Tb and Er dimers based on an asymmetric anilato ligand with slow magnetic relaxation

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Table S1. Bond lengths (Å) for complex **1**.

Atom	Atom	Distance (Å)	Atom	Atom	Distance (Å)
Tb1	O16[1]	2.465(4)	N11	O11A	1.148(10)
Tb1	O12	2.413(5)	N1	C1	1.607(8)
Tb1	O2	2.439(5)	N1	O1B	1.195(9)
Tb1	O3	2.418(5)	N1	O1A	1.121(11)
Tb1	O15W	2.335(5)	O16	C16	1.245(8)
Tb1	O14W	2.420(5)	O12	C12	1.252(8)
Tb1	O12W	2.420(6)	O2	C2	1.260(8)
Tb1	O13W	2.422(6)	O3	C3	1.265(8)
Tb1	O11W	2.469(6)	O5	C5	1.232(8)
Cl4	C4	1.709(7)	O6	C6	1.225(8)
Cl4	O4A	1.104(15)	C11	C12	1.402(9)
Cl4	O4B	1.093(17)	C11	C16	1.409(9)
N4	C4	1.709(7)	C12	C16[1]	1.532(10)
N4	O4A	1.104(15)	C3	C4	1.397(10)
N4	O4B	1.093(17)	C3	C2	1.527(10)
Cl11	C11	1.650(7)	C4	C5	1.417(9)
Cl11	O11B	1.168(10)	C1	C2	1.394(9)
Cl11	O11A	1.148(10)	C1	C6	1.436(10)
N11	C11	1.650(7)	C6	C5	1.554(10)
N11	O11B	1.168(10)	O3W	O4W	1.39(2)

[1]1-x, -y, 2-z

Table S2. Bond angles (°) for complex **1**.

Atom	Atom	Atom	Angle (º)	Atom	Atom	Atom	Angle (º)
O16[1]	Tb1	O11W	116.0(2)	O11A	Cl11	C11	110.7(6)
O12	Tb1	O16[1]	64.07(15)	O11A	Cl11	O11B	138.1(8)
O12	Tb1	O2	135.66(16)	O11B	N11	C11	111.0(6)
O12	Tb1	O3	142.21(17)	O11A	N11	C11	110.7(6)
O12	Tb1	O14W	76.05(18)	O11A	N11	O11B	138.1(8)
O12	Tb1	O12W	90.9(2)	O1B	N1	C1	110.1(5)
O12	Tb1	O13W	72.37(18)	O1A	N1	C1	114.6(6)
O12	Tb1	O11W	69.7(2)	O1A	N1	O1B	135.1(8)
O2	Tb1	O16[1]	131.24(16)	C16	O16	Tb1[1]	121.9(4)
O2	Tb1	O11W	112.7(2)	C12	O12	Tb1	123.8(4)
O3	Tb1	O16[1]	133.53(16)	C2	O2	Tb1	122.1(4)
O3	Tb1	O2	64.36(16)	C3	O3	Tb1	122.7(4)
O3	Tb1	O14W	137.66(18)	C12	C11	Cl11	119.1(5)
O3	Tb1	O12W	72.22(18)	C12	C11	N11	119.1(5)
O3	Tb1	O13W	98.6(2)	C12	C11	C16	121.4(6)
O3	Tb1	O11W	72.7(2)	C16	C11	Cl11	119.5(5)
O15W	Tb1	O16[1]	69.99(16)	C16	C11	N11	119.5(5)
O15W	Tb1	O12	133.35(17)	O12	C12	C11	125.9(6)
O15W	Tb1	O2	72.82(18)	O12	C12	C16[1]	114.8(6)
O15W	Tb1	O3	78.20(18)	C11	C12	C16[1]	119.3(6)
O15W	Tb1	O14W	81.3(2)	O3	C3	C4	125.5(7)
O15W	Tb1	O12W	80.6(2)	O3	C3	C2	115.3(6)
O15W	Tb1	O13W	137.3(2)	C4	C3	C2	119.2(6)
O15W	Tb1	O11W	142.9(2)	O16	C16	C11	125.5(6)
O14W	Tb1	O16[1]	69.90(17)	O16	C16	C12[1]	115.2(6)
O14W	Tb1	O2	74.35(17)	C11	C16	C12[1]	119.3(6)
O14W	Tb1	O12W	139.5(2)	C3	C4	Cl4	119.3(5)
O14W	Tb1	O13W	72.8(2)	C3	C4	N4	119.3(5)
O14W	Tb1	O11W	135.7(2)	C3	C4	C5	122.2(6)
O12W	Tb1	O16[1]	69.93(18)	C5	C4	Cl4	118.4(5)
O12W	Tb1	O2	132.5(2)	C5	C4	N4	118.4(5)
O12W	Tb1	O13W	139.6(3)	C2	C1	N1	119.7(5)
O12W	Tb1	O11W	69.1(3)	C2	C1	C6	121.8(6)
O13W	Tb1	O16[1]	127.73(19)	C6	C1	N1	118.5(5)
O13W	Tb1	O2	67.80(18)	O2	C2	C3	114.1(6)
O13W	Tb1	O11W	70.7(3)	O2	C2	C1	126.0(6)
O4A	Cl4	C4	104.4(8)	C1	C2	C3	119.8(6)
O4B	Cl4	C4	107.5(9)	O6	C6	C1	126.4(7)
O4B	Cl4	O4A	134.5(12)	O6	C6	C5	115.7(6)
O4A	N4	C4	104.4(8)	C1	C6	C5	117.8(6)
O4B	N4	C4	107.5(9)	O5	C5	C4	125.1(7)
O4B	N4	O4A	134.5(12)	O5	C5	C6	116.1(6)
O11B	Cl11	C11	111.0(6)	C4	C5	C6	118.8(6)

