Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Single Molecule Magnets with *m*-Fluorobenzoate and Difluoromethylacetate as Polar Ligands

Norihisa Hoshino, Takuya Shiga, Hiroki Oshio and Tomoyuki Akutagawa

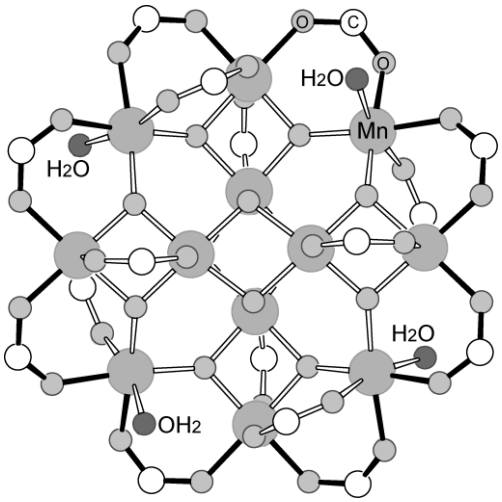

Figure S1. Coordination scheme of $[Mn_{12}O_{12}(CHF_2COO)_{16}(H_2O)_4]$ (**1**). Four coordination sites of H_2O ligands are labeled. $-CHF_2$ groups are omitted for clarity.

