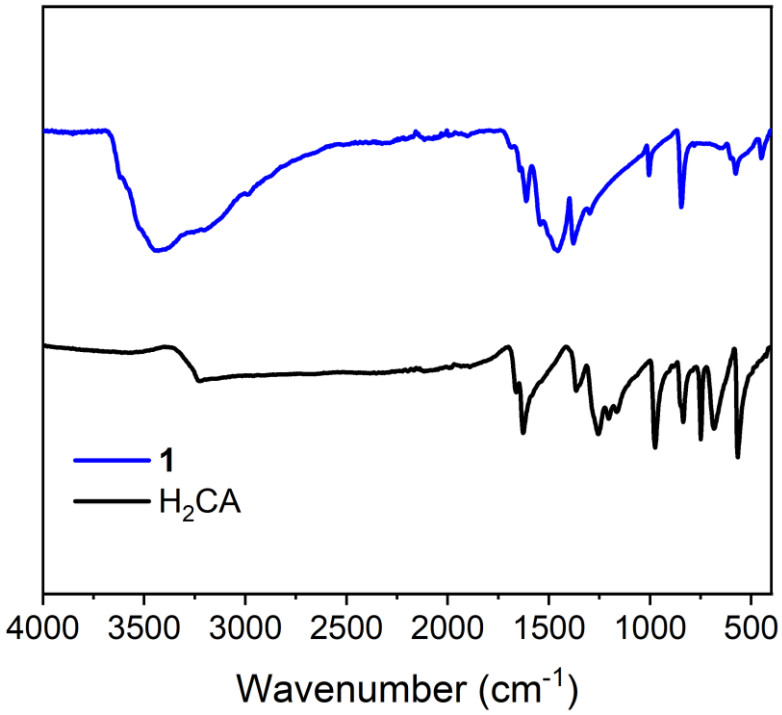


Fig. S6 Thermogravimetric analysis for **2** under N_2 atmosphere (heating rate = 5 °C/min).



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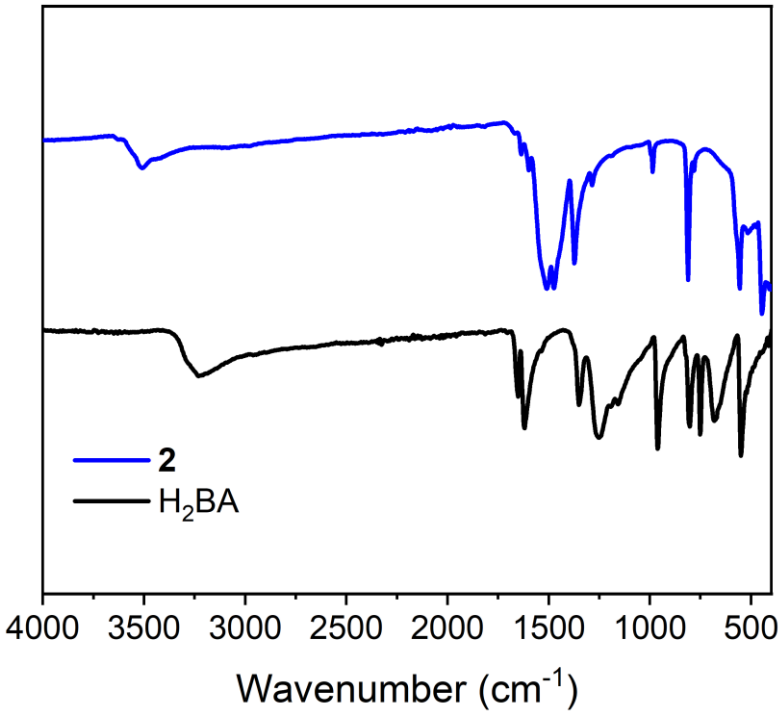

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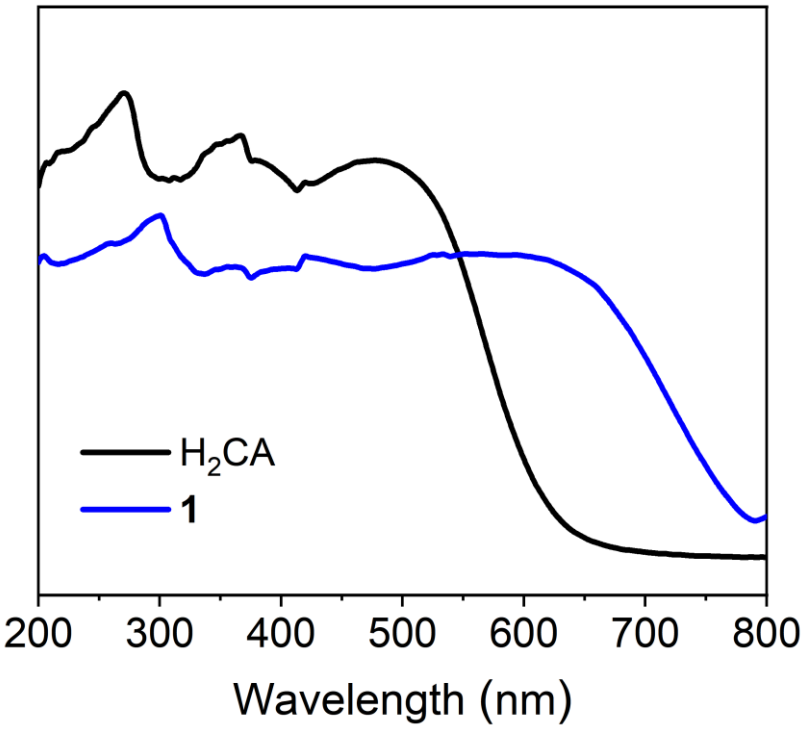

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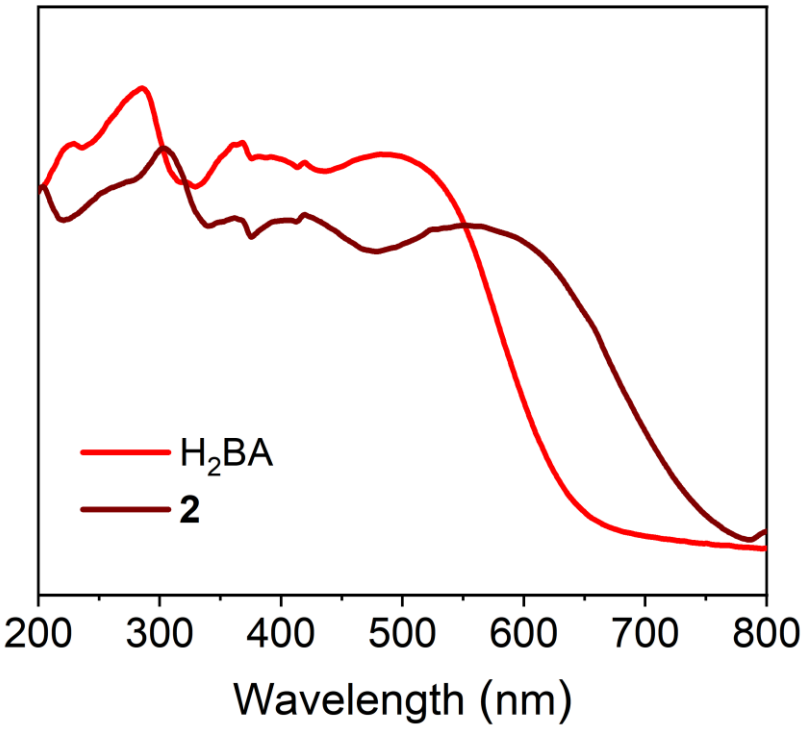