[1]1-x, -y, 2-z

Table S3. Bond lengths (Å) for complex **2**.

Atom	Atom	Distance (Å)	Atom	Atom	Distance (Å)
Er1	O16[1]	2.431(5)	N1	O1B	1.176(9)
Er1	O12	2.382(5)	N1	O1A	1.117(10)
Er1	O3	2.377(5)	Cl1	C1	1.611(8)
Er1	O2	2.403(5)	Cl1	O1B	1.176(9)
Er1	O13W	2.384(5)	Cl1	O1A	1.117(10)
Er1	O11W	2.293(6)	O16	C16	1.242(8)
Er1	O12W	2.357(7)	O12	C12	1.242(8)
Er1	O15W	2.346(8)	O3	C5	1.254(8)
Er1	O14W	2.466(8)	O2	C6	1.268(8)
Cl4	C4	1.704(7)	O6	C2	1.229(8)
Cl4	O4A	1.084(16)	O5	C3	1.226(8)
Cl4	O4B	1.024(17)	C16	C11	1.420(9)
N4	C4	1.704(7)	C16	C12[1]	1.535(10)
N4	O4A	1.084(16)	C11	C12	1.407(10)
N4	O4B	1.024(17)	C5	C6	1.527(10)
N11	C11	1.638(7)	C5	C4	1.394(10)
N11	O11B	1.183(9)	C1	C6	1.388(10)
N11	O11A	1.148(10)	C1	C2	1.433(10)
Cl11	C11	1.638(7)	C2	C3	1.558(10)
Cl11	O11B	1.183(9)	C4	C3	1.419(9)
Cl11	O11A	1.148(10)	O3W	O3W'	1.33(2)
N1	C1	1.611(8)			

[1]1-x, -y, 2-z

Table S4. Bond angles (°) for complex **2**.

