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Supporting Information

Nitronyl nitroxide based 2p-3d-4f chains with magnetocaloric effect and slow magnetic relaxation

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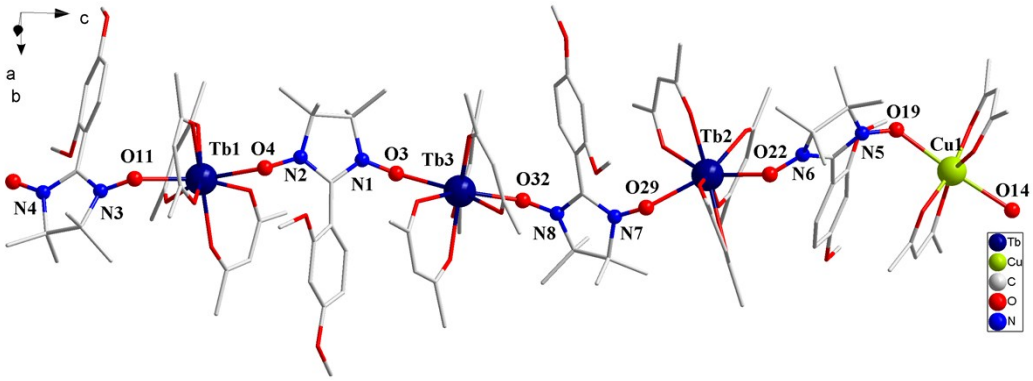

Figure S1. Crystal structure of complex **2.** All hydrogen and fluorine atoms are omitted for clarity

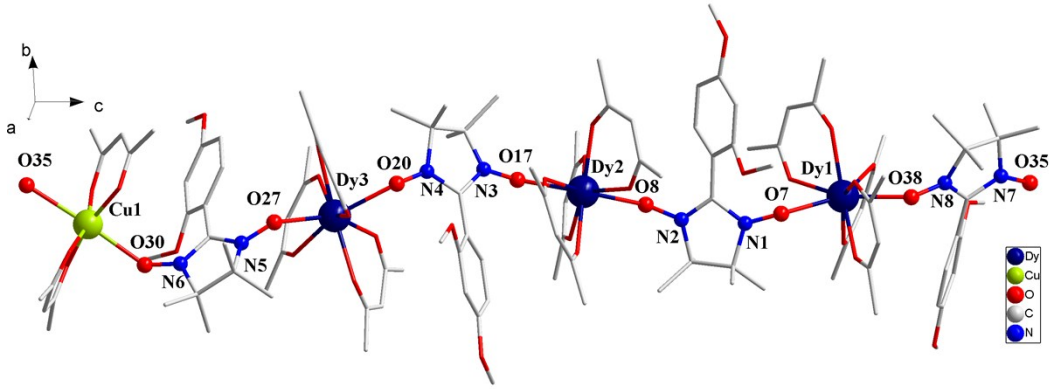

Figure S2. Crystal structure of complex **3.** All hydrogen and fluorine atoms are omitted for clarity

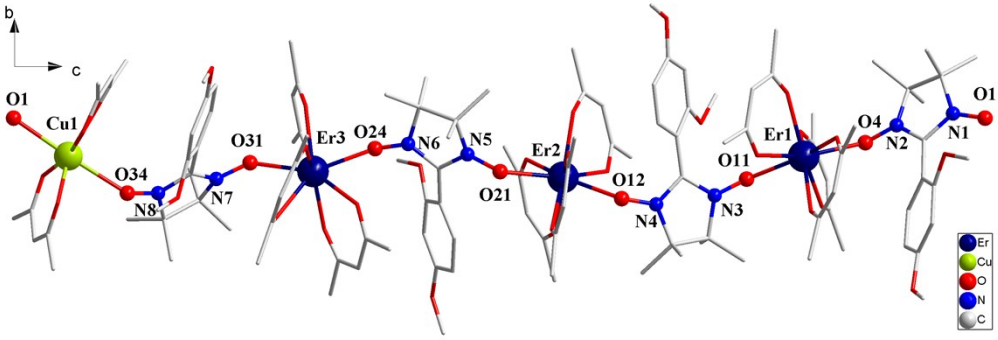

Figure S3. Crystal structure of complex **4**. All hydrogen and fluorine atoms are omitted for clarity