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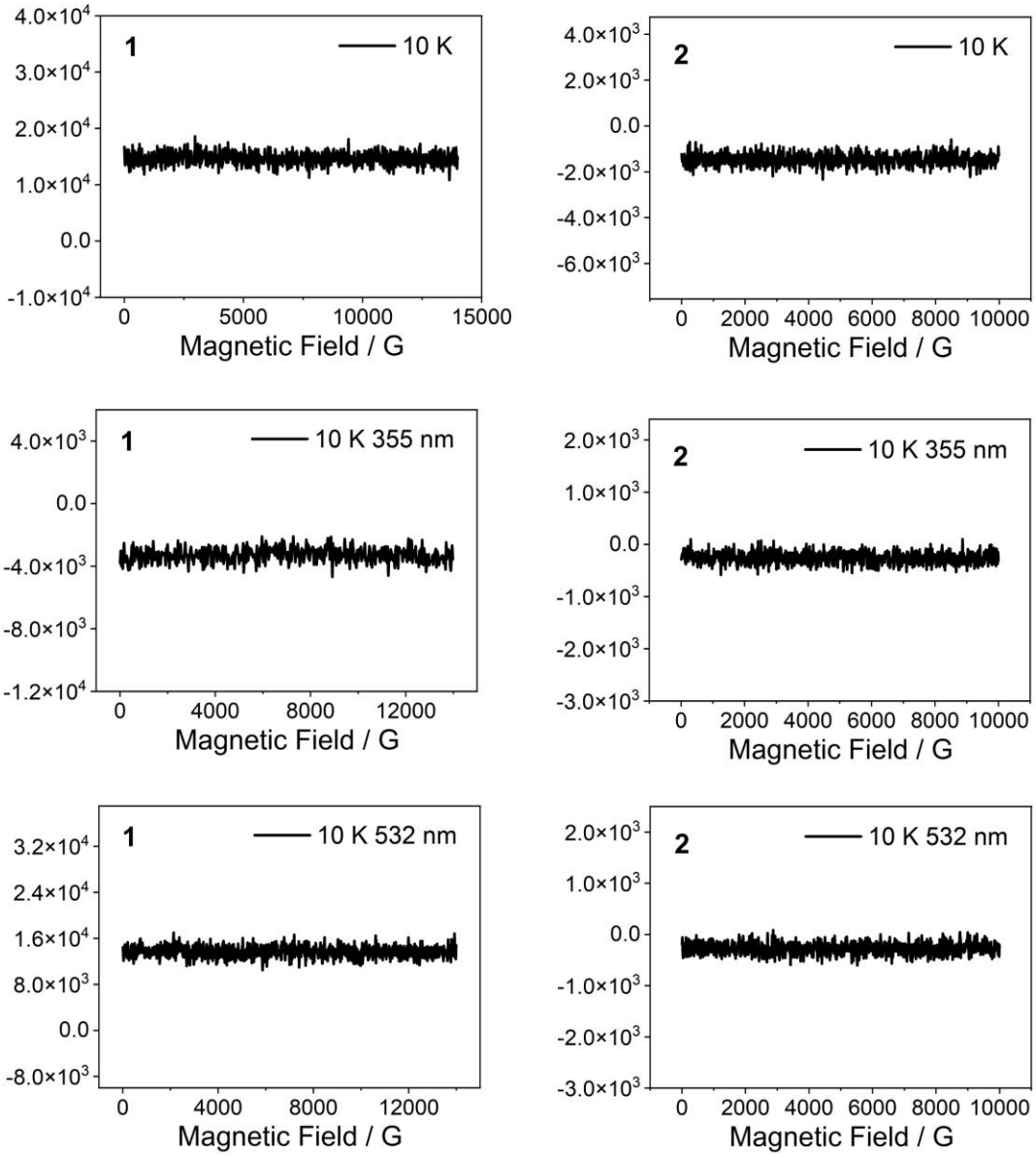

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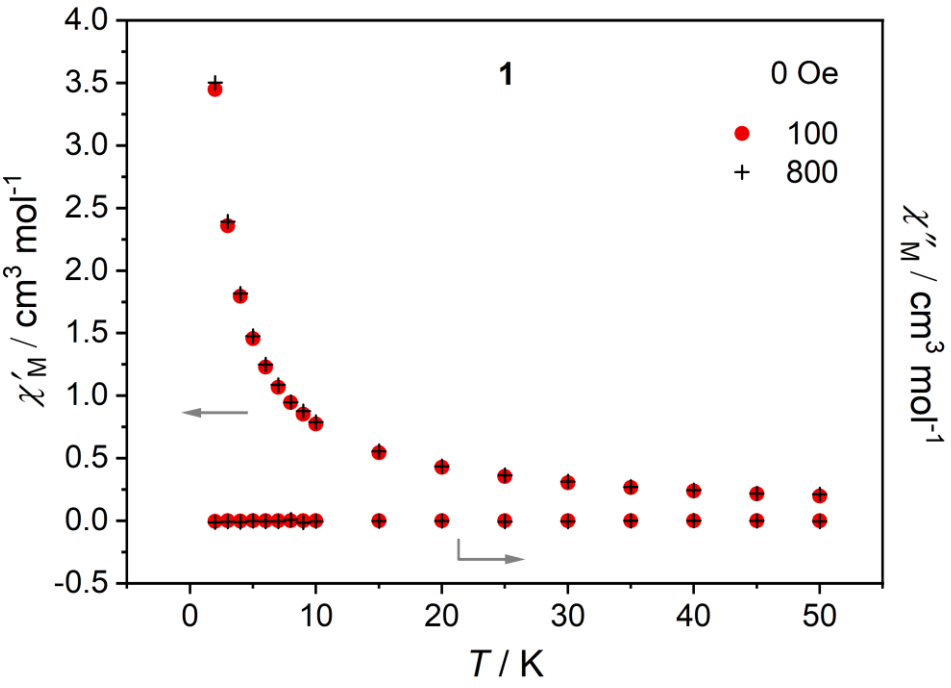


Fig. S12 Temperature dependence of the χ' and χ'' for **1** at zero dc field in the temperature range of 2–50 K, ν = 100, 800 Hz.

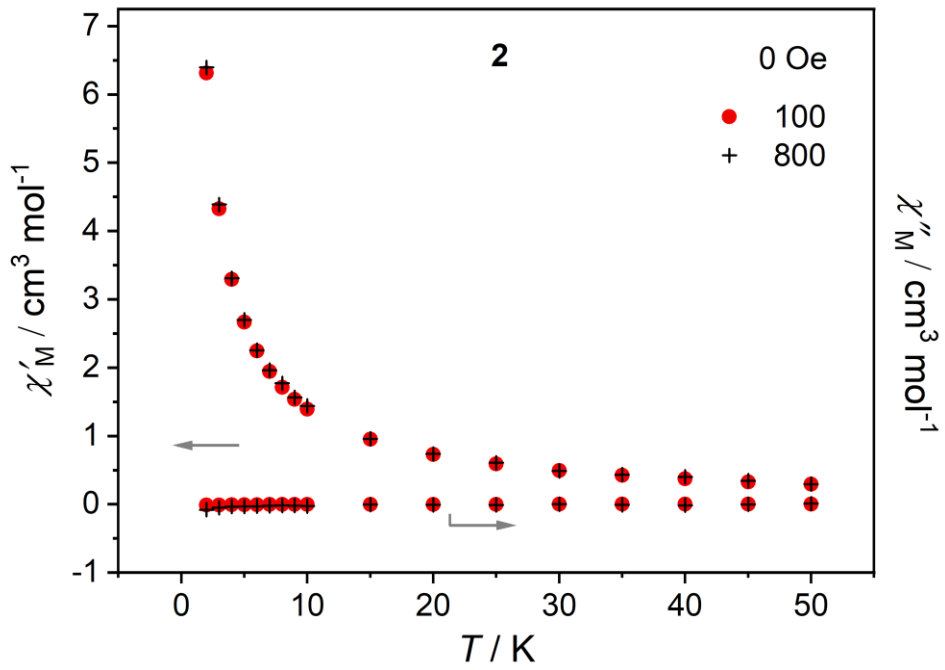
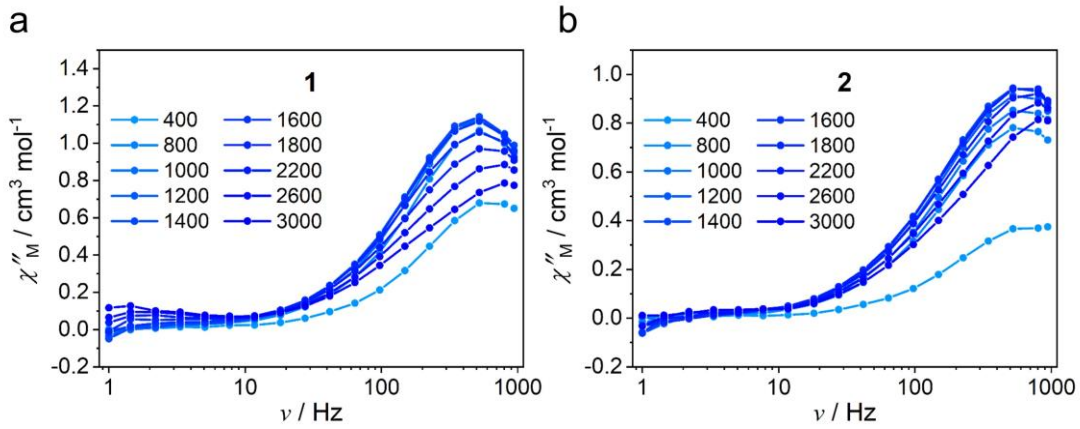


