Supplementary Materials: 1D Chains of Lanthanoid Ions and a Dithienylethene Ligand Showing Slow Relaxation of the Magnetization

Mudasir Ahmad Yatoo [1], Goulven Cosquer [1,2], Masakazu Morimoto [3], Masahiro Irie [3], Brian K. Breedlove [1] and Masahiro Yamashita [1,2,*]

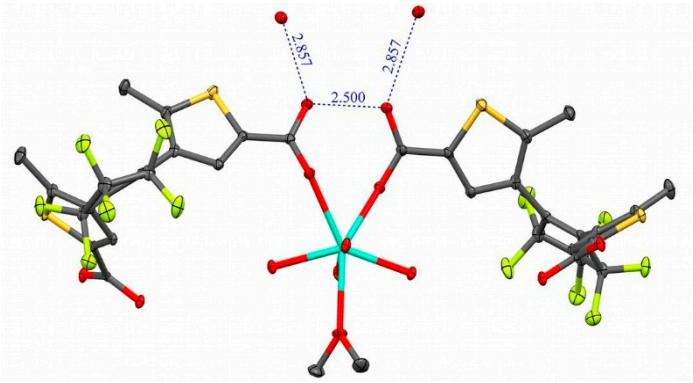

Figure S1. Hydrogen bond between O6–O2 and O2–O2. Water and MeOH molecule have occupancy of 0.5.

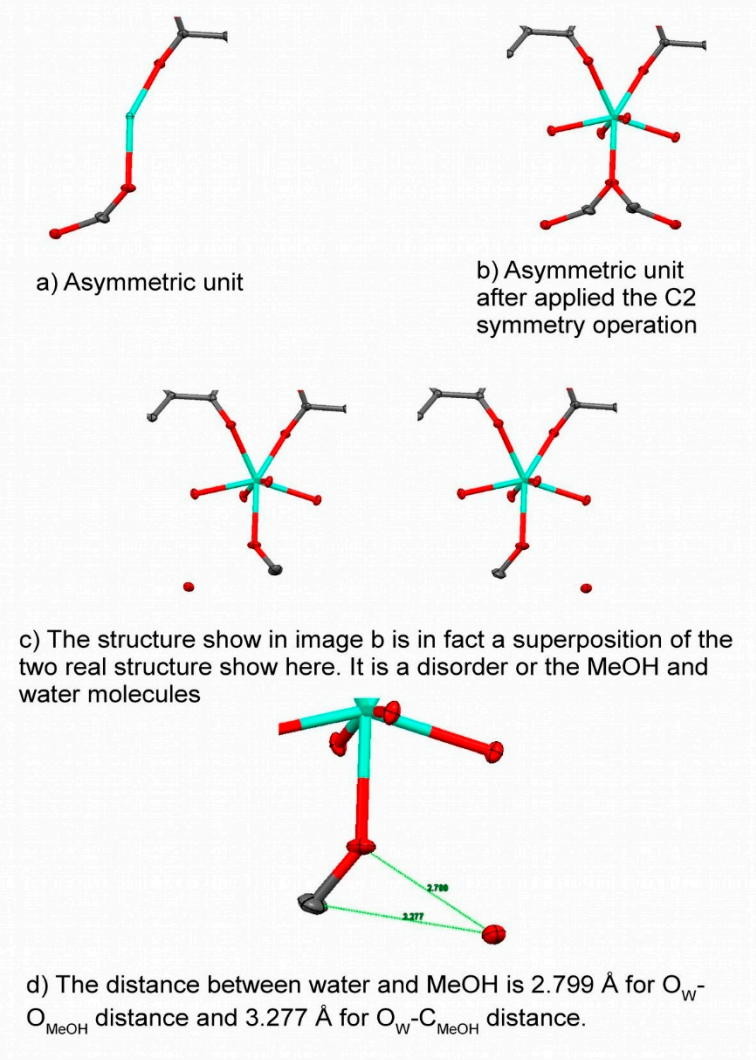

Figure S2. Disorder of MeOH and water molecule.

