

Supporting Information

Chiral weak ferromagnets formed in one-dimensional organic-inorganic hybrid manganese chloride hydrates

Kouji Taniguchi*^{1,2}, Po-Jung Huang³, Shojiro Kimura³, and Hitoshi Miyasaka³

¹*Department of Chemistry, School of Science, Tokyo Institute of Technology, 2-12-1 Ookayama, Tokyo, 152-8551, Japan*

²*PRESTO, Japan Science and Technology Agency (JST), 5-3 Yonbancho, Chiyoda-ku, Tokyo 102-8666, Japan*

³*Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Sendai, 980-8577, Japan*

Corresponding author*

Kouji Taniguchi

Department of Chemistry, School of Science, Tokyo Institute of Technology, 2-12-1 Ookayama, Tokyo, 152-8551, Japan

E-mail: taniguchi.k.ap@m.titech.ac.jp

Table S1**Crystallographic Data for S-1.**

Compound	(S- β -MePhC ₂ H ₃ NH ₃) ₂ MnCl ₄ (H ₂ O)
Empirical formula	C ₁₈ H ₃₀ Cl ₄ MnN ₂ O
Formula weight	487.18
Temperature/K	103
Crystal system	monoclinic
Space group	<i>P</i> 2 ₁ (#4)
a/Å	17.5072(5)
b/Å	7.27776(19)
c/Å	17.6298(7)
α /°	90
β /°	90.488(3)
γ /°	90
Volume/Å ³	2246.19(12)
Z	4
ρ_{calc} /g cm ⁻³	1.441
<i>F</i> ₀₀₀	1012.00
λ /Å	0.71073
μ (Mo K α)/cm ⁻¹	1.073
measured reflections	7764
unique reflections	9912 (<i>R</i> _{int} = 0.0278)
<i>R</i> ₁ (<i>I</i> > 2.00 σ (<i>I</i>))	0.0334
<i>R</i> ₁ (all data)	0.0385
<i>wR</i> ₂ (all data),	0.0783
GOF	1.021
Flack parameter	-0.002(13)
CCDC	2190484

Table S2**Crystallographic Data for R-1.**

Compound	(<i>R</i> - β -MePhC ₂ H ₃ NH ₃) ₂ MnCl ₄ (H ₂ O)
Empirical formula	C ₁₈ H ₃₀ Cl ₄ MnN ₂ O
Formula weight	487.18
Temperature/K	103
Crystal system	monoclinic
Space group	<i>P</i> 2 ₁ (#4)
<i>a</i> /Å	17.5439(4)
<i>b</i> /Å	7.2896(2)
<i>c</i> /Å	17.6559(5)
α /°	90
β /°	90.502(2)
γ /°	90
Volume/Å ³	2257.89(10)
<i>Z</i>	4
ρ_{calc} /g cm ⁻³	1.433
<i>F</i> ₀₀₀	1012
λ /Å	0.71073
μ (Mo K α)/cm ⁻¹	1.068
measured reflections	33573
unique reflections	11472 (<i>R</i> _{int} = 0.0427)
<i>R</i> ₁ (<i>I</i> > 2.00 σ (<i>I</i>))	0.0307
<i>R</i> ₁ (all data)	0.0398
<i>wR</i> ₂ (all data),	0.0644
GOF	1.009
Flack parameter	-0.016(9)
CCDC	2190483