Fig. S13 Temperature dependence of the χ' and χ'' for **2** at zero dc field in the temperature range of 2–50 K, ν = 100, 800 Hz.



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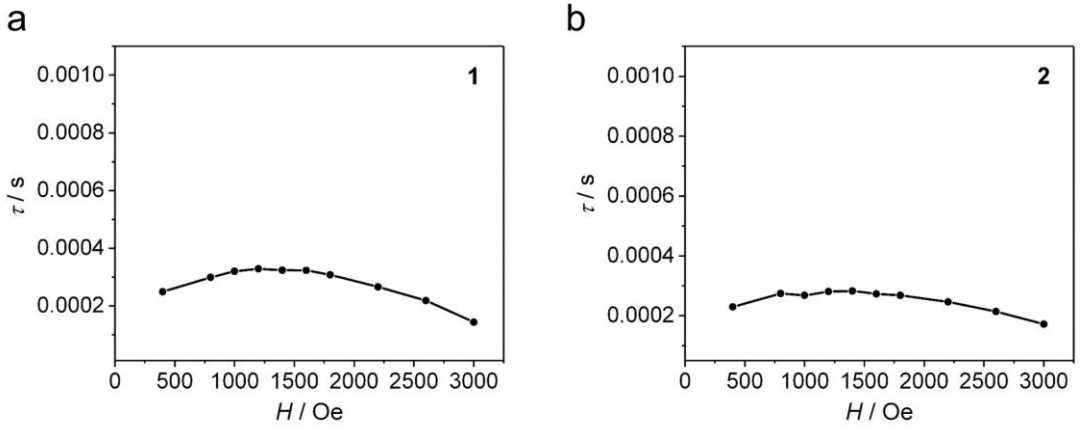

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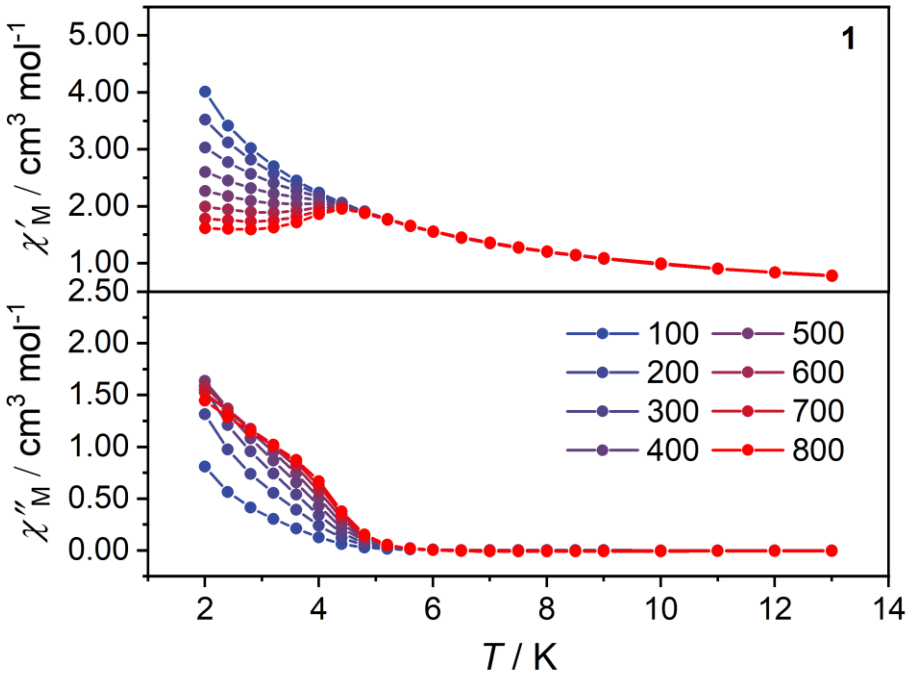
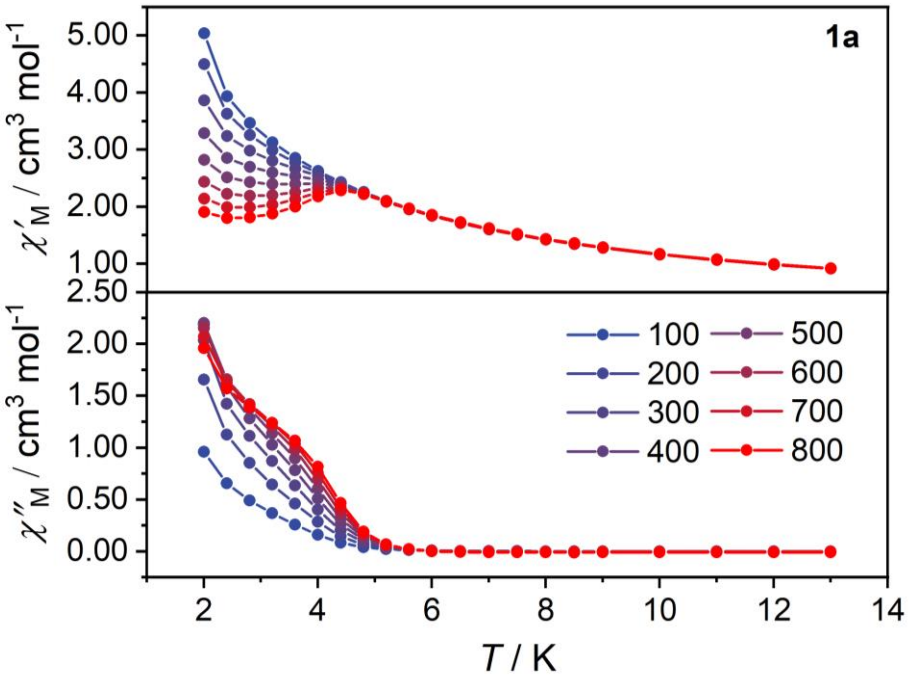


Fig. S16 Temperature dependence of the in-phase χ' and out-of-phase χ'' molar magnetic susceptibility for **1** at 1200 Oe dc field in the temperature range of 2–14 K, ν = 100–800 Hz.



