

Supplementary Materials: Metal-Organic Framework of Lanthanoid Dinuclear Clusters Undergoes Slow Magnetic Relaxation

Hikaru Iwami, Ryo Nakanishi, Yoji Horii, Keiichi Katoh, Brian K. Breedlove and Masahiro Yamashita

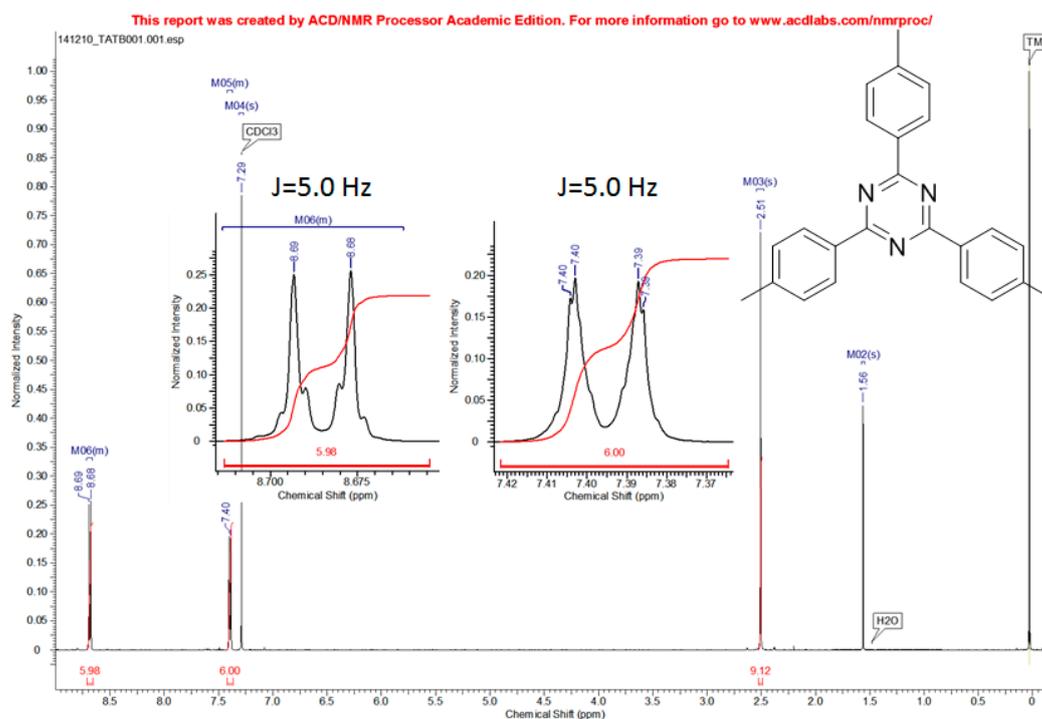


Figure S1. ^1H NMR spectrum of 2,4,6-tri-*p*-tolyl-1,3,5-triazine in CDCl_3 at 500 MHz on a Bruker AV-500 spectrometer.