Atom	Atom	Atom	Angle (º)	Atom	Atom	Atom	Angle (º)
O16[1]	Er1	O14W	115.3(3)	O11A	Cl11	C11	111.1(6)
O12	Er1	O16[1]	64.93(16)	O11A	Cl11	O11B	137.5(8)
O12	Er1	O2	134.68(18)	O1B	N1	C1	110.3(6)
O12	Er1	O13W	76.80(19)	O1A	N1	C1	113.3(7)
O12	Er1	O14W	69.3(3)	O1A	N1	O1B	136.3(8)
O3	Er1	O16[1]	134.22(17)	O1B	Cl1	C1	110.3(6)
O3	Er1	O12	140.56(17)	O1A	Cl1	C1	113.3(7)
O3	Er1	O2	64.92(16)	O1A	Cl1	O1B	136.3(8)
O3	Er1	O13W	137.76(18)	C16	O16	Er1[1]	121.2(5)
O3	Er1	O14W	71.3(3)	C12	O12	Er1	123.7(5)
O2	Er1	O16[1]	131.64(17)	C5	O3	Er1	123.1(4)
O2	Er1	O14W	113.0(3)	C6	O2	Er1	122.4(4)
O13W	Er1	O16[1]	70.31(18)	O16	C16	C11	125.1(7)
O13W	Er1	O2	73.74(18)	O16	C16	C12[1]	115.6(6)
O13W	Er1	O14W	136.9(3)	C11	C16	C12[1]	119.3(6)
O11W	Er1	O16[1]	69.90(18)	C16	C11	N11	120.1(5)
O11W	Er1	O12	134.19(18)	C16	C11	Cl11	120.1(5)
O11W	Er1	O3	79.2(2)	C12	C11	N11	119.2(5)
O11W	Er1	O2	73.8(2)	C12	C11	Cl11	119.2(5)
O11W	Er1	O13W	81.5(2)	C12	C11	C16	120.7(6)
O11W	Er1	O12W	82.8(3)	O3	C5	C6	115.3(6)
O11W	Er1	O15W	140.9(3)	O3	C5	C4	126.3(7)
O11W	Er1	O14W	141.5(3)	C4	C5	C6	118.4(6)
O12W	Er1	O16[1]	71.0(2)	C6	C1	N1	120.2(6)
O12W	Er1	O12	89.5(2)	C6	C1	Cl1	120.2(6)
O12W	Er1	O3	72.3(2)	C6	C1	C2	121.2(6)
O12W	Er1	O2	134.1(2)	C2	C1	N1	118.7(5)
O12W	Er1	O13W	141.2(2)	C2	C1	Cl1	118.7(5)
O12W	Er1	O14W	65.3(4)	O2	C6	C5	113.2(6)
O15W	Er1	O16[1]	129.4(2)	O2	C6	C1	125.9(7)
O15W	Er1	O12	71.0(2)	C1	C6	C5	120.8(6)
O15W	Er1	O3	95.8(2)	O12	C12	C16[1]	114.3(6)
O15W	Er1	O2	69.2(2)	O12	C12	C11	125.7(7)
O15W	Er1	O13W	76.7(3)	C11	C12	C16[1]	120.0(6)
O15W	Er1	O12W	133.0(4)	O6	C2	C1	126.0(7)
O15W	Er1	O14W	67.8(4)	O6	C2	C3	115.8(6)
O4A	Cl4	C4	105.8(9)	C1	C2	C3	118.2(6)
O4B	Cl4	C4	106.1(10)	C5	C4	Cl4	119.5(5)
O4B	Cl4	O4A	135.0(13)	C5	C4	N4	119.5(5)
O4A	N4	C4	105.8(9)	C5	C4	C3	122.5(6)
O4B	N4	C4	106.1(10)	C3	C4	Cl4	117.8(5)
O4B	N4	O4A	135.0(13)	C3	C4	N4	117.8(5)
O11B	N11	C11	111.3(6)	O5	C3	C2	115.4(6)
O11A	N11	C11	111.1(6)	O5	C3	C4	126.2(7)
O11A	N11	O11B	137.5(8)	C4	C3	C2	118.4(6)

[1]1-x, -y, 2-z

Table S5. Interdimer H-Bond distances (Å) for complex **1**.

Atom1	Atom2	Symm. op. 1	Symm. op. 2	Distance (Å)
O3W'	O3W'	x,y,z	2-x,-y,1-z	2.502
O3W	O3W'	x,y,z	2-x,-y,1-z	2.512
O11W	O4B	x,y,z	1-x,-y,1-z	2.660
O12W	O1A	x,y,z	x,-1+y,z	2.669
O15W	O2W	1-x,-y,2-z	-1+x,-1+y,1+z	2.722
O13W	O3W'	x,y,z	-1+x,y,z	2.748
O11A	O3W	x,y,z	-1+x,y,z	2.753
O1W	O11A	x,y,z	1+x,y,z	2.774
O2W	O11B	x,y,z	1-x,-y,1-z	2.775
O14W	O2W	x,y,z	x,y,1+z	2.798
O4A	O11B	1-x,-y,2-z	x,y,1+z	2.811
O13W	O3W	x,y,z	-1+x,y,z	2.826
O4B	O3W	1-x,-y,2-z	-1+x,y,1+z	2.842
O5	O13W	1-x,-y,2-z	x,-1+y,1+z	2.846
O2	O1W	1-x,-y,2-z	-1+x,-1+y,z	2.886
O14W	O14W	1-x,-y,2-z	x,-1+y,z	2.889
O12W	O11W	x,y,z	1-x,-y,1-z	2.921
O1W	O1B	x,y,z	2-x,1-y,2-z	2.930
O12W	O6	x,y,z	x,-1+y,z	2.943
O11W	O11W	x,y,z	1-x,-y,1-z	2.976
O11W	O3W	x,y,z	-1+x,y,z	2.978
O1W	O11B	x,y,z	1-x,-y,2-z	3.000
O16	O1A	1-x,-y,2-z	x,-1+y,z	3.024