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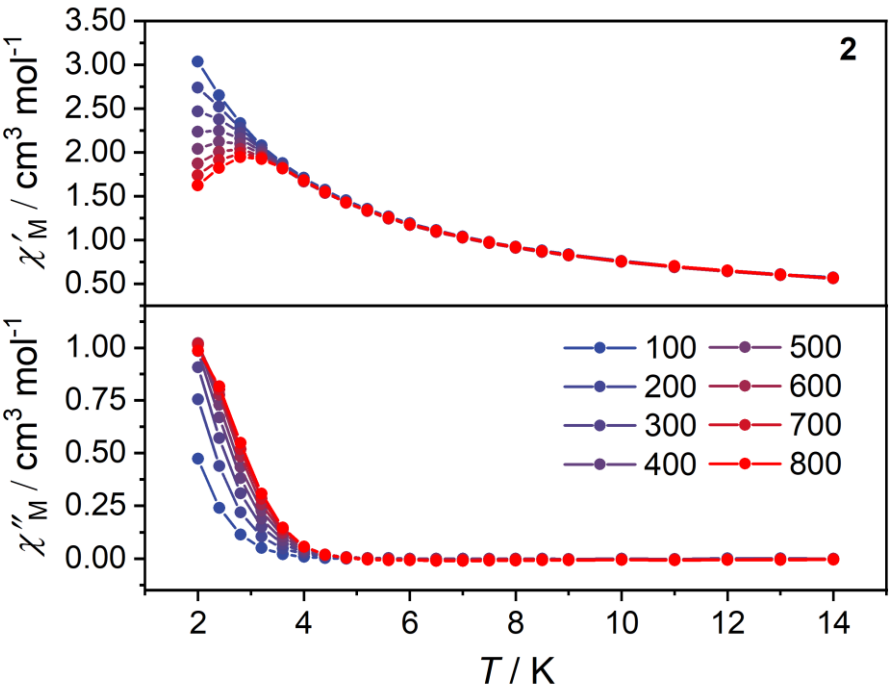

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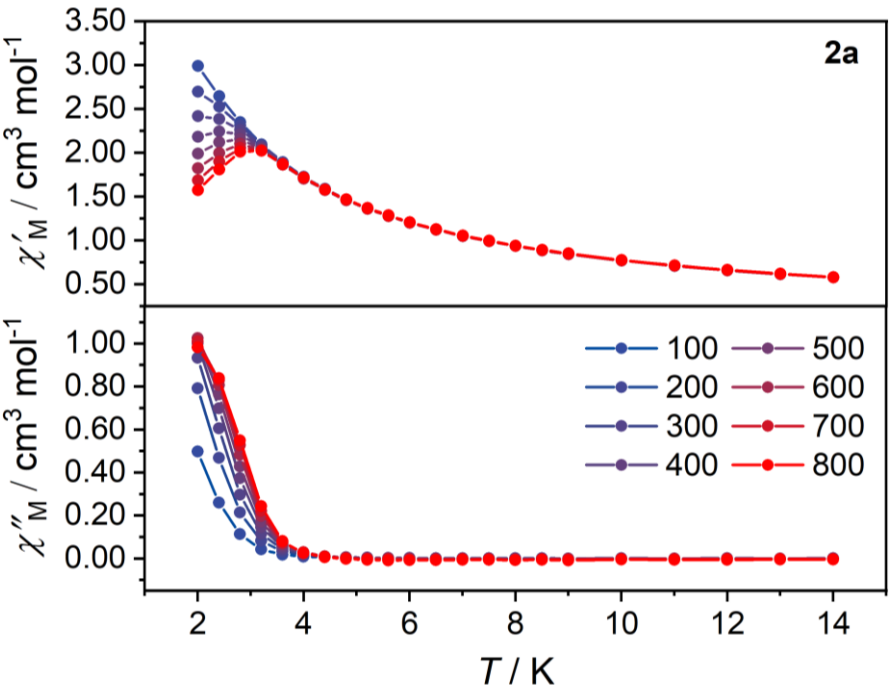

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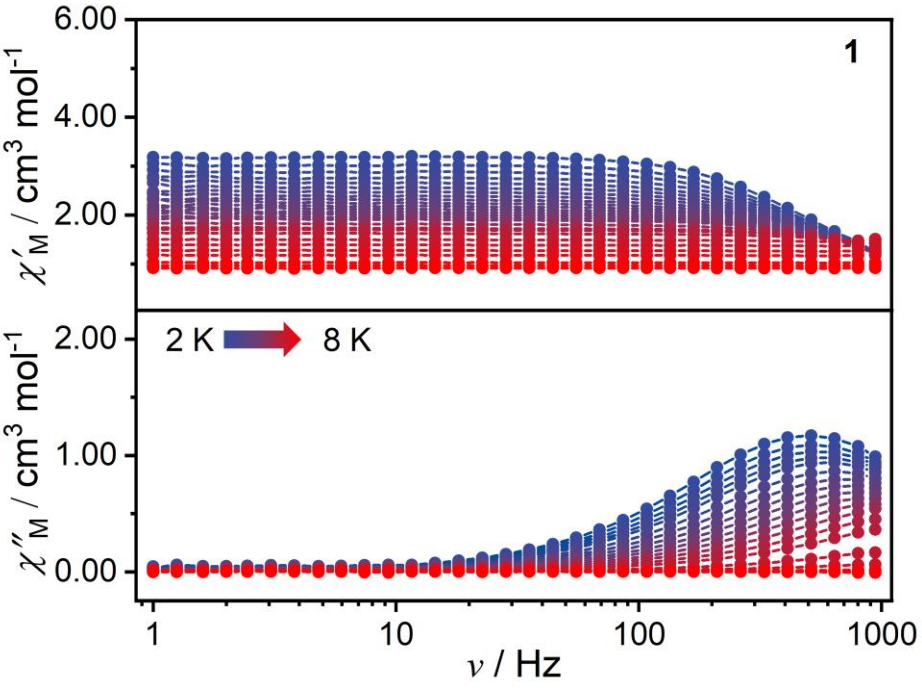
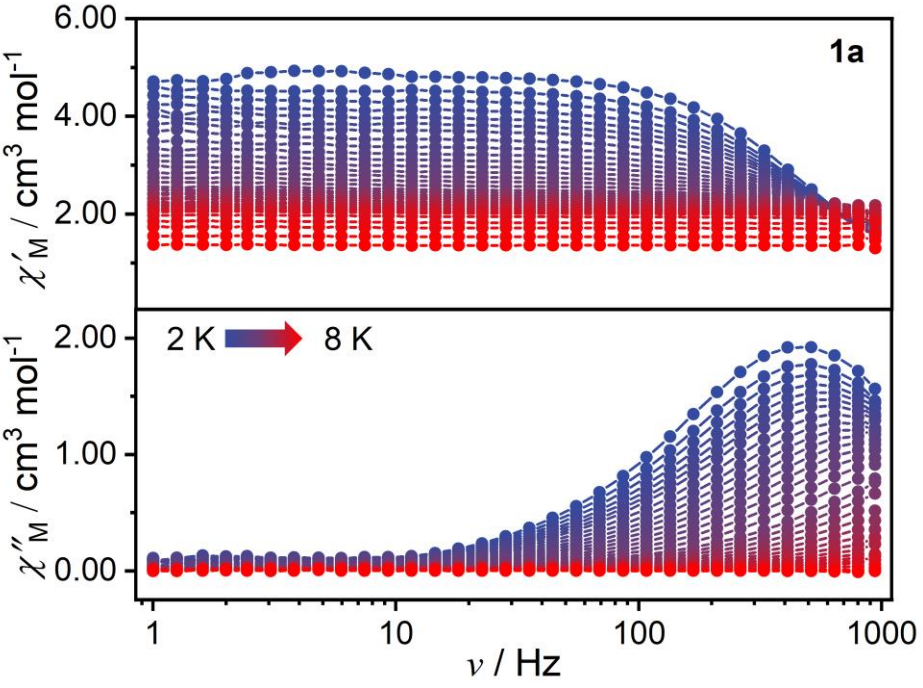


Fig. S20 Frequency dependence of the in-phase χ' and out-of-phase χ'' molar magnetic susceptibility for **1** at 1200 Oe dc field.