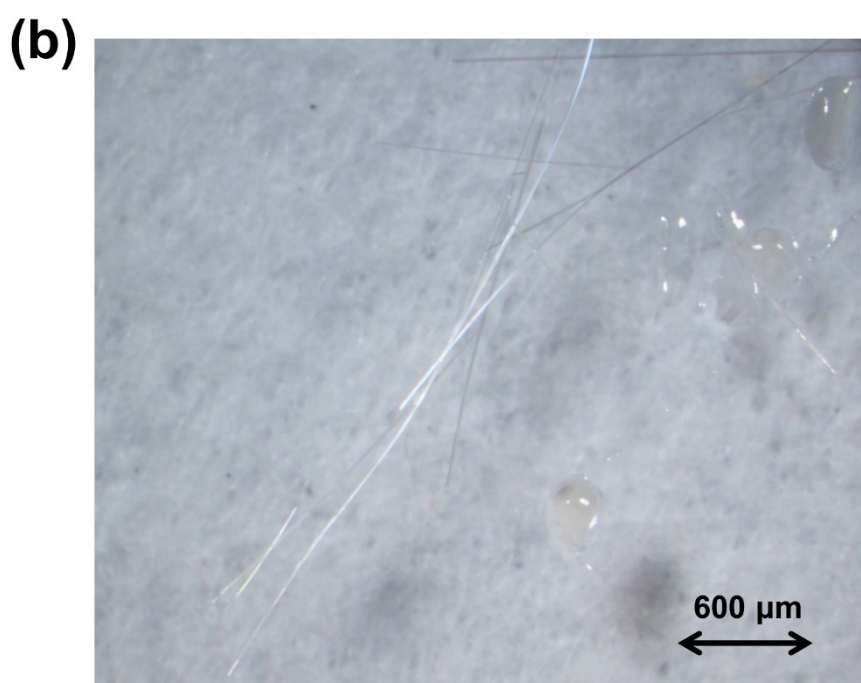
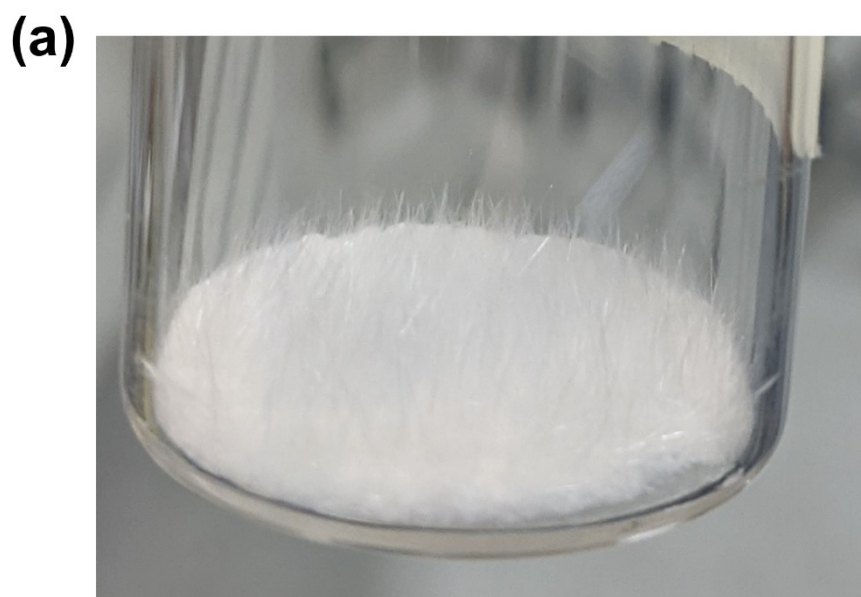


Figure S1. The picture of *R-1* crystals. (a) As grown crystals, (b) Expanded picture of needle like *R-1* crystals.