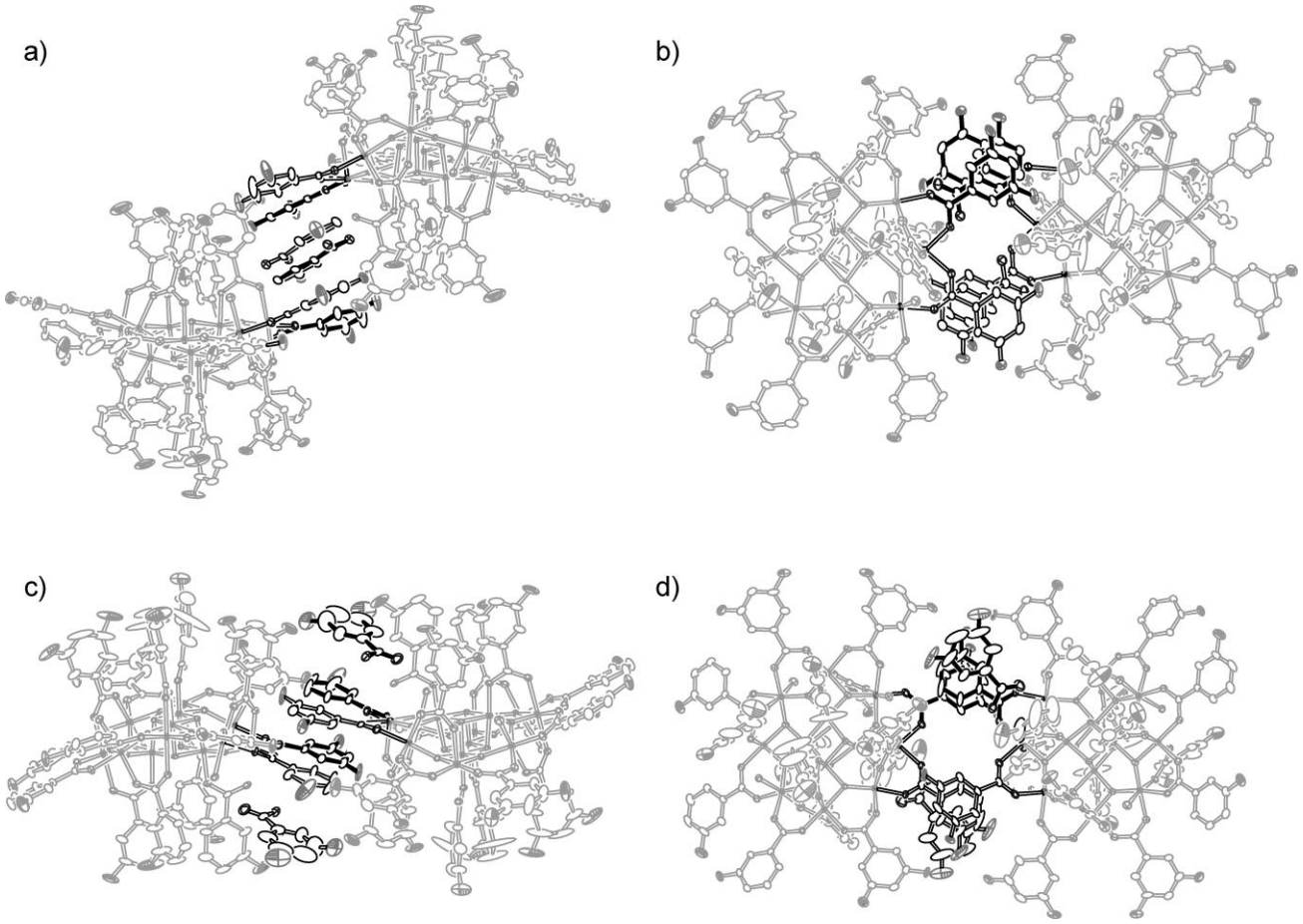

Figure S2. ORTEP diagrams of intermolecular π-trimer structures of crystal **2**. a) Side view and b) top view of π-trimers in which neutral *m*-FPhCOOH molecules were inserted between neighboring equatorial *m*-FPhCOO$^-$ ligands. c) Side view and d) top view in which neutral *m*-FPhCOOH molecules were attached on the π-dimers of *m*-FPhCOO$^-$ ligands.

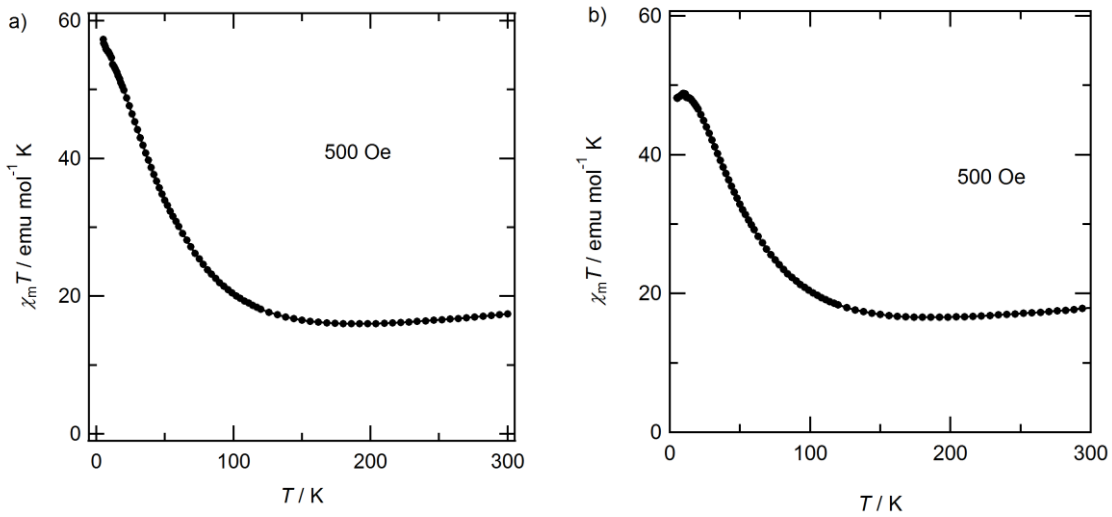

Figure S3. $\chi_m T$ *vs*. temperature (T) plots for (a) crystals **1** and (b) **2**.