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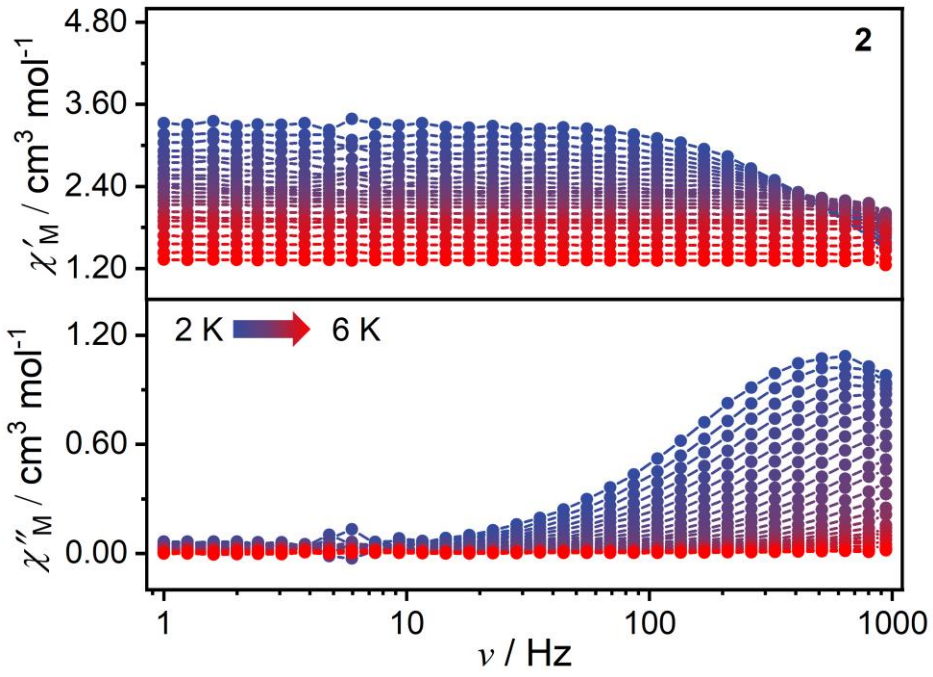

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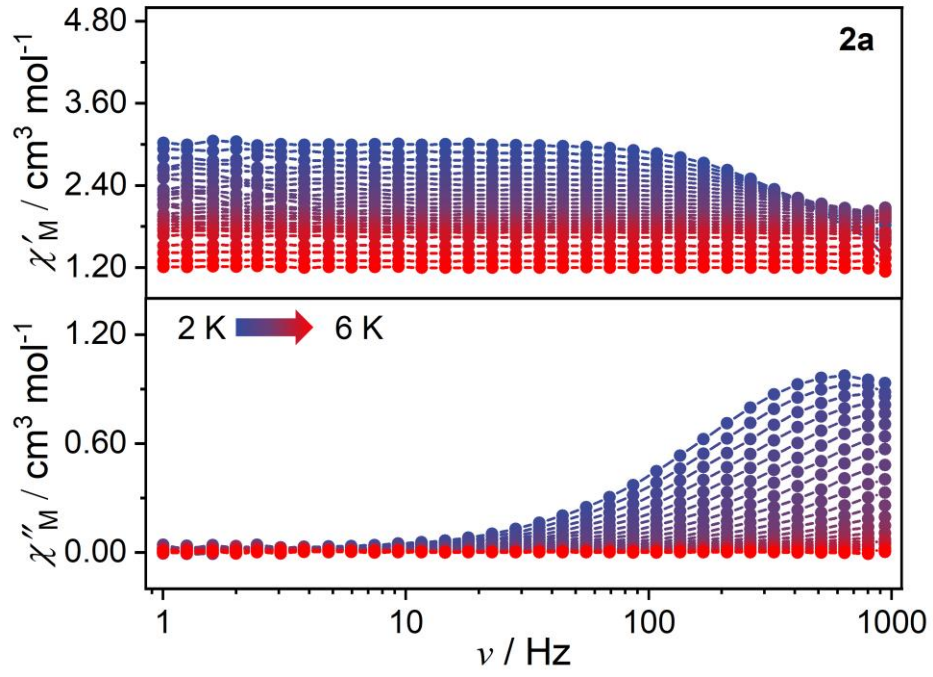

Fig. S23 Frequency dependence of the in-phase χ' and out-of-phase χ'' molar magnetic susceptibility for **2a**, collected in 1400 Oe dc field.

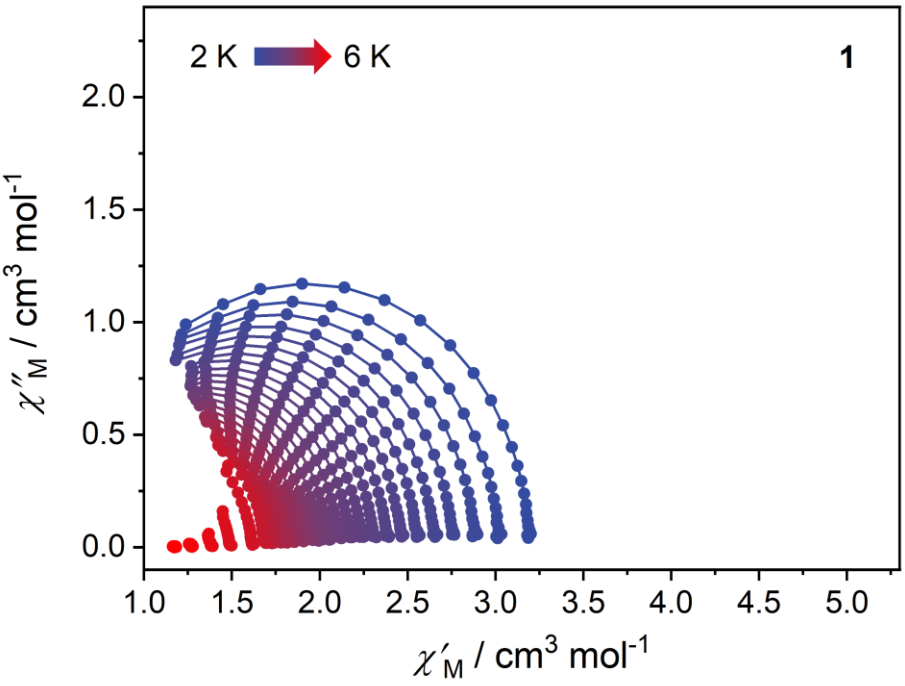

Fig. S24 Cole-Cole plots of **1**.

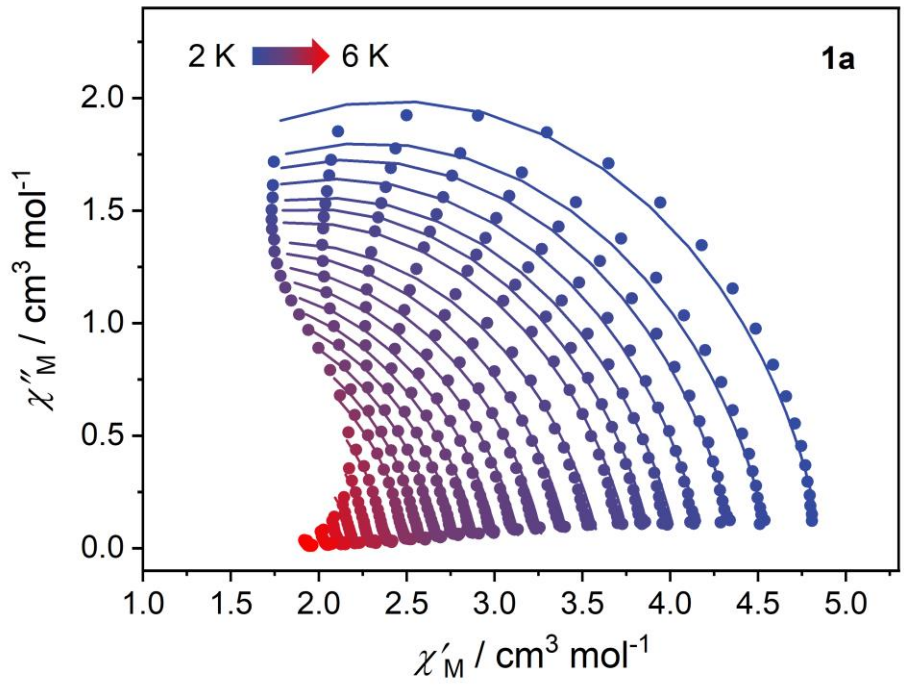

Fig. S25 Cole-Cole plots of **1a**.