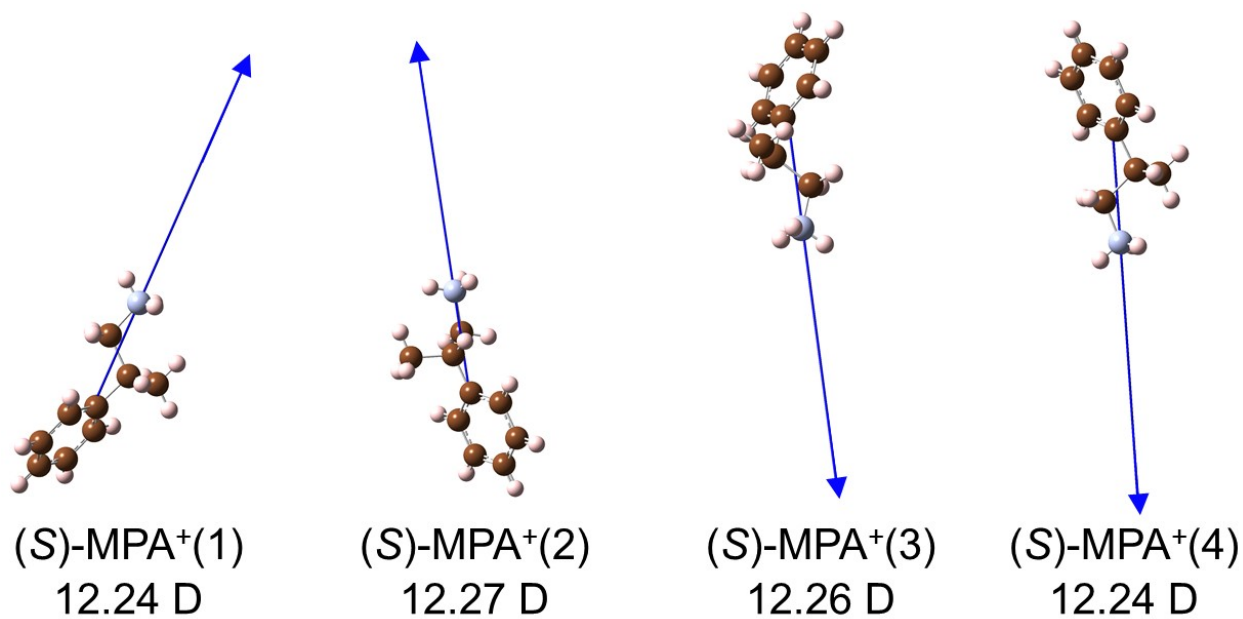


Figure S2. Calculated electric dipole moments of (S)-MPA⁺ ions in the unit cells of **S-1**. The blue arrows indicate the direction of electric dipole moments. The structures of molecular cations are displayed with color codes C (brown), N (grey), H (pale pink).

