

Supplementary Tables and Figures

Ferrimagnetic structures with rare-earth induced spin-reorientation in the Mn self-doped perovskite (Er_{0.7}Mn_{0.3})MnO₃

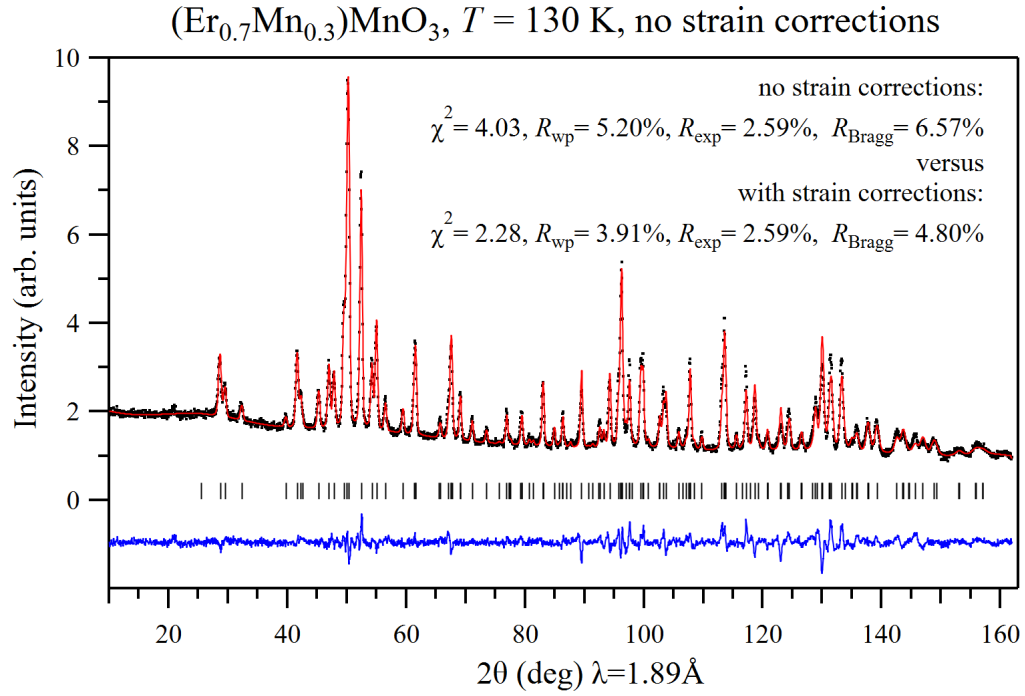
Andreas Dönni, Vladimir Y. Pomjakushin, Martin Rotter, Lei Zhang, Kazunari Yamaura, Alexei A. Belik

Supplementary Table S1. Energy levels of the crystal field (CF) splitting of Er³⁺ in (Er_{0.7}Mn_{0.3})MnO₃ and (Er_{0.8}Mn_{0.2})MnO₃ based on the point charge model, calculated by McPhase.