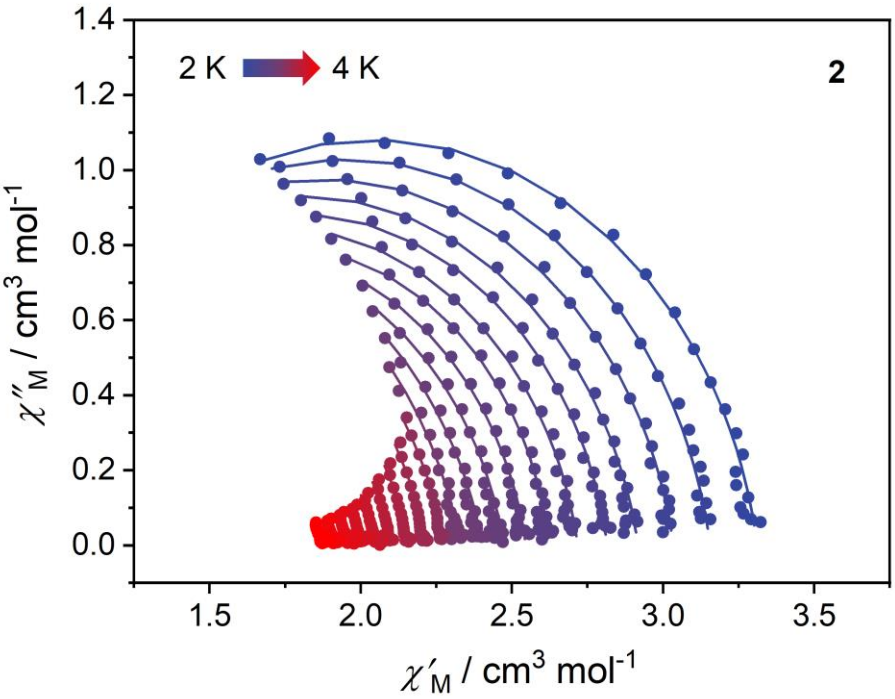

Fig. S26 Cole-Cole plots of **2**.

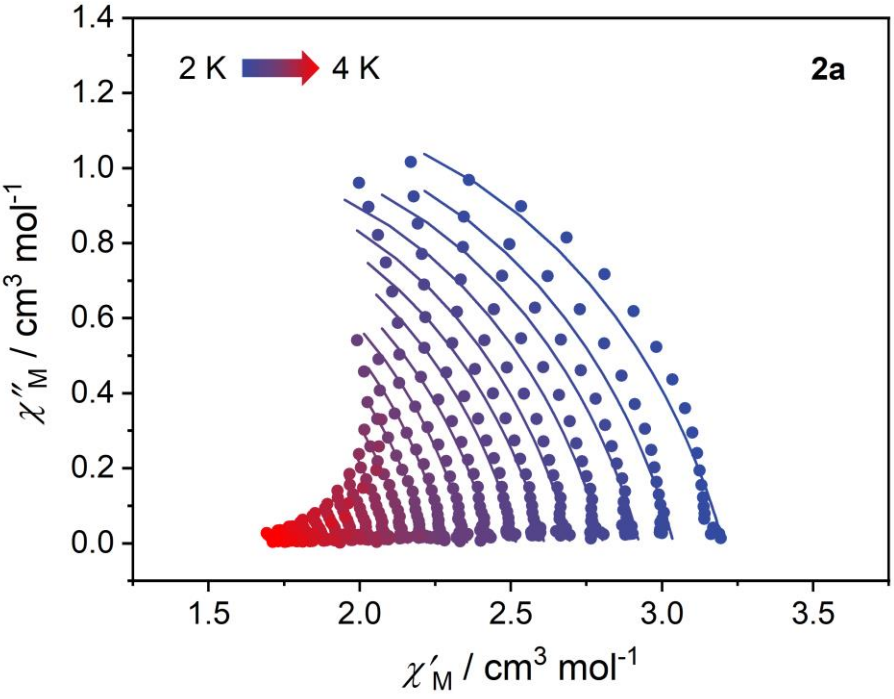

Fig. S27 Cole-cole plots of **2a**.

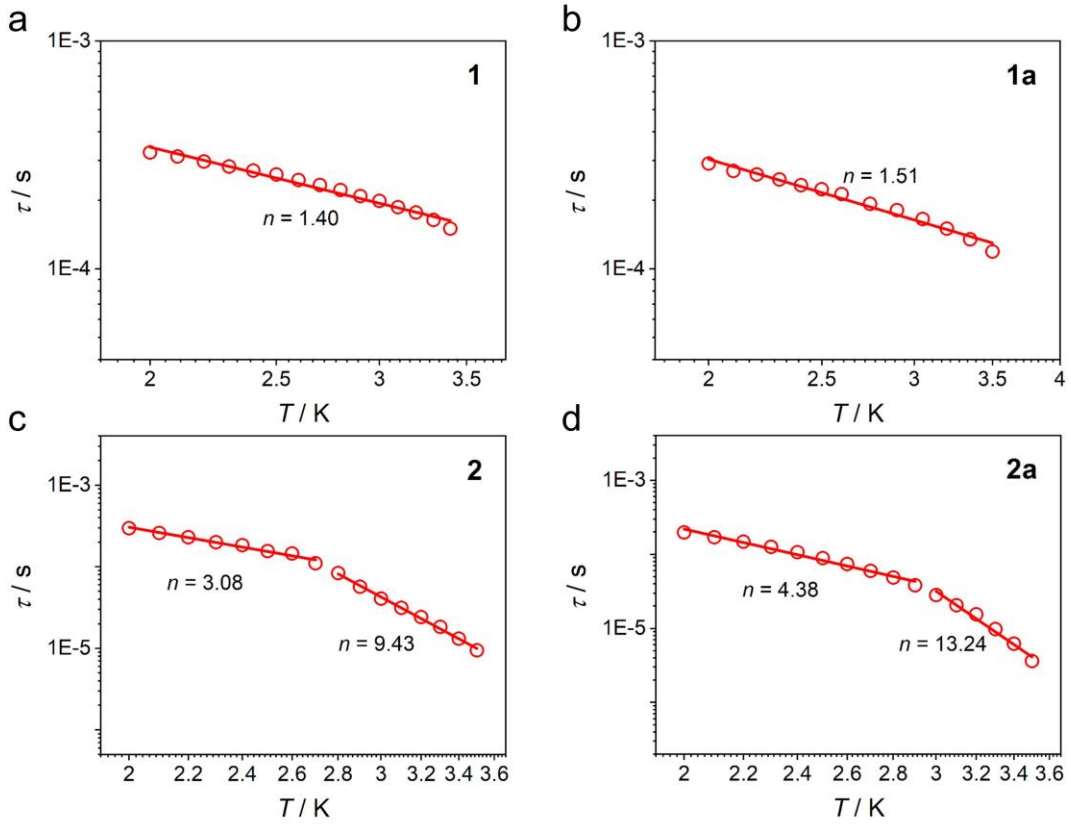

Fig. S28 The plots of the relaxation time τ vs T on a log−log scale for **1**, **1a**, **2** and **2a**.