Table S6. Interdimer H-Bond distances (Å) for complex **2**.

Atom1	Atom2	Symm. op. 1	Symm. op. 2	Distance (Å)
O3W	O3W'	x,y,z	2-x,-y,1-z	2.536
O15W	O3W'	x,y,z	-1+x,y,z	2.625
O12W	O1A	x,y,z	x,-1+y,z	2.665
O3W'	O3W'	x,y,z	2-x,-y,1-z	2.687
O11W	O2W	1-x,-y,2-z	-1+x,-1+y,1+z	2.713
O14W	O4B	x,y,z	1-x,-y,1-z	2.741
O11A	O3W	x,y,z	-1+x,y,z	2.776
O1W	O11A	x,y,z	1+x,y,z	2.786
O4A	O11B	1-x,-y,2-z	x,y,1+z	2.787
O13W	O2W	x,y,z	x,y,1+z	2.793
O2W	O11B	x,y,z	1-x,-y,1-z	2.802
O15W	O3W	x,y,z	-1+x,y,z	2.804
O14W	O14W	x,y,z	1-x,-y,1-z	2.805
O4A	O2W	x,y,z	x,y,z	2.819
O4B	O3W	1-x,-y,2-z	-1+x,y,1+z	2.869
O2	O1W	1-x,-y,2-z	-1+x,-1+y,z	2.870
O5	O15W	1-x,-y,2-z	x,-1+y,1+z	2.889
O13W	O13W	1-x,-y,2-z	x,-1+y,z	2.896
O1W	O1B	x,y,z	2-x,1-y,2-z	2.898
O12W	O6	x,y,z	x,-1+y,z	2.937
O1W	O11B	x,y,z	1-x,-y,2-z	2.966
O12W	O14W	x,y,z	1-x,-y,1-z	3.013
O13W	O1B	1-x,-y,2-z	x,-1+y,z	3.029
O3W	O3W	x,y,z	2-x,-y,1-z	3.032

Table S7. Parameters obtained for compound **1** from the fit of the AC susceptibility to the Debye model with an applied DC field of 160 mT

T (K)	α_1	χ_{ad} ($cm^3\ mol^{-1}$)	χ_{T1} ($cm^3\ mol^{-1}$)	χ_{T2} ($cm^3\ mol^{-1}$)	τ_1 (s)	α_2	τ_2 (s)
1.9	0.0359	3.1180	5.6206	6.1666	0.3579	0.4378	0.000967
2.0	0.0897	3.2780	5.4823	5.9933	0.3076	0.4975	0.001002
2.2	0.0535	3.5024	5.3679	5.8613	0.2741	0.4995	0.000872
2.4	0.0081	3.7141	5.2807	5.7190	0.2225	0.5517	0.000736
2.6	0.0036	3.8834	5.2194	5.6318	0.1999	0.5544	0.000614
2.8	0.0584	4.0290	5.1723	5.5510	0.1638	0.5126	0.000511
3.0	0.0628	4.1554	5.1267	5.4920	0.1452	0.5218	0.000441
3.2	0.0513	4.2641	5.0901	5.4269	0.1340	0.5185	0.000361
3.4	0.0137	4.3701	5.0561	5.3663	0.1265	0.5694	0.000320
3.6	0.0233	4.4583	5.0293	5.3100	0.1138	0.5547	0.000353
3.8	0.0459	4.5286	5.0136	5.2645	0.1079	0.6127	0.000307
4.0	0.0496	4.6227	4.9854	5.2073	0.1063	0.5950	0.000333
4.2	0.1481	4.6965	4.9632	5.1627	0.1067	0.5840	0.000337
4.4	0.1888	4.7366	4.9573	5.1339	0.1076	0.5455	0.000387
4.6	0.1591	4.7789	4.9514	5.0990	0.1108	0.6024	0.000395

χ_{ad} = total adiabatic susceptibility; χ_{T1} and χ_{T2} = isothermal susceptibility for relaxation process 1 and 2, respectively; α_1 and α_2 = magnetic relaxation time distribution parameter for relaxation process 1 and 2, respectively; τ_1 and τ_2 = magnetic relaxation time for relaxation processes 1 and 2, respectively.