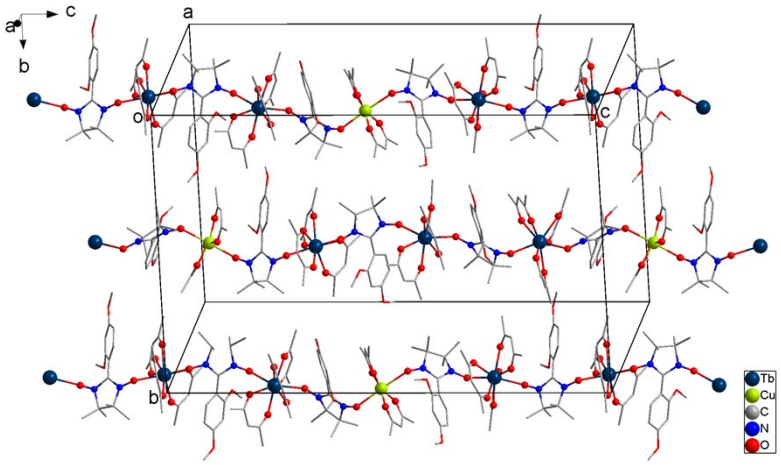

Figure S4. Packing diagram of complex **2**. All hydrogen and fluorine atoms are not shown for the sake of clarity.

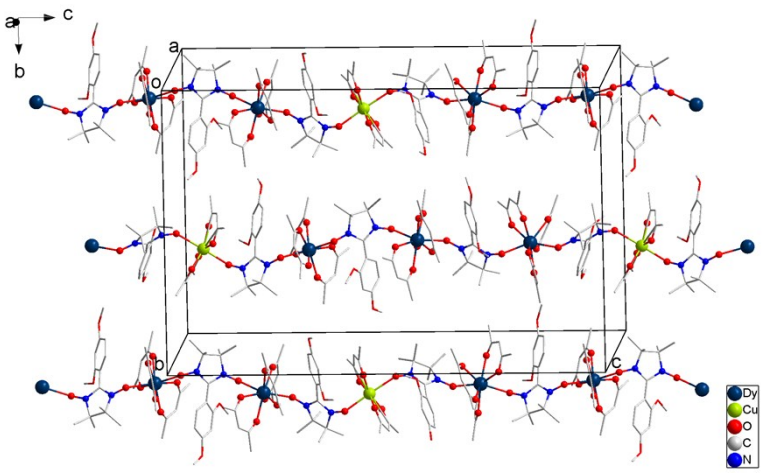

Figure S5. Packing diagram of complex **3**. All hydrogen and fluorine atoms are not shown for the sake of clarity.

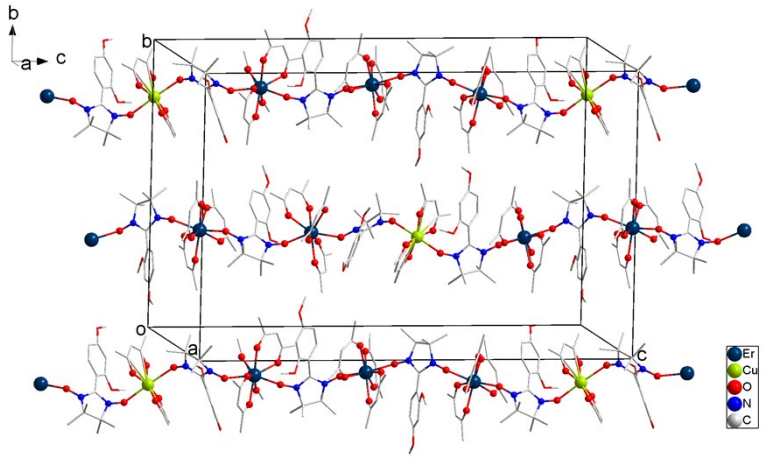

Figure S6. Packing diagram of complex **4**. All hydrogen and fluorine atoms are not shown for the sake of clarity.