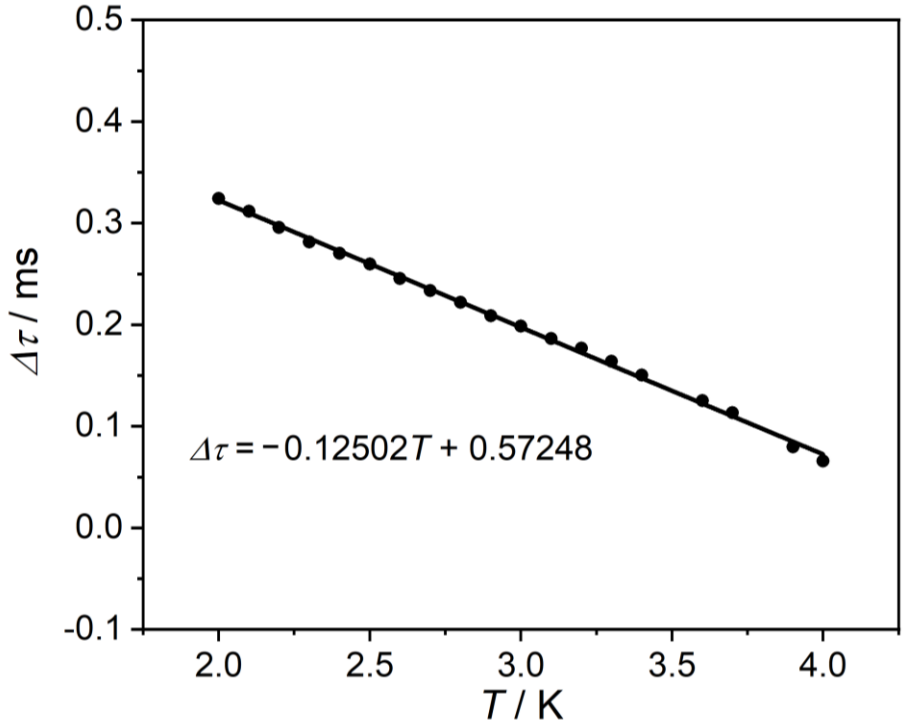

Fig. S29 The plot of the relaxation time difference ($\Delta\tau$) between **1** and **1a**. The straight solid line shows the linear fitting by $\Delta\tau$ = -0.12502T + 0.57248, R^2 = 0.9983.

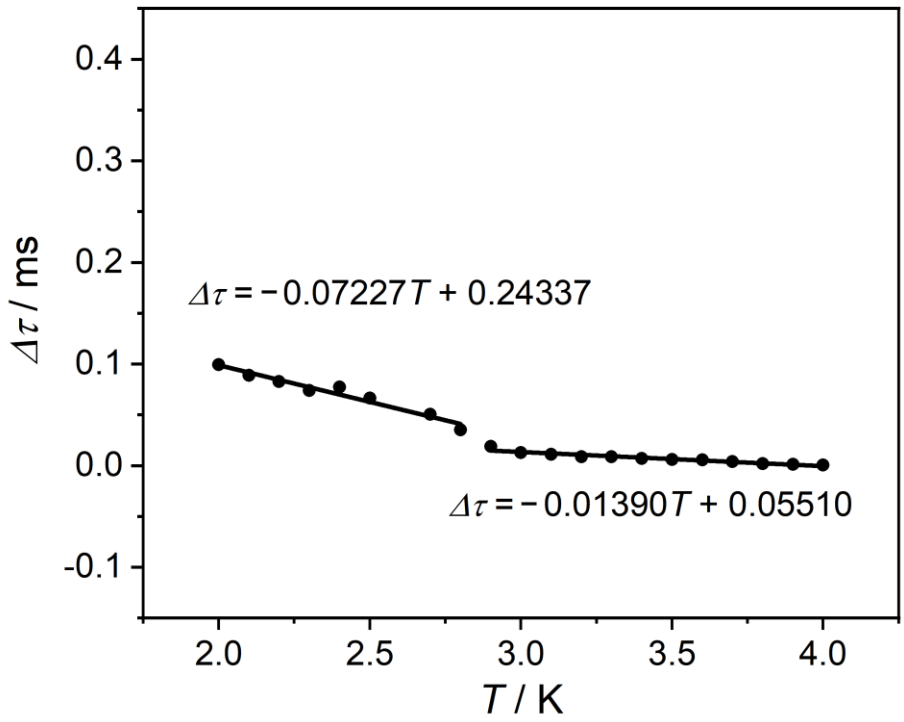

Fig. S30 The plot of the relaxation time difference ($\Delta\tau$) between **2** and **2a**. The straight solid lines show the linear fitting by $\Delta\tau$ = -0.07227T + 0.24337, R^2 = 0.9577 (2–2.7 K) and $\Delta\tau$ = -0.01390T + 0.05510, R^2 = 0.9167 (2.7–4 K).

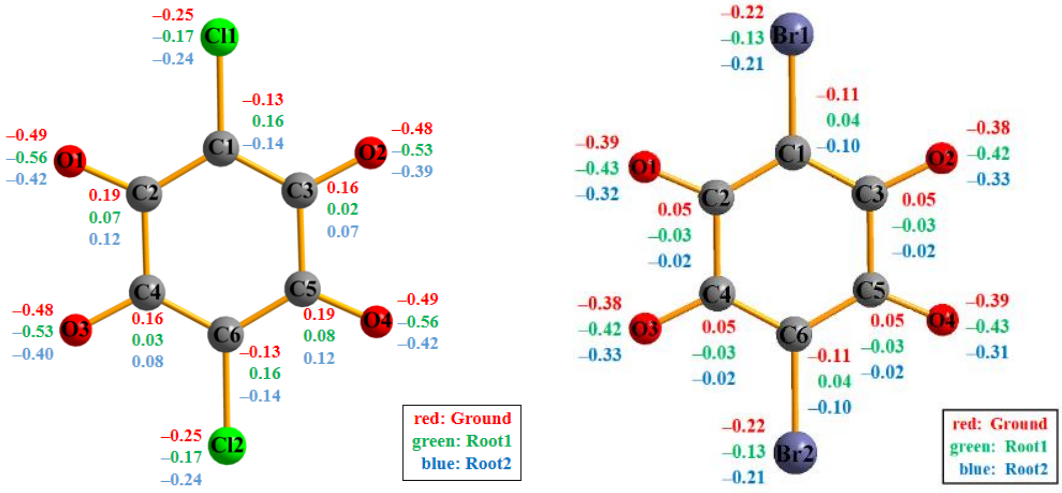

Fig. S31 Calculated ligand structure with charges per atom in the lowest three states.

Table S1. Crystal data and structure refinement details for **1** and **2**.

Compounds	**1**	**2**
CCDC	2161869	2161860
Formula	$C_9H_{12}Cl_3ErO_{12}$	$C_9H_{12}Br_3ErO_{12}$
Formula weight	585.80	719.18
Temperature (K)	298(2)	298(2)
Crystal colour	Black	Black
Wavelength (Å)	0.71073	0.71073
Crystal system	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$
a (Å)	9.1911(3)	9.1947(3)
b (Å)	10.1363(3)	10.2230(3)
c (Å)	11.0340(4)	11.0842(4)
α (deg)	64.916(3)	65.914(3)
β (deg)	69.776(3)	70.234(3)
γ (deg)	81.116(3)	80.603(3)
Z	2	2
V (Å^3)	873.58(6)	894.75(6)
ρ_{calc} (g/cm^3)	2.227	2.669
μ (mm^{-1})	5.319	11.445
F(000)	562.0	670.0
R_{int}	0.0245	0.0441
Goodness-of-fit on F^2	1.077	1.039
[a] R_1, [b] wR_2 (I ≥ 2σ(I))	0.0185, 0.0447	0.0293, 0.0520
[a] R_1, [b] wR_2 (all data)	0.0199, 0.0451	0.0429, 0.0546

[a] $R_1 = \sum||F_o|-|F_c|| / \sum|F_o|$, [b] $wR_2 = \left|\sum w(|F_o|^2-|F_c|^2)\right| / \sum\left|w(F_o)^2\right|^{1/2}$

Table S2. Symmetries and deviated values of Er(III) centers for **1** and **2**.

Shape	Symmetry	**1**	**2**
Enneagon	D_{9h}	36.484	36.330
Octagonal pyramid	C_{8v}	21.385	21.462
Heptagonal bipyramid	D_{7h}	19.929	20.085
Johnson triangular cupola J3	C_{3v}	15.004	14.882
Capped cube J8	C_{4v}	10.963	10.716
Spherical-relaxed capped cube	C_{4v}	9.769	9.799
Capped square antiprism J10	C_{4v}	1.697	1.691
Spherical capped square antiprism	C_{4v}	0.671	0.694
Tricapped trigonal prism J51	D_{3h}	1.869	1.858
Spherical tricapped trigonal prism	D_{3h}	0.555	0.561
Tridiminished icosahedron J63	C_{3v}	12.105	11.977
Hula-hoop	C_{2v}	12.705	12.250
Muffin	C_s	1.240	1.387

Table S3. Relaxation fitting parameters for **1**.