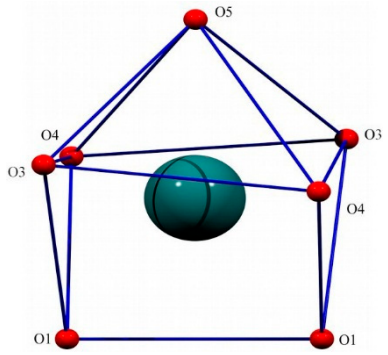

Figure S3. Coordination polyhedron around the Tb ion.

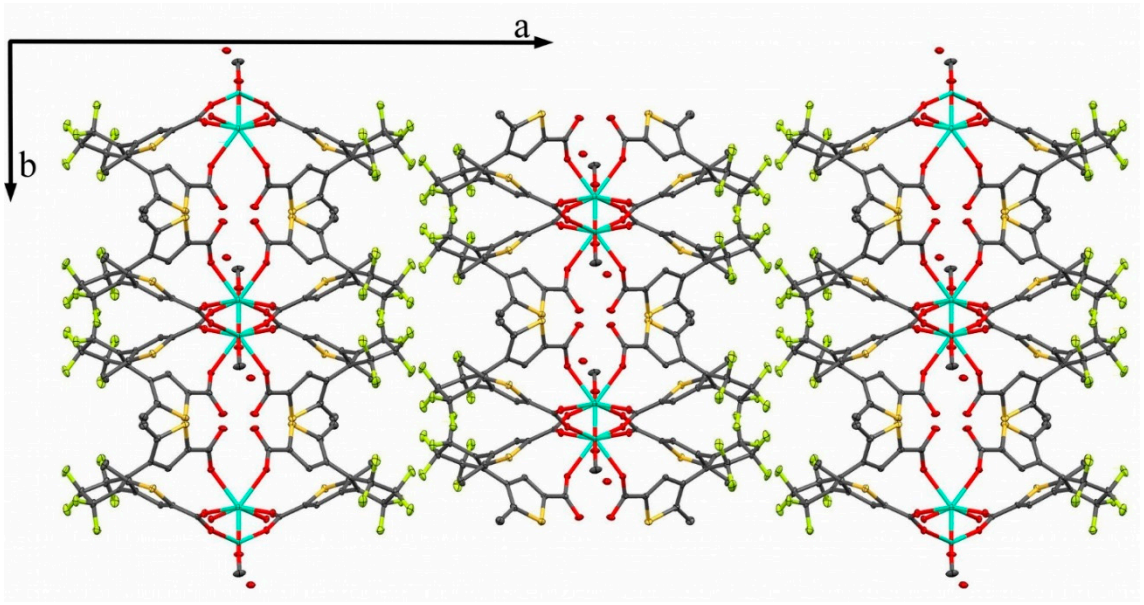

Figure S4. Crystal packing of Tb crystal in the *ab* plane.

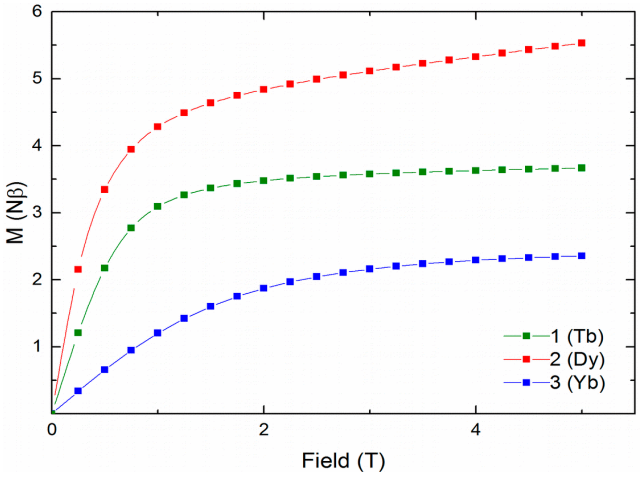

Figure S5. Magnetization curves of the three complexes at 1.82 K.