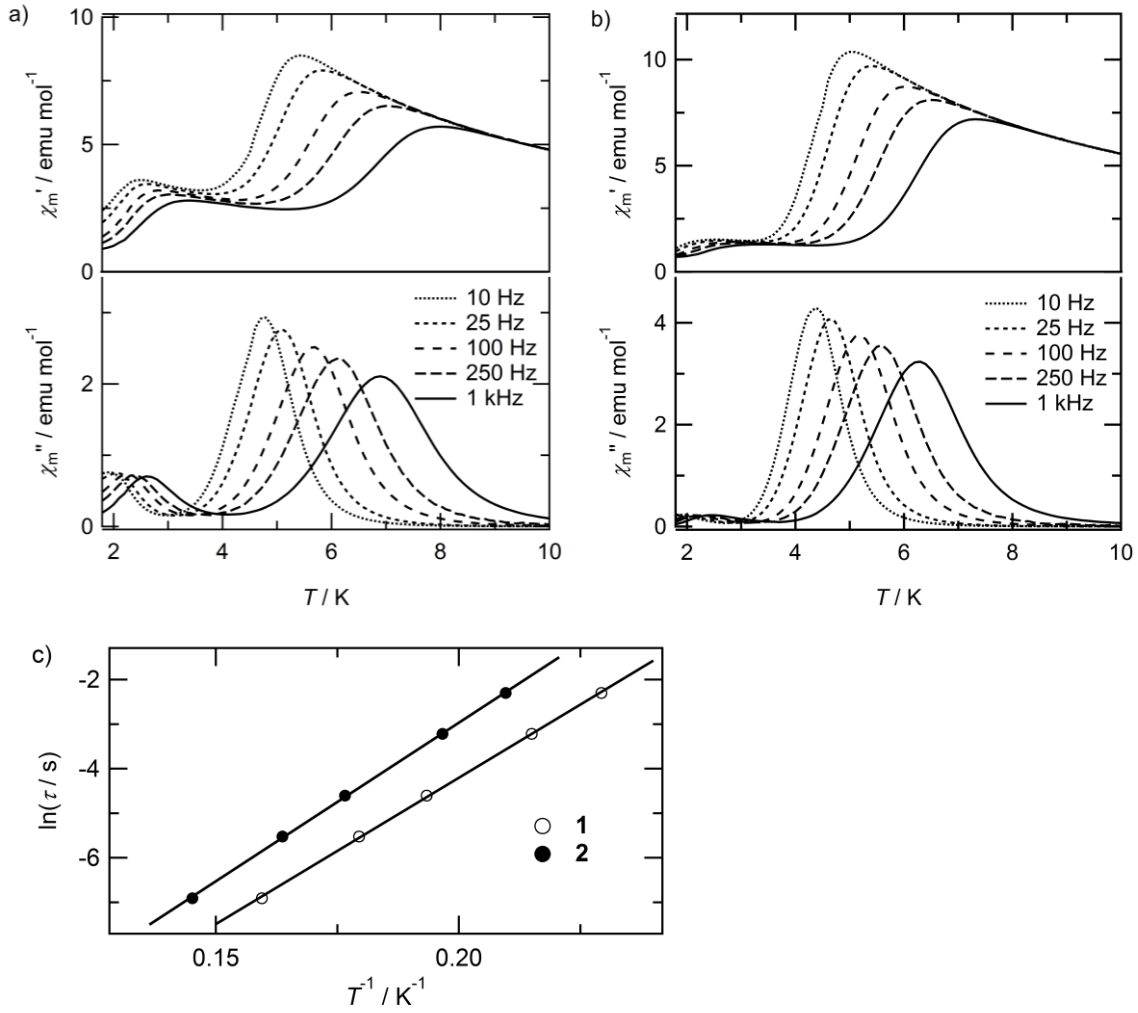

Figure S4. χ' (in-phase) and χ" (out-of-phase) *vs*. temperature (T) plots for (a) crystals **1** and (b) **2**. (c) Arrhenius plots for **1** and **2**.

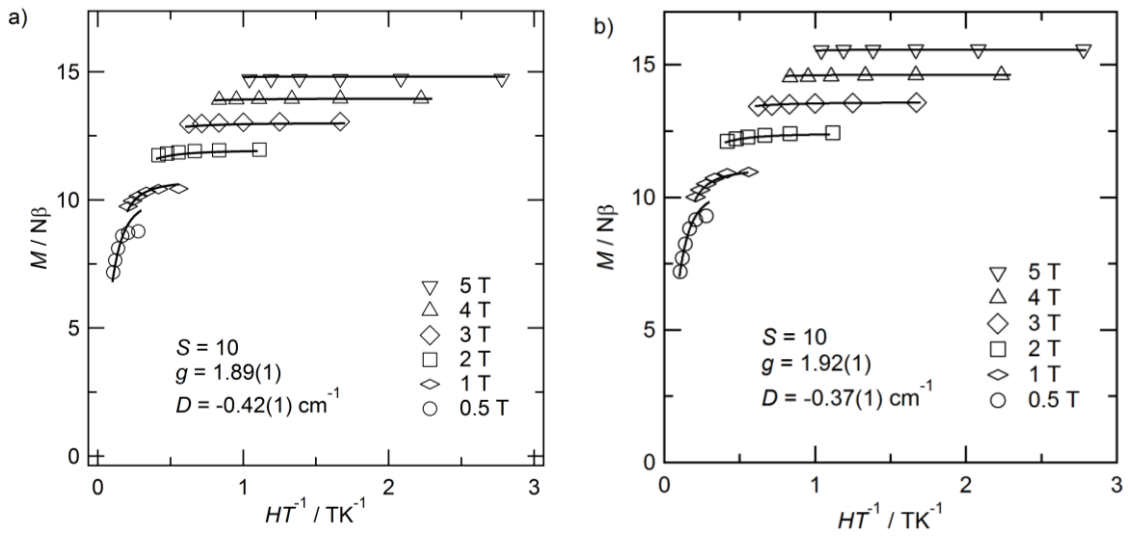

Figure S5. Temperature- and frequency-dependent magnetization for (a) crystals **1** and (b) **2**.

