Supporting Information

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

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Figure S1. Coordination scheme of \([\text{Mn}_{12}\text{O}_{12}(\text{CHF}_2\text{COO})_{16}(\text{H}_2\text{O})_4]\) (1). Four coordination sites of \(\text{H}_2\text{O}\) ligands are labeled. –\(\text{CHF}_2\) 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.** $\chi'$ (in-phase) and $\chi''$ (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.
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]. $\varepsilon_1$ 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.