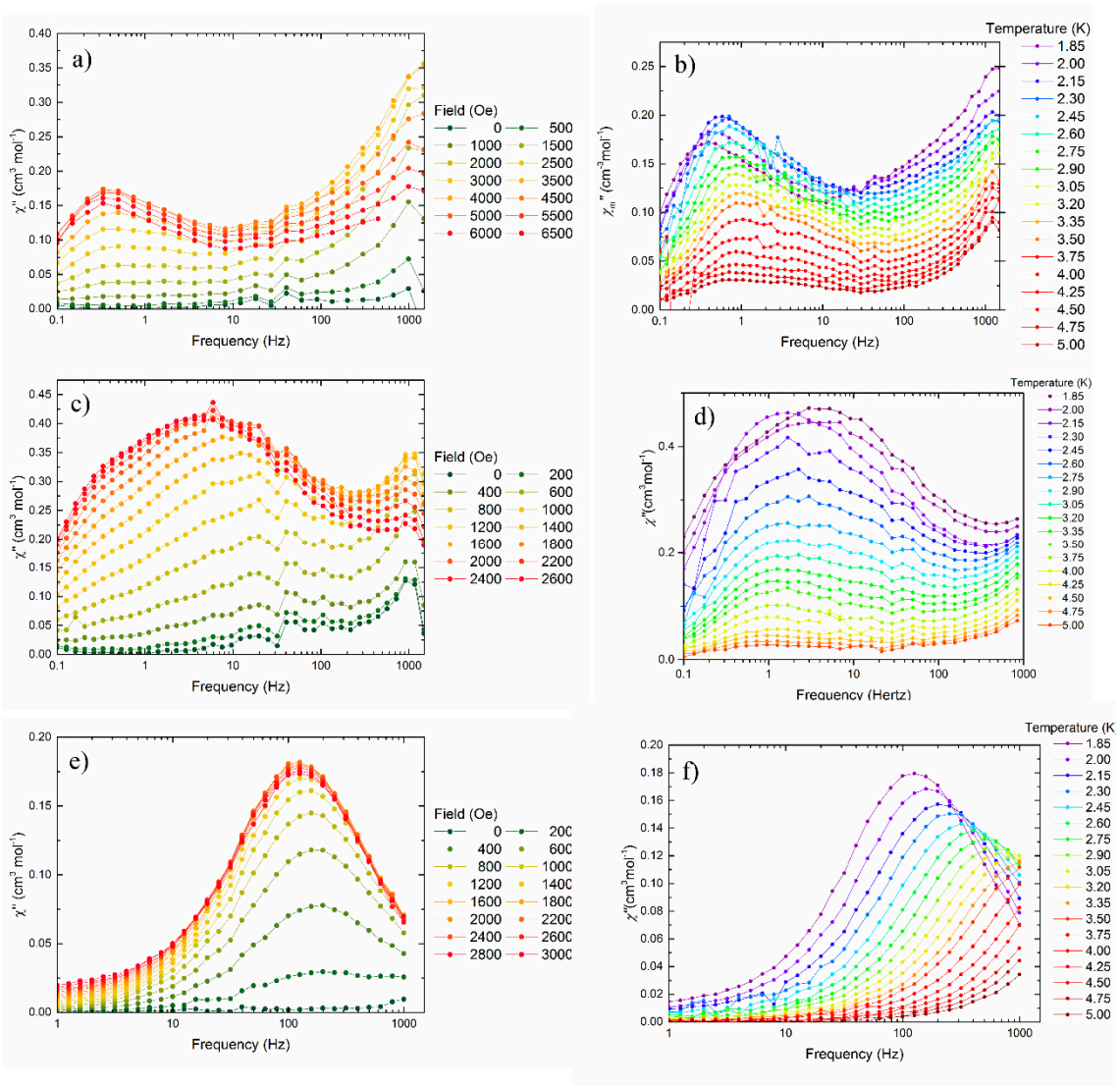

Figure S6. Out-of-phase signal of ac susceptibility at 1.85 K in various fields (**a**, **c**, **e**), and at various temperature in optimum field (**b**, **d**, **f**), for complexes 1 (**a**, **b**), 2 (**c**, **d**) and 3 (**e**, **f**). The optimum field, defined as the field where the intensity of peak is maximized and the peak have lowest frequency, was determined to be 5000 Oe for 1, 2500 Oe for 2 and 2000 Oe for 3.

Table S1. Determination of polyhedron geometry by using SHAPE 2.1 software.