T	χ_S	χ_T	τ / s	α	Residual
2	0.69352	3.1882	3.24491E-4	0.0343	0.00875
2.1	0.66475	3.02175	3.11815E-4	0.04322	0.01043
2.2	0.63614	2.88659	2.95957E-4	0.04784	0.01358
2.3	0.6102	2.76494	2.81794E-4	0.05282	0.01839
2.4	0.59276	2.66867	2.70312E-4	0.06123	0.02476
2.5	0.58687	2.57041	2.60056E-4	0.06038	0.02628
2.6	0.57969	2.4799	2.45625E-4	0.06544	0.01554
2.7	0.56358	2.39916	2.33562E-4	0.06878	0.01769
2.8	0.55463	2.3223	2.22202E-4	0.06951	0.01305
2.9	0.52819	2.26073	2.09058E-4	0.08121	0.02087
3	0.52468	2.18857	1.9879E-4	0.07707	0.01376
3.1	0.51579	2.12907	1.86566E-4	0.08272	0.01355
3.2	0.50879	2.06921	1.77015E-4	0.0798	0.01104
3.3	0.49156	2.01594	1.64172E-4	0.0851	0.00894
3.4	0.47458	1.95984	1.50317E-4	0.0865	0.00816

Table S4. Relaxation fitting parameters for **1a**.

T	χ_S	χ_T	τ / s	α	Residual
2	2.41482E-8	4.86439	2.90178E-4	0.1281	0.27789
2.1	3.26606E-8	4.56914	2.69493E-4	0.15057	0.20652
2.2	4.98888E-8	4.36936	2.59758E-4	0.14892	0.14668
2.3	7.30158E-8	4.187	2.47095E-4	0.15408	0.14354
2.4	1.01261E-7	4.04313	2.33119E-4	0.16453	0.15599
2.5	1.53802E-7	3.89749	2.24013E-4	0.16202	0.1459
2.6	2.08985E-7	3.77456	2.13305E-4	0.16691	0.13251
2.75	3.02983E-7	3.60319	1.9296E-4	0.17814	0.14055
2.9	4.29621E-7	3.43093	1.81248E-4	0.16924	0.08768
3.05	6.58519E-7	3.28367	1.65645E-4	0.1688	0.07039
3.2	9.39617E-7	3.15127	1.50241E-4	0.16877	0.05795
3.35	1.2497E-6	3.02798	1.34924E-4	0.16911	0.05289
3.5	1.75841E-6	2.91249	1.19177E-4	0.16808	0.04982

Table S5. Relaxation fitting parameters for **2**.

T	χ_S	χ_T	τ / s	α	Residual
2	0.78042	3.31096	2.97298E-4	0.10007	0.03565
2.1	0.74521	3.15548	2.59106E-4	0.10016	0.02676
2.2	0.72317	3.0344	2.30778E-4	0.10724	0.03738
2.3	0.69317	2.91696	2.00038E-4	0.11294	0.03681
2.4	0.75112	2.81448	1.83857E-4	0.09883	0.02208
2.5	0.713	2.71694	1.55463E-4	0.10599	0.03371
2.6	0.81227	2.6213	1.45446E-4	0.07977	0.02327
2.7	0.67136	2.546	1.10148E-4	0.10838	0.0244
2.8	0.54897	2.47357	8.36881E-5	0.12465	0.0261
2.9	0.29443	2.40261	5.69546E-5	0.14234	0.01969
3	0.08821	2.32917	4.07978E-5	0.14172	0.02572
3.1	8.08744E-14	2.34523	3.14507E-5	0.15048	0.01423
3.2	1.22129E-13	2.27996	2.41374E-5	0.15268	0.0119
3.3	1.74125E-13	2.22003	1.83882E-5	0.16065	0.00972
3.4	2.64525E-13	2.16598	1.31743E-5	0.18586	0.00802
3.5	4.00433E-13	2.11171	9.45335E-6	0.20731	0.00889

Table S6. Relaxation fitting parameters for **2a**.

T	χ_S	χ_T	τ / s	α	Residual
2	7.53477E-6	3.20149	1.97967E-4	0.20565	0.10974
2.1	1.03976E-5	3.03808	1.70466E-4	0.20312	0.08538
2.2	1.41068E-5	2.92456	1.47965E-4	0.20423	0.0602
2.3	2.13861E-5	2.80518	1.2623E-4	0.19904	0.04866
2.4	3.27051E-5	2.69681	1.06613E-4	0.19485	0.03744
2.5	4.88834E-5	2.61078	8.907E-5	0.19837	0.02693
2.6	7.57031E-5	2.5177	7.39878E-5	0.18986	0.02524
2.7	1.06454E-4	2.43707	5.98485E-5	0.18924	0.01995
2.8	1.63054E-4	2.35502	4.84814E-5	0.17742	0.01381
2.9	2.41248E-4	2.28005	3.81673E-5	0.17113	0.01163
3	3.50079E-4	2.22145	2.82269E-5	0.18913	0.01948
3.1	5.0664E-4	2.15829	2.04919E-5	0.20186	0.01773
3.2	7.77148E-4	2.09355	1.55206E-5	0.19567	0.00729
3.3	0.00115	2.0425	9.78397E-6	0.24106	0.00964
3.4	0.00174	1.98874	6.2022E-6	0.27331	0.00563
3.5	0.0025	1.93895	3.61472E-6	0.31206	0.00501

Table S7. The fitting parameters of relaxation processes for **1**, **1a**, **2** and **2a**.

Complexes	A (s^{-1} K^{-n})	n	U_{eff} (K)	τ_0 (s)	R^2
1	1105 ± 66	1.40 ± 0.06			0.9769
1a	1156 ± 78	1.51 ± 0.07			0.9782
2	1141 ± 39	1.61 ± 0.45	37.73 ± 2.11	2.18×10^{-10} ± 1.35×10^{-11}	0.9981
2a	417 ± 6	3.56 ± 0.16	56.52 ± 0.14	4.66×10^{-13} ± 2.78×10^{-14}	0.9984

Table S8. Calculated energy levels (eV) of the lowest ten states of H_2CA and H_2BA, where Root* represent the different excited states.

Excited states	**Energy levels**	
	H_2CA	H_2BA
Ground	0.00	0.00
Root1	2.83	2.97
Root2	3.02	3.08
Root3	3.44	3.51
Root4	3.47	3.57
Root5	4.07	4.15
Root6	4.16	4.24
Root7	5.18	4.35
Root8	5.24	4.49
Root9	5.87	5.31

Table S9. Calculated ADCH charges (e) per atom in the lowest three states of H_2CA and H_2BA, where Ground, Root1 and Root2 represent the ground, first and second excited states, respectively.

	Ground	Root1	Root2
C1	–0.13/–0.11	0.16/0.04	–0.14/–0.10
C2	0.19/0.05	0.07/–0.03	0.12/–0.02
C3	0.16/0.05	0.02/–0.03	0.07/–0.02
C4	0.16/0.05	0.03/–0.03	0.08/–0.02
C5	0.19/0.05	0.08/–0.03	0.12/–0.02
C6	–0.13/–0.11	0.16/0.04	–0.14/–0.10
O1	–0.49/–0.39	–0.56/–0.43	–0.42/–0.32
O2	–0.48/–0.38	–0.53/–0.42	–0.39/–0.33
O3	–0.48/–0.38	–0.53/–0.42	–0.40/–0.33
O4	–0.49/–0.39	–0.56/–0.43	–0.42/–0.31
Cl1/Br1	–0.25/–0.22	–0.17/–0.13	–0.24/–0.21
Cl2/Br2	–0.25/–0.22	–0.17/–0.13	–0.24/–0.21