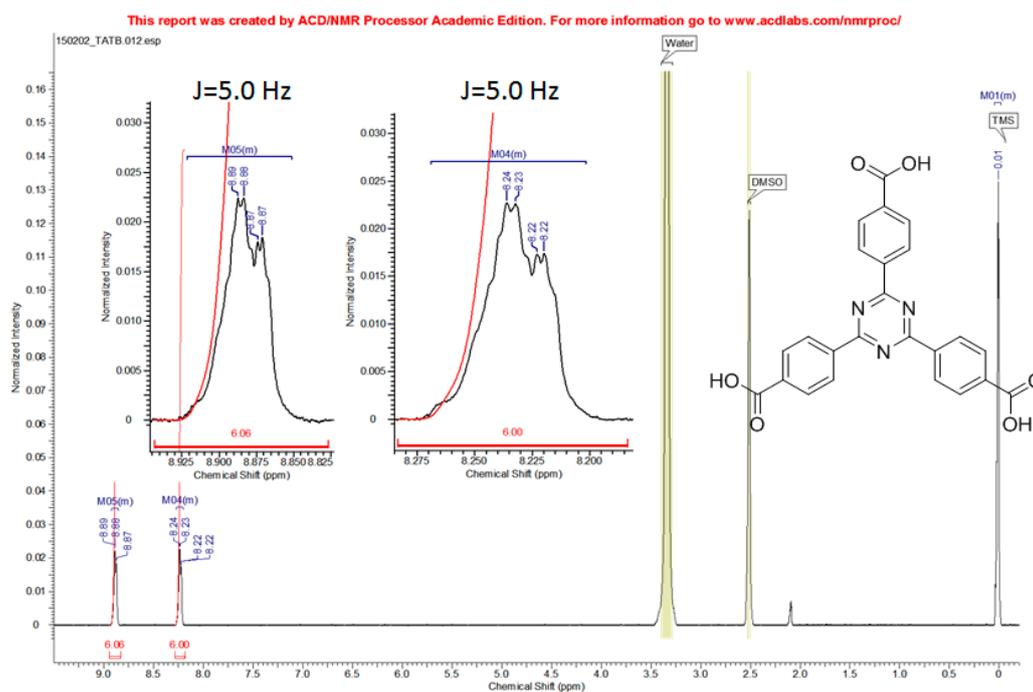


Figure S2. ^1H NMR spectrum of 4,4',4''-*s*-triazine-2,4,6-triyl-tribenzoic acid (H_3TATB) in CDCl_3 at 500 MHz on a Bruker AV-500 spectrometer.

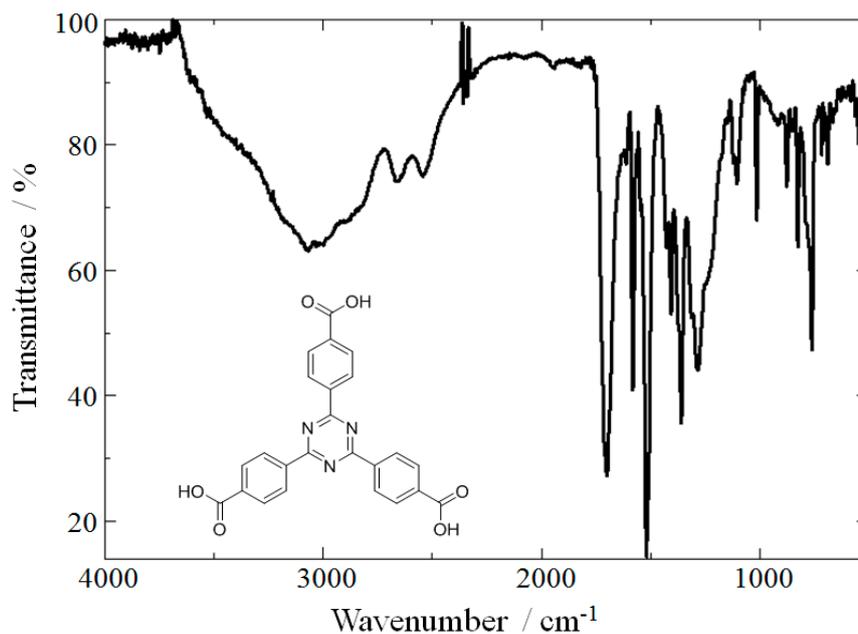


Figure S3. IR spectrum of H₃TATB.