Complex	HP-7	HPY-7	PBPY-7	COC-7	CTPR-7	JPBPY-7	JETPY-7
1	31.896	22.621	4.080	2.305	0.490	7.425	20.136
2	32.200	22.449	3.939	2.320	0.562	7.332	20.203
3	32.392	22.378	3.704	2.417	0.704	7.161	20.327

The in-phase and out-of-phase susceptibility data of 1 and 2 were fitted simultaneously by using a dual relaxation Debye model, as show in the following Equations:

$$\chi_m' = \chi_{adia} + g(\chi_{iso1},\alpha_1,\tau_1) + g(\chi_{iso2},\alpha_2,\tau_2)$$
$$\chi_m'' = f(\chi_{iso\,1},\alpha_1,\tau_1) + f(\chi_{iso\,2},\alpha_2,\tau_2) \quad (1)$$

with

$$g(\chi_{iso},\alpha,\tau) = (\chi_{iso}-\chi_{adia})\frac{1+(\omega\tau)^{1-\alpha}\sin\frac{\pi\alpha}{2}}{1+2(\omega\tau)^{1-\alpha}\sin\frac{\pi\alpha}{2}+(\omega\tau)^{2(1-\alpha)}} \quad (2)$$

$$f(\chi_{iso},\alpha,\tau) = (\chi_{iso}-\chi_{adia})\frac{1+(\omega\tau)^{1-\alpha}\cos\frac{\pi\alpha}{2}}{1+2(\omega\tau)^{1-\alpha}\sin\frac{\pi\alpha}{2}+(\omega\tau)^{2(1-\alpha)}} \quad (3)$$

where χ_{iso} and χ_{adia} are the isotrope and adiabatic susceptibilities, τ is the relaxation time, and α is the distribution of τ.

In the case of 3, only one relaxation process was necessary to obtain a correct fitting of the data by using the following equations.

$$\chi_m' = \chi_{adia} + g(\chi_{iso},\alpha,\tau) \qquad \chi_m'' = f(\chi_{iso},\alpha,\tau) \quad (4)$$

τ was fitted using the following equation with direct, Orbach, and quantum tunneling relaxation processes. For each complex, not all of the processes were used (see Table S2).

$$\tau^{-1}(T,H) = A T^2 H^4 + \tau_0^{-1}\exp(-\Delta/k_B T) + \mathrm{QTM} \quad (5)$$

Table S2. Summary of the parameters used in Equations S1–S5 to fit τ.

Complex	1		2		3
A	9.87×10^{-12}	-	5.75×10^{-9}	-1.66×10^{-14}	1.47×10^{-11}
H	5000	-	2500	2500	2000
Δ	33.3	6.9	59.0	-	27.0
$\tau 0$	6.93×10^{-9}	2.48×10^{-2}	3.12×10^{-12}	-	8.13×10^{-7}
QTM	-	-	-	17.73136	-

Table S3. Fitting parameters for complex 3.

Temperature (K)	χ_{adia} ($cm^3 \cdot mol^{-1}$)	χ_{iso} ($cm^3 \cdot mol^{-1}$)	α	τ (s)
1.85	3.44×10^{-2}	0.46	0.16	1.23×10^{-3}
2.00	3.13×10^{-2}	0.43	0.16	9.60×10^{-4}
2.15	2.76×10^{-2}	0.41	0.16	7.40×10^{-4}
2.30	2.26×10^{-2}	0.39	0.16	5.94×10^{-4}
2.45	2.68×10^{-2}	0.36	0.15	4.79×10^{-4}
2.60	2.53×10^{-2}	0.34	0.13	3.84×10^{-4}
2.75	2.79×10^{-2}	0.32	0.12	3.18×10^{-4}
2.90	3.00×10^{-2}	0.30	0.11	2.65×10^{-4}
3.05	2.63×10^{-2}	0.29	0.10	2.15×10^{-4}
3.20	2.75×10^{-2}	0.27	0.09	1.81×10^{-4}
3.35	2.57×10^{-2}	0.26	0.08	1.50×10^{-4}
3.50	2.25×10^{-2}	0.26	0.07	1.26×10^{-4}
3.75	1.28×10^{-2}	0.25	0.07	9.02×10^{-5}
4.00	3.12×10^{-2}	0.21	0.04	7.73×10^{-5}
4.25	6.41×10^{-3}	0.23	0.05	5.42×10^{-5}

4.50	4.29×10^{-3}	0.22	0.04	4.11×10^{-5}
4.75	2.08×10^{-2}	0.19	0.02	3.88×10^{-5}
5.00	3.11×10^{-2}	0.17	0.02	3.25×10^{-5}
5.50	0	0.18	0.06	1.30×10^{-5}

Table S4. Fitting parameters for complex 1.