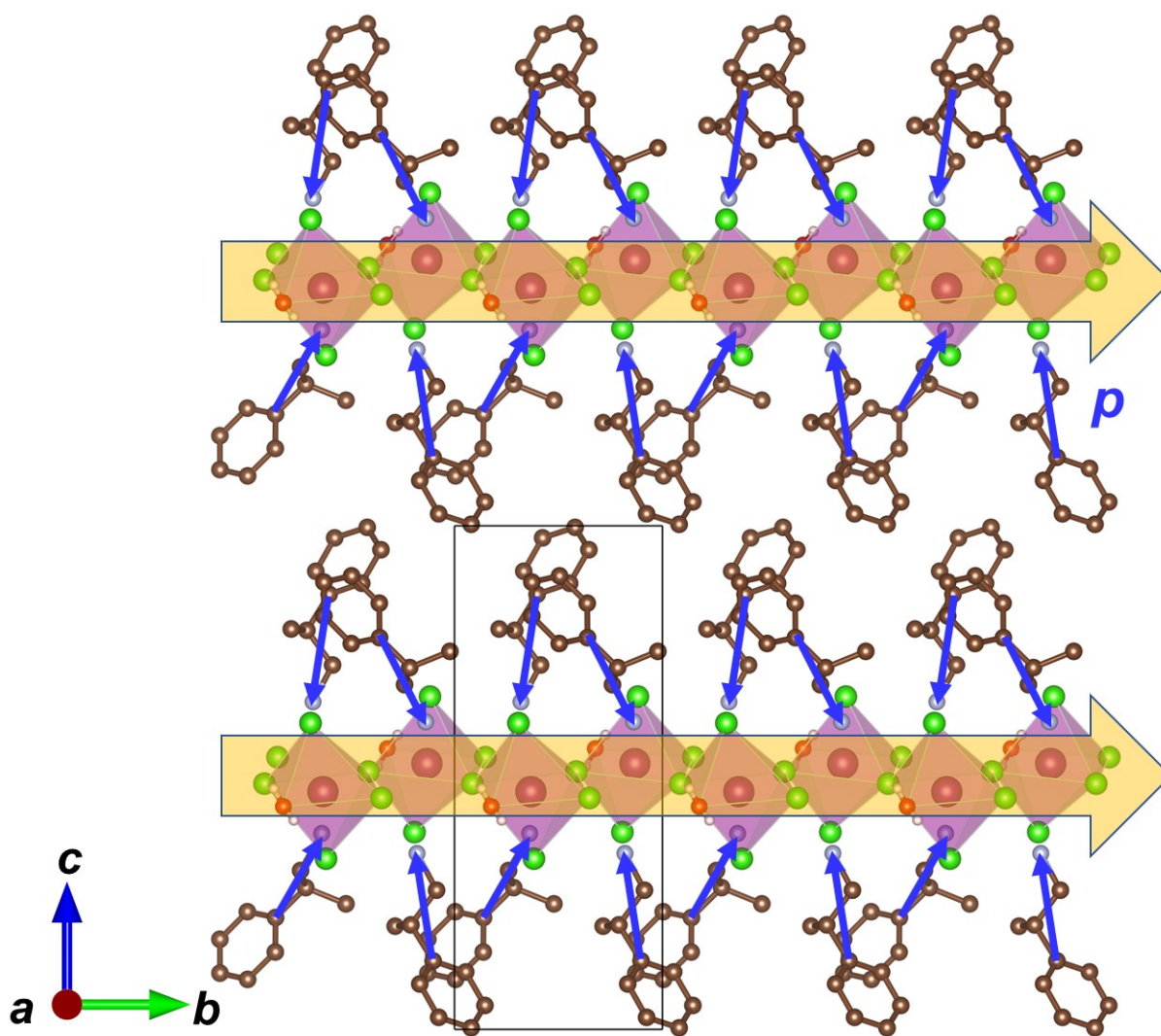


Figure S3. Arrangement of electric dipole moments of (*S*)-MPA⁺ ions in crystal structures of **S-1**. The small blue arrows and the large transparent orange arrows represent electric dipole moments (*p*) of (*S*)-MPA⁺ and electric polarization of each 1D-chain of manganese chloride hydrates from molecule components of **S-1**. The crystal structure of **S-1** projected along the [100] is displayed with color codes Mn (purple), Cl (yellowish green), C (brown), N (grey). Hydrogen atoms are omitted except for those in H₂O for clarity.

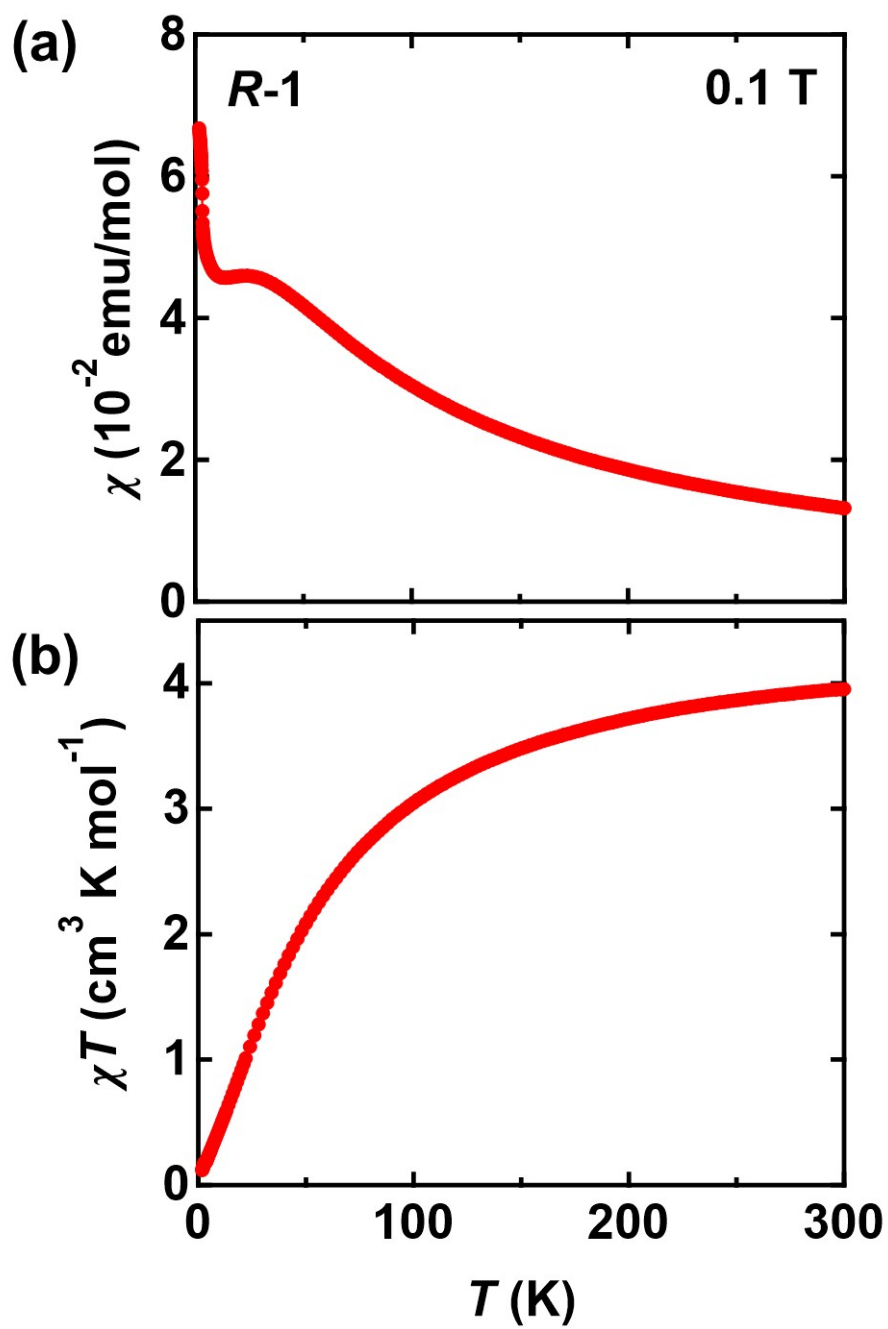


Figure S4. (a) Temperature dependence of magnetic susceptibility (χ) of $R-1$ in 0.1 T. (b) Temperature dependences of χT for $R-1$.