Table S1. Crystallographic data and structure refinement summary for **1**–**4**.

	1Gd	**2** Tb	**3** Dy	**4** Er
Formula	$C_{115}H_{95}CuF_{66}Ln_3N_8O_{38}$			
Formula weight	3986.29	3991.29	4002.03	4016.31
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
a **/Å**	19.808(2)	19.8010(14)	19.771(2)	19.7419(18)
b **/Å**	22.168(3)	22.1604(16)	22.179(2)	22.174(2)
c **/Å**	33.918(4)	33.851(3)	33.842(4)	33.727(3)
α**, deg**	90	90	90	90
β**, deg**	90	90	90	90
γ**, deg**	90	90	90	90
V **/Å^3**	14894(3)	14853.6(19)	14840(3)	14764(2)
Z	4	4	4	4
D_{calcd} **/g cm^{-3}**	1.778	1.785	1.791	1.807
F(000)	7839	7852	7864	7888
θ_{min}, θ_{max} **deg**	1.38, 25.01	1.38, 27.88	1.38, 25.01	1.10, 25.01
Reflections collected	118846	152963	109275	124405
Unique reflns/ R_{int}	26236/0.0595	35392/0.0449	26082/0.0623	26033/0.0506
GOF (F^2**)**	0.999	1.038	0.992	1.012
R_1/wR_2 **[**$I > 2\sigma(I)$**]**[a]	0.0449/0.1151	0.0357/0.0784	0.0517/0.1362	0.0376/0.0984
R_1/wR_2 **(all data)**[a]	0.0473/0.1168	0.0385/0.0799	0.0563/0.1396	0.0396/0.0998

[a] $R_1 = \Sigma(||Fo| - |Fc||)/\Sigma|Fo|$. $wR_2 = [\Sigma w(|Fo|^2 - |Fc|^2)^2/\Sigma w(|Fo|^2)^2]^{1/2}$.

Table S2 SHAPE analysis for complexes **1-4**.

complex	Ln	SAPR-8	TDD-8	BTPR-8
	Gd1	2.250	**0.116**	2.310
1	Gd2	2.025	**0.135**	1.978
	Gd3	1.871	**0.205**	1.866
	Tb1	2.165	**0.119**	2.277
2	Tb2	1.937	**0.174**	1.957
	Tb3	2.069	**0.117**	2.030
	Dy1	2.224	**0.105**	2.366
3	Dy2	2.054	**0.111**	2.028
	Dy3	1.928	**0.175**	1.953
	Er1	1.935	**0.168**	1.967
4	Er2	2.024	**0.112**	2.061
	Er3	2.178	**0.103**	2.322