Table S8. Parameters obtained for compound **2** from the fit of the AC susceptibility to the Debye model with an applied DC field of 60 mT

T (K)	α_1	χ_{ad} (cm^3 mol^{-1})	χ_{T1} (cm^3 mol^{-1})	χ_{T2} (cm^3 mol^{-1})	τ_1 (s)	α_2	τ_2 (s)
1.90	0.44568	2.7547	3.2635	6.5888	0.0066897	0.17916	2.8768e-05
1.95	0.41913	2.8490	3.3231	6.4815	0.0082383	0.17869	3.0128e-05
2.00	0.54071	3.0317	3.5015	6.4739	0.0094188	0.16155	2.8620e-05
2.05	0.59033	2.9124	3.3505	6.4871	0.010433	0.13527	2.8412e-05
2.10	0.62912	3.0953	3.4992	6.4767	0.011248	0.12796	2.6821e-05
2.20	0.60925	3.1200	3.4812	6.5831	0.0082923	0.10444	2.5027e-05
2.30	0.60528	3.1515	3.4779	6.5486	0.0077010	0.10772	2.2134e-05
2.40	0.54755	3.2027	3.4995	6.5121	0.0068161	0.12542	1.9614e-05
2.50	0.50254	3.2486	3.5216	6.4964	0.0064775	0.13882	1.7038e-05
2.60	0.56920	3.3043	3.5658	6.4640	0.0055698	0.11105	1.5030e-05
2.70	0.56349	3.2334	3.4717	6.2666	0.0050722	0.11593	1.2912e-05
2.80	0.56931	3.2597	3.4821	6.2237	0.0051877	0.12412	1.0760e-05
2.90	0.58261	3.0644	3.2716	5.7696	0.0046721	0.11015	1.0221e-05

χ_{ad} = total adiabatic susceptibility; χ_{T1} and χ_{T2} = isothermal susceptibility for relaxation process 1 and 2, respectively; α_1 and α_2 = magnetic relaxation time distribution parameter for relaxation process 1 and 2, respectively; τ_1 and τ_2 = magnetic relaxation time for relaxation processes 1 and 2, respectively.

Table S9. Parameters obtained for compound **2** from the fit of the AC susceptibility to the Debye model with an applied DC field of 100 mT

T (K)	α_1	χ_{ad} (cm^3 mol^{-1})	χ_{T1} (cm^3 mol^{-1})	χ_{T2} (cm^3 mol^{-1})	τ_1 (s)	α_2	τ_2 (s)
2.0	0.40791	2.9631	3.1397	3.5960	0.012155	0.22056	6.2330e-06
2.1	0.44031	2.9469	3.1117	3.6324	0.011910	0.20779	5.6901e-06
2.2	0.48396	2.9500	3.1019	3.5840	0.010896	0.14776	7.6697e-06
2.3	0.46872	2.9340	3.0808	3.6312	0.0095553	0.15554	6.6886e-06
2.4	0.48169	2.9166	3.0601	3.7040	0.010300	0.18551	5.2481e-06
2.5	0.56420	2.9440	3.0823	3.6168	0.012488	0.10792	7.9004e-06
2.6	0.58236	2.9480	3.0790	3.6233	0.011239	0.085025	8.1911e-06
2.7	0.54909	2.9427	3.0650	3.6579	0.0087645	0.12120	7.2528e-06
2.8	0.56188	2.9398	3.0579	3.6708	0.0092002	0.13405	6.7688e-06
2.9	0.55049	2.9079	3.0179	3.6899	0.0081447	0.15437	5.8115e-06
3.0	0.59210	2.9211	3.0256	3.7152	0.0095532	0.14630	5.5716e-06
3.1	0.58466	2.9409	3.0356	3.7244	0.0097409	0.18128	5.2095e-06
3.2	0.61143	2.9281	3.0144	3.6662	0.0087590	0.15886	5.7498e-06
3.3	0.54937	2.9586	3.0372	3.8131	0.0082417	0.22464	3.8673e-06
3.4	0.61381	2.9981	3.0654	3.6333	0.0072301	0.16963	6.3705e-06
3.6	0.55301	2.9702	3.0188	3.6967	0.0059901	0.25324	3.7036e-06
3.8	0.50822	3.0763	3.1161	3.5520	0.0040934	0.20682	6.8071e-06
4.0	0.42937	3.1336	3.1664	3.5308	0.0039771	0.22526	6.9507e-06