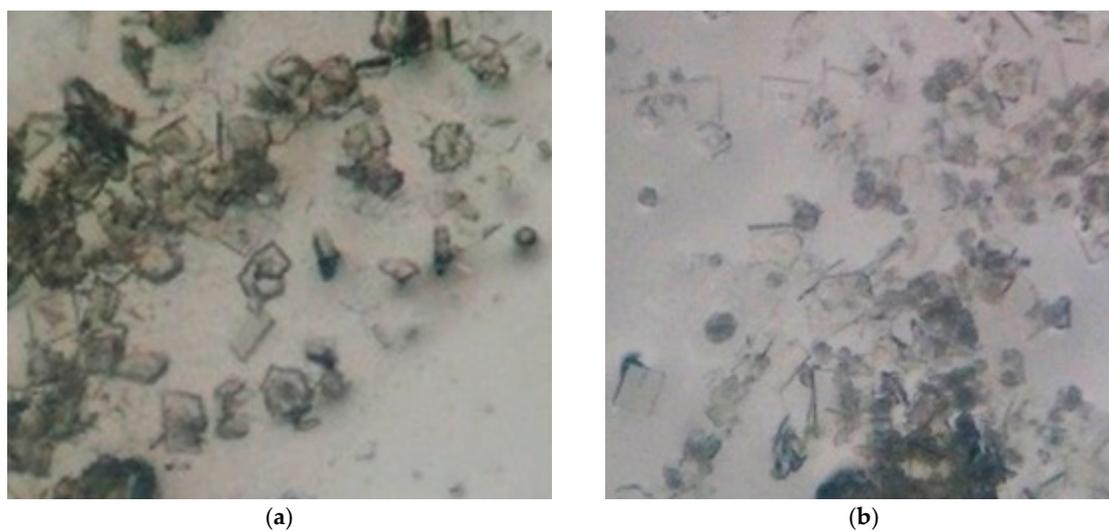


Figure S4. Obtained transparent crystals of (a) 1 and (b) 2.

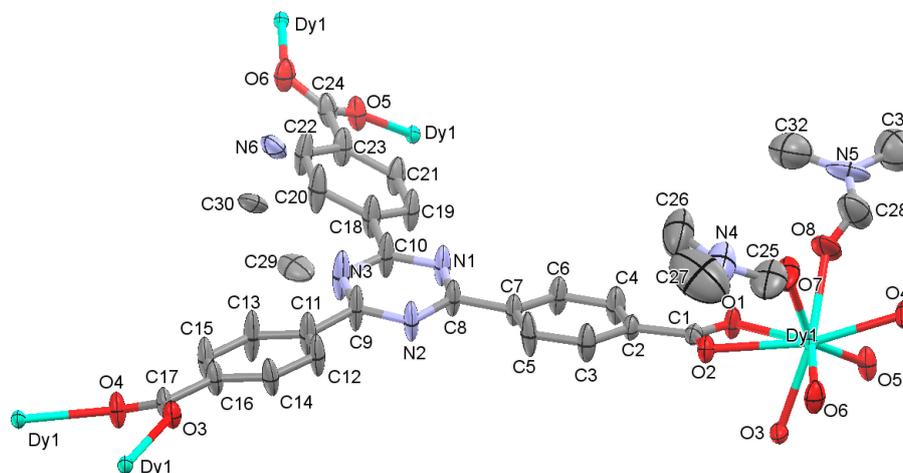


Figure S5. ORTEP drawing of asymmetric unit of 1 with thermal ellipsoid of 50% probability. Hydrogen atoms are omitted for clarity.

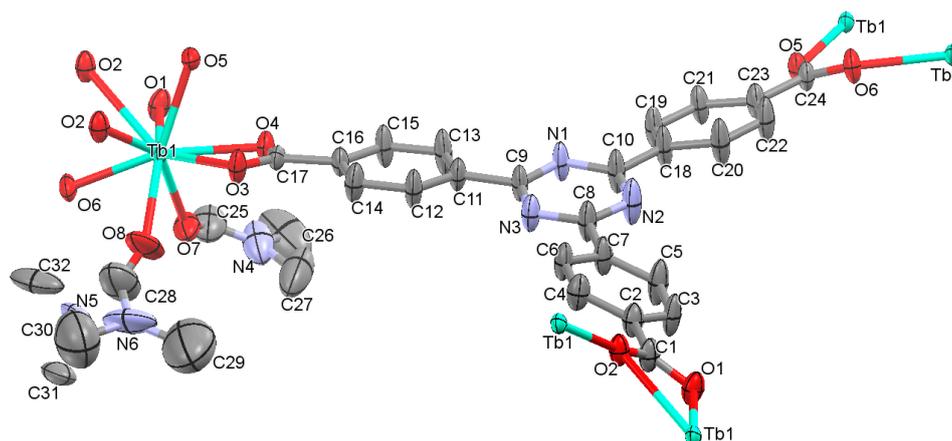


Figure S6. ORTEP drawing of asymmetric unit of **2** with thermal ellipsoid of 50% probability. Hydrogen atoms are omitted for clarity.