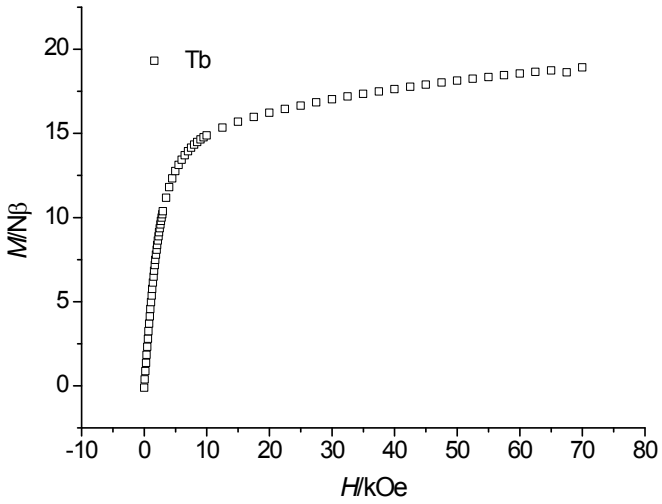

Figure S7. *M* versus *H* plots for **2** at 2 K

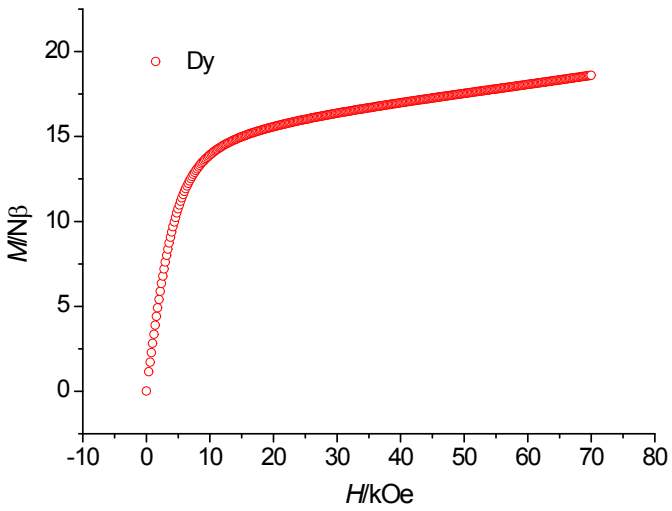

Figure S8. *M* versus *H* plots for **3** at 2 K

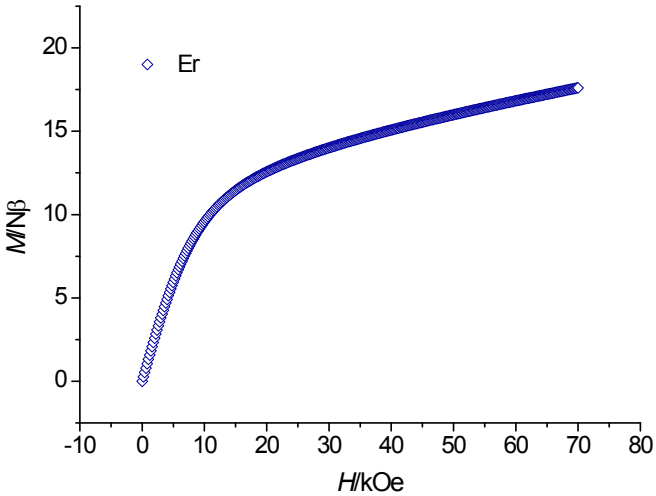

Figure S9. *M* versus *H* plots for **4** at 2 K

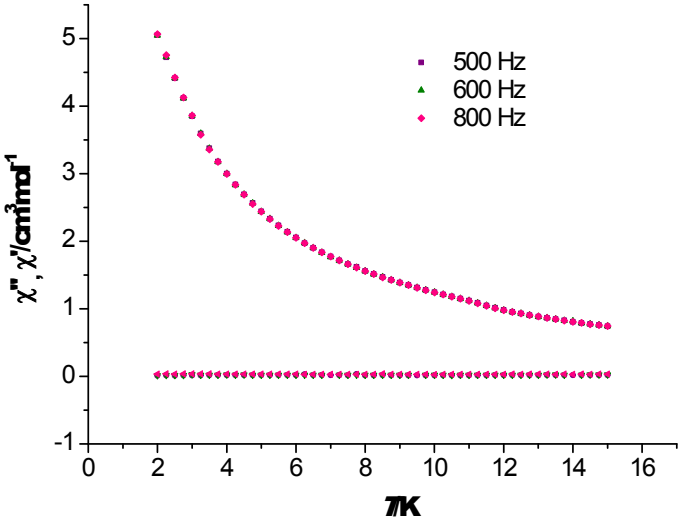

Figure S10. Temperature dependence of the out-of-phase signals of the ac susceptibility under different frequency (Hz) for **3** (H_{ac}=3 Oe, H_{dc}=0).