χ_{ad} = total adiabatic susceptibility; χ_{T1} and χ_{T2} = isothermal susceptibility for relaxation process 1 and 2, respectively; α_1 and α_2 = magnetic relaxation time distribution parameter for relaxation process 1 and 2, respectively; τ_1 and τ_2 = magnetic relaxation time for relaxation processes 1 and 2, respectively.

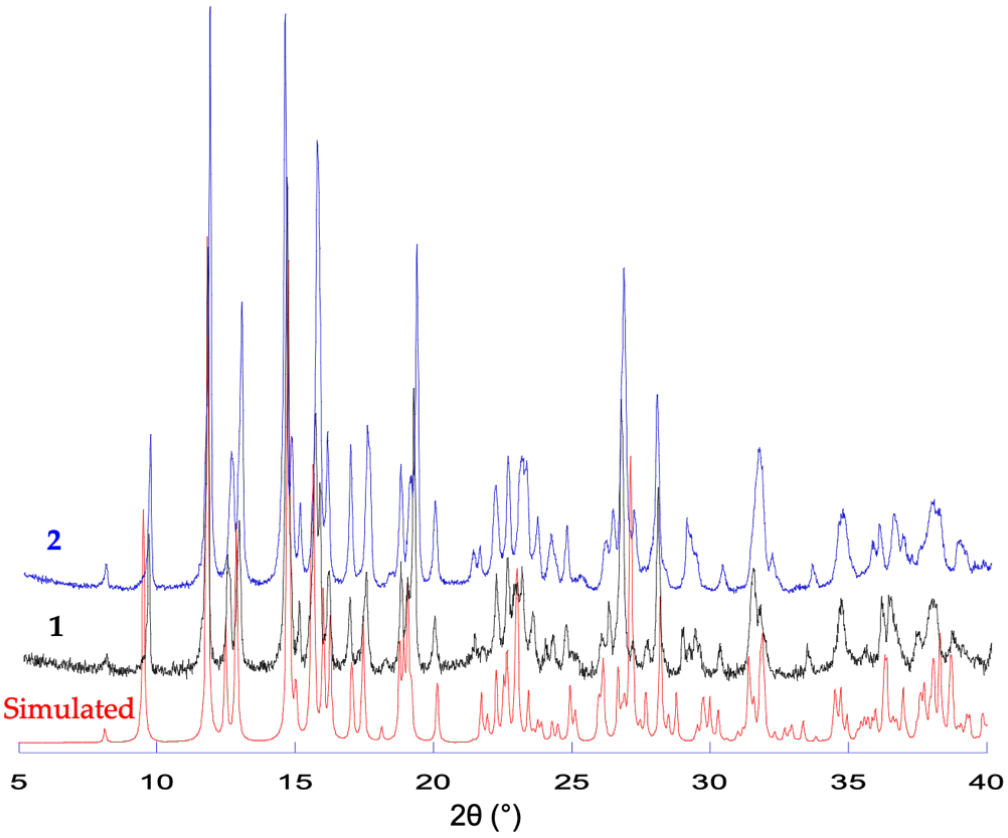

Figure S1. Experimental X-ray powder diffractograms for compounds **1** and **2** and and simulated one from the crystal structure of compound **1**.