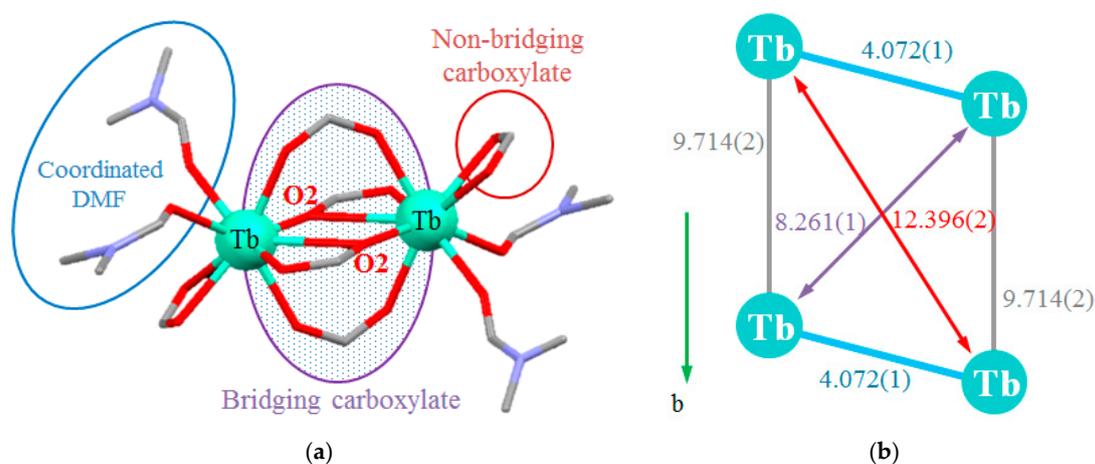


Figure S7. Drawings of (a) Tb(III) dinuclear clusters in **2**; and (b) their Tb-Tb distances. The unit of length is Å.

Table S1. Crystal structure parameters for **1** and **2**.

Compounds	1 [Dy(TATB)(DMF) ₂]	2 [Tb(TATB)(DMF) ₂]
Formula	C ₃₀ H ₂₆ N ₅ O ₈ Dy	C ₃₀ H ₂₆ N ₅ O ₈ Tb
Formula mass/g·mol ⁻¹	747.06	743.48
T/K	110	110
Crystal system	monoclinic	monoclinic
Space group	C2/c	C2/c
a/Å	33.138(10)	33.137(7)
b/Å	9.893(3)	9.7145(17)
c/Å	26.959(8)	27.314(6)
α/°	90	90
β/°	106.751(5)	107.642(3)
γ/°	90	90
V/Å ³	8463(4)	8379(3)
Z	8	8
R ₁ [<i>I</i> > 2s(<i>I</i>)] ^a	0.0476	0.0461
ωR ₂ (all) ^b	0.1328	0.1237
GoF on F ²	1.011	1.098
CCDC number	151,5211	1,516,111

$${}^a R_1 = \frac{\sum(F_0 - F_c)}{\sum F_0}; \quad {}^b wR_2 = \sqrt{\frac{\sum[w(F_0^2 - F_c^2)]}{\sum[w(F_0^2)^2]}}$$

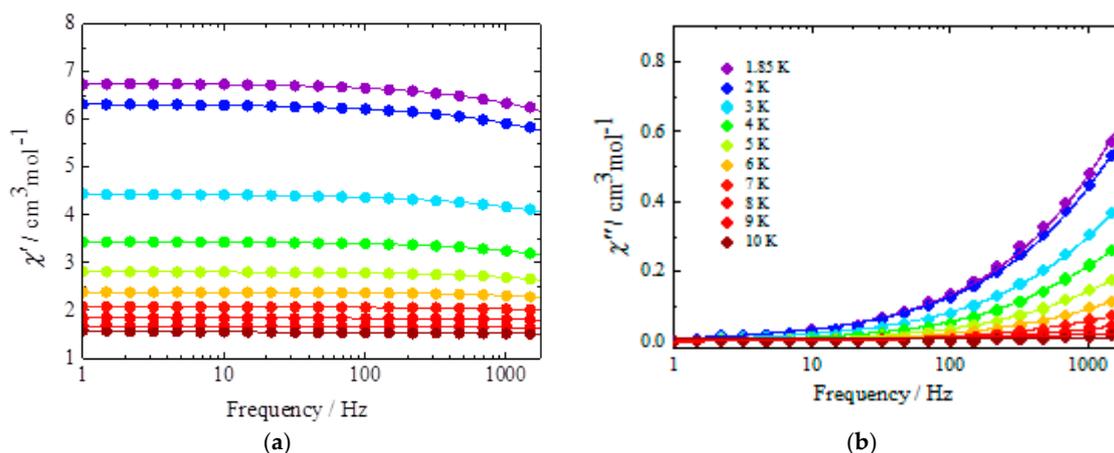


Figure S8. Frequency dependences of the (a) χ' and (b) χ'' AC magnetic susceptibilities of **1** in an H_{DC} of 0 Oe. The measurements were performed in an H_{AC} of 3 Oe and T range of 10–1.85 K.