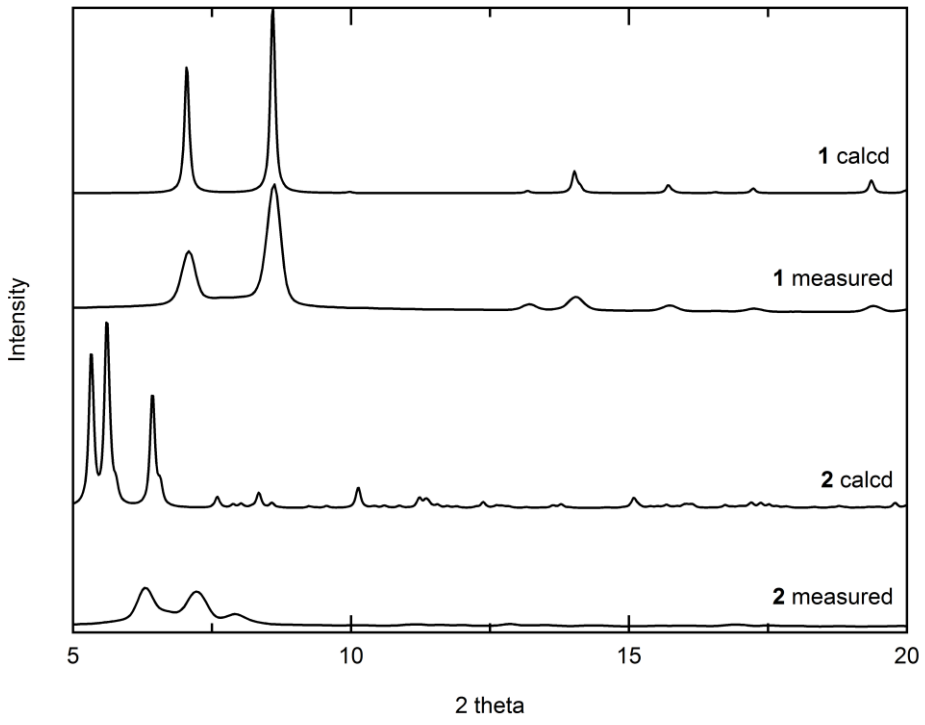

Figure S6. Powder X-ray data for the granule sample of **1** and **2** at 100 K.

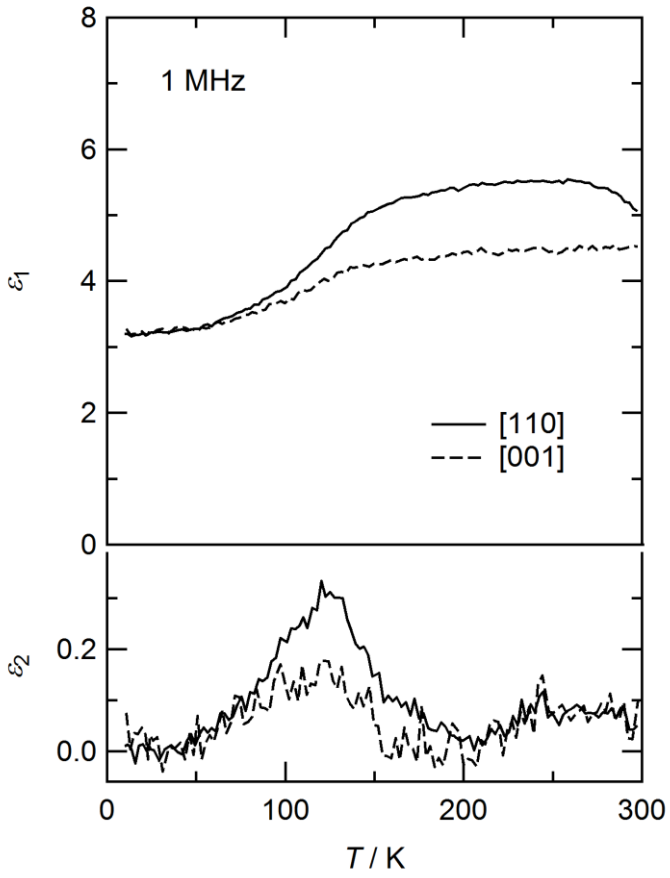

Figure S7. Temperature-dependent dielectric constants of single crystal **1**. Electric field was applied along [110] or [001] using gold paste. The sizes of crystals were (3.06 x 0.46 x 0.40 mm) for the measurement along [110] and (0.33 x 0.36 x 0.38 mm) for [001]. ε_1 values were normalized with the value of compressed pellet (Fig. 6) at 10 K, because of too small dielectric capacitances for determination of accurate absolute values.