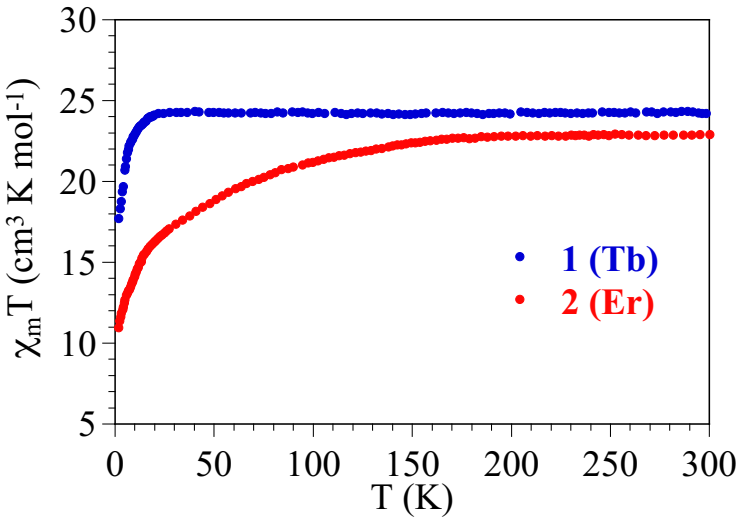

Figure S2. Thermal variation of the $\chi_m T$ product for compounds **1** and **2**.

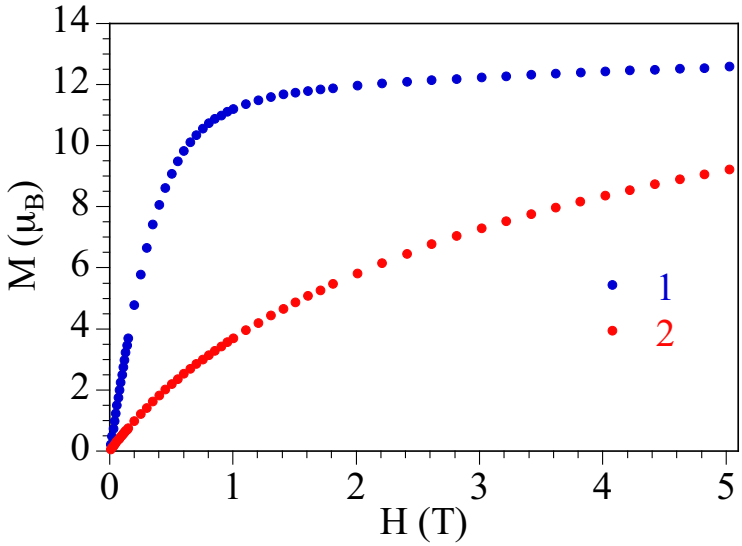

Figure S3. Isothermal magnetization at 2 K for compounds **1** and **2**.

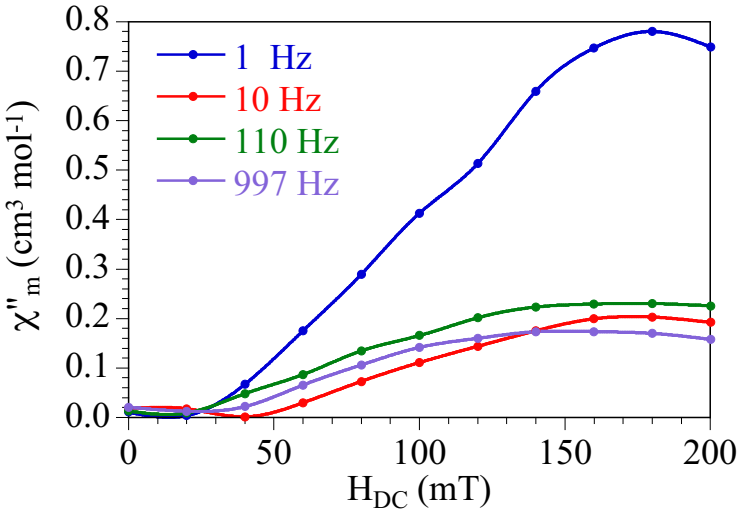

Figure S4. Variation of the out-of-phase magnetic susceptibility (χ''_m) with the external DC field (H_{dc}) for compound **1** at 1.9 K at different frequencies. Solid lines are guides for the eyes.