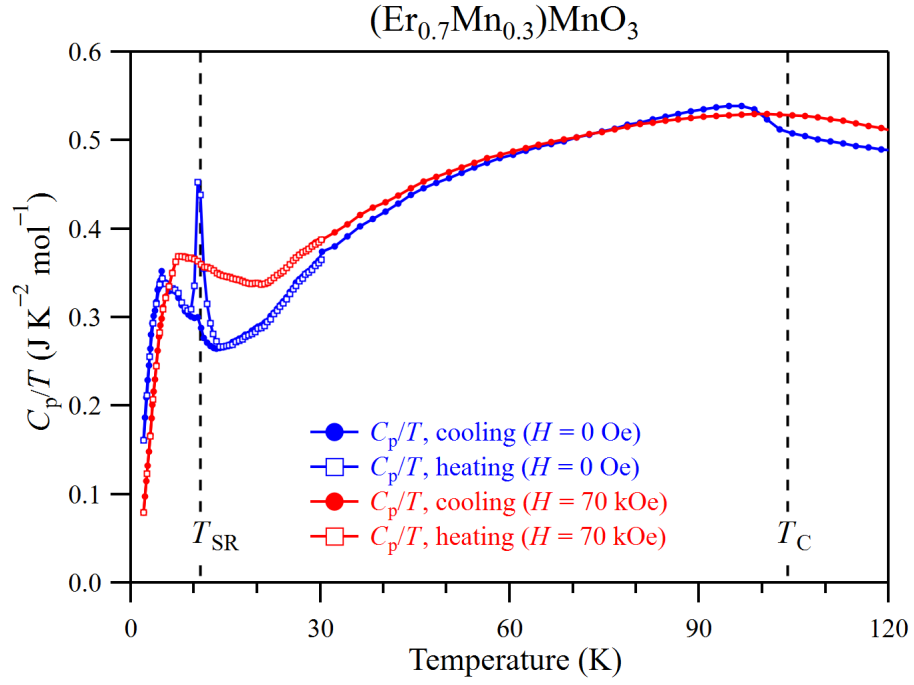
Number of CF level	(Er _{0.7} Mn _{0.3})MnO ₃		(Er _{0.8} Mn _{0.2})MnO ₃	
	Er ³⁺ energy (meV)		Er ³⁺ energy (meV)	
16	23.72	36.96(39)	23.25	36.36(39)
15	23.72	36.96(39)	23.25	36.36(39)
14	12.63	25.87(25)	12.36	25.48(23)
13	12.63	25.87(25)	12.36	25.48(23)
12	4.12	17.36(20)	3.63	16.75(16)
11	4.12	17.36(20)	3.63	16.75(16)
10	-0.70	12.54(25)	-0.99	12.13(27)
9	-0.70	12.54(25)	-0.99	12.13(27)
8	-6.54	6.70(16)	-6.13	6.99(17)
7	-6.54	6.70(16)	-6.13	6.99(17)
6	-9.69	3.55(25)	-8.76	4.36(32)
5	-9.69	3.55(25)	-8.76	4.36(32)
4	-10.32	2.92(27)	-10.24	2.88(13)
3	-10.32	2.92(27)	-10.24	2.88(13)
2	-13.24	0.00(0)	-13.12	0.00(0)
1	-13.24	0.00	-13.12	0.00

Supplementary Table S2. Induced magnetic Er^{3+} moments in $(\text{Er}_{0.8}\text{Mn}_{0.2})\text{MnO}_3$ at $T = 1$ K in an external magnetic field of $H = 10$ T applied along the three axes a , b , c calculated by McPhase. Uncertainties due to the experimental errors in the crystal-structural parameters were evaluated using gauss law of error propagation and are shown in parentheses only for Er_{11} for simplicity.

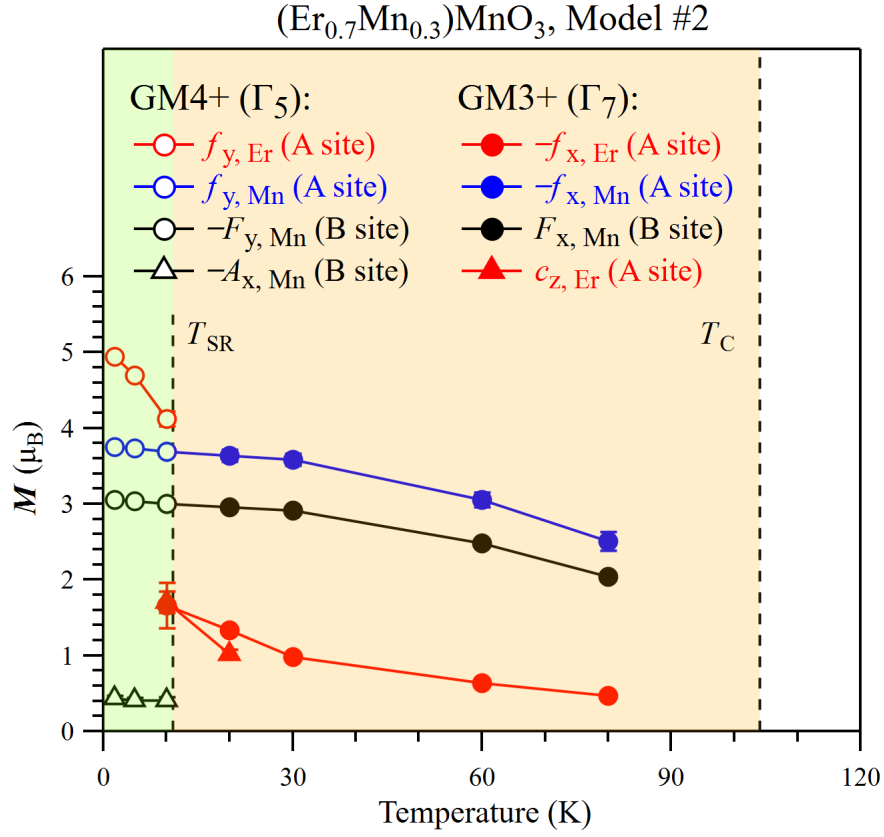
$H \parallel a$	$\langle M_a \rangle$	$\langle M_b \rangle$	$\langle M_c \rangle$	$\langle M \rangle$
Er_{11}	3.112(755)	0(0)	-1.795(210)	3.592(763)
Er_{12}	3.112	0	1.795	3.592
Er_{13}	3.112	0	-1.795	3.592
Er_{14}	3.112	0	1.795	3.592
$H \parallel b$	$\langle M_a \rangle$	$\langle M_b \rangle$	$\langle M_c \rangle$	$\langle M \rangle$
Er_{11}	0(0)	8.269(33)	0(0)	8.269(33)
Er_{12}	0	8.269	0	8.269
Er_{13}	0	8.269	0	8.269
Er_{14}	0	8.269	0	8.269
$H \parallel c$	$\langle M_a \rangle$	$\langle M_b \rangle$	$\langle M_c \rangle$	$\langle M \rangle$
Er_{11}	-0.838(43)	0(0)	5.765(168)	5.826(172)
Er_{12}	0.838	0	5.765	5.826
Er_{13}	-0.838	0	5.765	5.826
Er_{14}	0.838	0	5.765	5.826