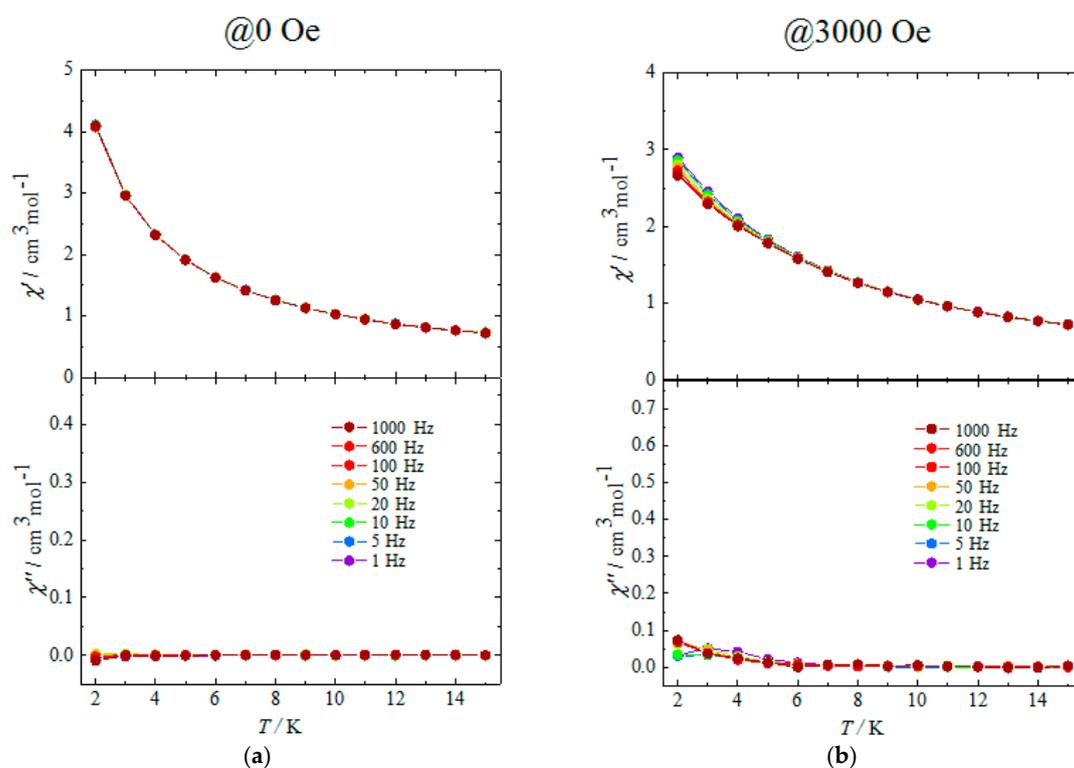


Figure S9. Temperature dependences of the χ' and χ'' AC magnetic susceptibilities of **2** in H_{DC} of (a) 0 and (b) 3000 Oe. The measurements were performed in an H_{AC} of 3 Oe and T range of 10–1.85 K.

The Generalized Debye Model (Equations (S1) and (S2))

$$\chi'(\omega) = \chi_S + (\chi_T - \chi_S) \frac{1 + (\omega\tau)^{1-\alpha} \sin(\pi\alpha/2)}{1 + 2(\omega\tau)^{1-\alpha} \sin(\pi\alpha/2) + (\omega\tau)^{2-2\alpha}} \quad (\text{S1})$$

$$\chi''(\omega) = (\chi_T - \chi_S) \frac{(\omega\tau)^{1-\alpha} \cos(\pi\alpha/2)}{1 + 2(\omega\tau)^{1-\alpha} \sin(\pi\alpha/2) + (\omega\tau)^{2-2\alpha}} \quad (\text{S2})$$

where χ_S is the adiabatic susceptibility, χ_T is the isothermal susceptibility, $\omega = 2\pi\nu$, (ν is the frequency) is the angular frequency, τ is the magnetization relaxation time, and α is the quantitative parameter for the width of the τ distribution.