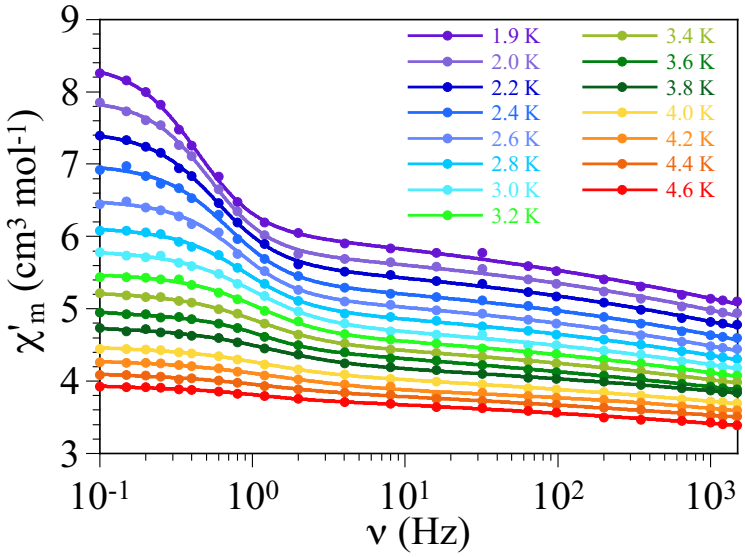

Figure S5. Frequency dependence of the in-phase magnetic susceptibility (χ'_m) for compound **1** with a DC magnetic field of 160 mT at different temperatures. Solid lines are the best fit to the Debye model for two relaxation processes.

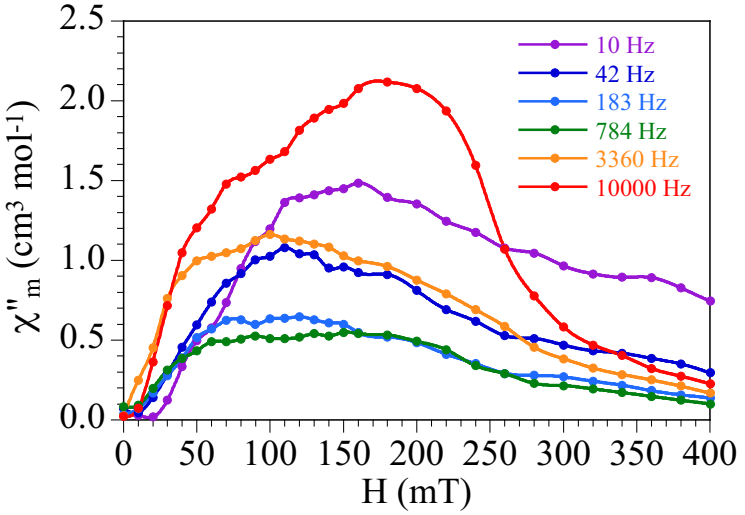

Figure S6. Variation of the out-of-phase magnetic susceptibility (χ''_m) with the external DC field (H_{dc}) for compound **2** at 2.0 K at different frequencies. Solid lines are guides for the eyes.

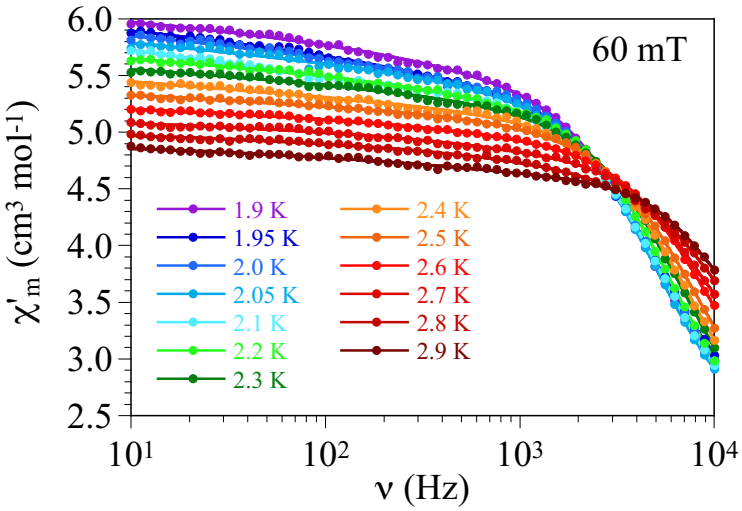

Figure S7. Frequency dependence of the in-phase magnetic susceptibility (χ'_m) for compound **2** at different temperatures with a DC magnetic field of 60 mT. Solid lines are the best fit to the Debye model for two relaxation processes.