Temperature (K)	χ_{adia} ($cm^3 \cdot mol^{-1}$)	$\chi iso1$ ($cm^3 \cdot mol^{-1}$)	$\chi iso2$ ($cm^3 \cdot mol^{-1}$)	$\alpha 1$	$\alpha 2$	$\tau 1$ (s)	$\tau 2$ (s)
1.85	0	0.51	1.41	0.32	0.59	0.34	4.39×10^{-5}
2.00	0	0.48	1.41	0.27	0.63	0.27	4.03×10^{-5}
2.15	0	0.52	1.36	0.26	0.65	0.22	3.41×10^{-5}
2.30	0	0.53	1.32	0.28	0.64	0.18	2.53×10^{-5}
2.45	0	0.52	1.29	0.28	0.62	0.17	1.98×10^{-5}
2.60	0	0.47	1.31	0.26	0.63	0.16	1.55×10^{-5}
2.75	0	0.44	1.30	0.28	0.62	0.14	1.19×10^{-5}
2.90	0	0.43	1.27	0.29	0.60	0.13	9.61×10^{-5}
3.05	0	0.42	1.25	0.30	0.58	0.12	7.37×10^{-6}
3.20	0	0.42	1.22	0.33	0.53	0.11	6.68×10^{-6}
3.35	0	0.37	1.22	0.30	0.53	0.10	5.31×10^{-6}
3.50	0	0.35	1.21	0.31	0.50	0.10	4.75×10^{-6}

Table S5. Fitting parameters for complex 2.

Temperature (K)	χ_{adia} ($cm^3 \cdot mol^{-1}$)	$\chi iso1$ ($cm^3 \cdot mol^{-1}$)	$\chi iso2$ ($cm^3 \cdot mol^{-1}$)	$\alpha 1$	$\alpha 2$	$\tau 1$ (s)	$\tau 2$ (s)
1.85	0	2.56	2.32	0.54	0.51	5.16×10^{-2}	1.82×10^{-6}
2.00	0	2.19	2.55	0.51	0.66	6.21×10^{-2}	8.47×10^{-7}
2.15	0	1.67	2.93	0.40	0.76	8.79×10^{-2}	1.04×10^{-6}
2.30	0	1.51	2.96	0.42	0.74	8.34×10^{-2}	8.74×10^{-7}
2.45	0	1.23	3.04	0.40	0.74	7.41×10^{-2}	7.53×10^{-7}
2.60	0	1.06	3.05	0.40	0.73	7.42×10^{-2}	6.14×10^{-7}
2.75	0	0.91	3.05	0.40	0.71	7.66×10^{-2}	5.47×10^{-7}
2.90	0	0.73	3.07	0.36	0.71	7.91×10^{-2}	4.63×10^{-7}
3.05	0	0.64	3.03	0.36	0.70	8.18×10^{-2}	4.11×10^{-7}
3.20	0	0.52	3.01	0.32	0.69	8.83×10^{-2}	3.47×10^{-7}
3.35	0	0.41	2.99	0.29	0.71	9.51×10^{-2}	1.93×10^{-7}
3.50	0	0.35	2.94	0.26	0.69	1.05×10^{-1}	2.09×10^{-7}

Table S6. Summary of some bonds length and distance in angstrom.

Complex	1	2	3
Ln–Ln	5.520	5.491	5.427
C5–C13	4.202	4.182	4.201
Ln–O1	2.359	2.340	2.297
Ln–O3	2.276	2.270	2.218
Ln–O4	2.290	2.251	2.174
Ln–O5	2.378	2.354	2.311
O2–O2	2.500	2.482	2.499
O6–O2	2.857	2.836	2.841
O6–O2	3.040	3.037	3.025