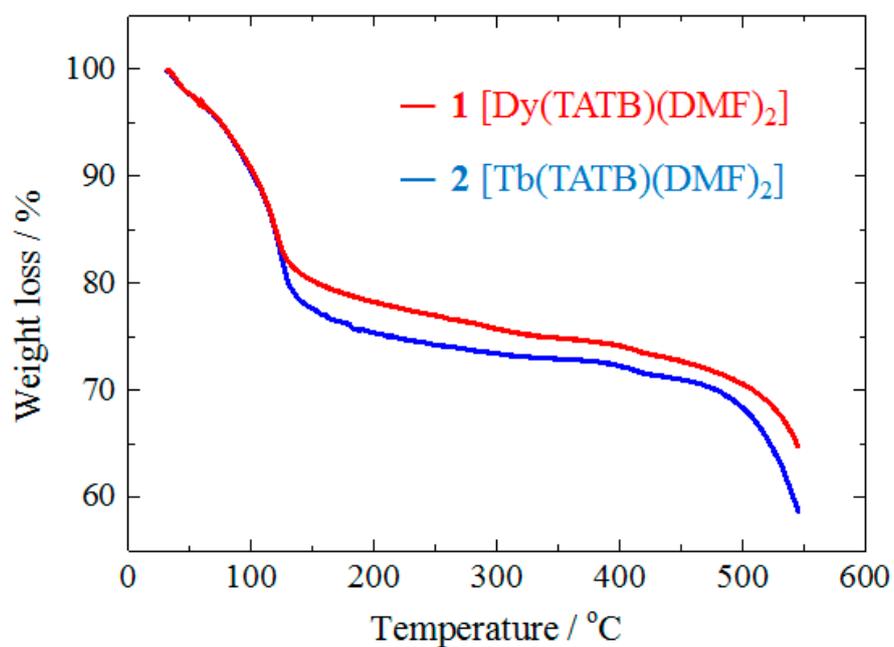


Figure S10. Thermogravimetric analyses of 1 and 2.

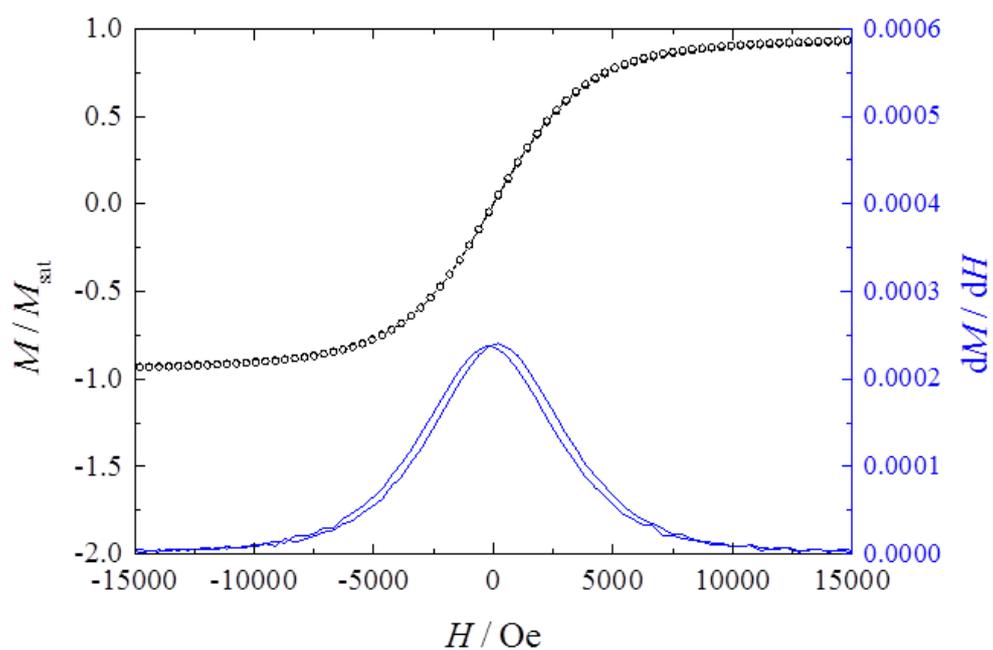


Figure S11. Field dependence of the magnetization of 1 at 1.8 K. Slight hysteresis was observed.