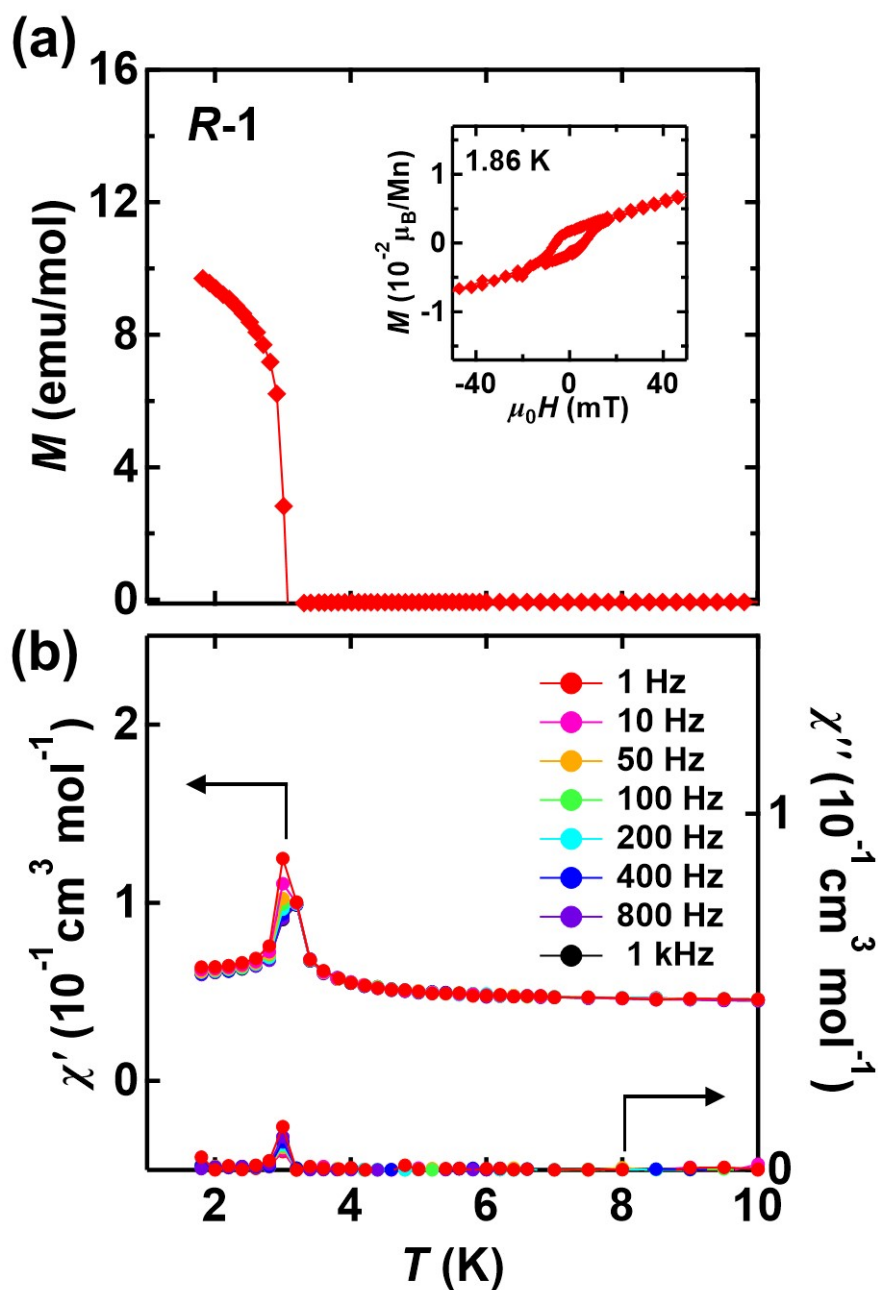


Figure S5. (a) Temperature dependence of the remnant magnetization of *R-1*. The inset shows magnetic field dependence of magnetization of *R-1* at 1.86 K. (b) Temperature dependence of AC susceptibility of *R-1*.