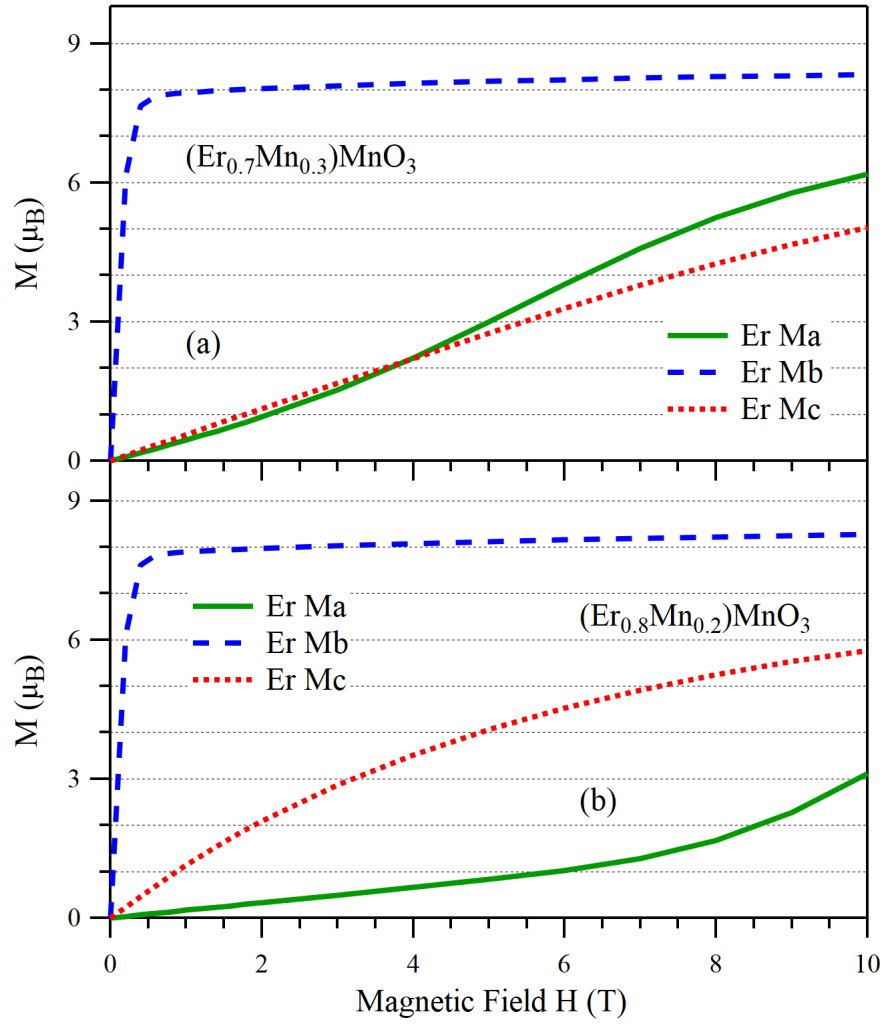
Supplementary Fig. S1. Experimental (black dots), calculated (red line), and difference (blue line) neutron diffraction pattern of $(\text{Er}_{0.7}\text{Mn}_{0.3})\text{MnO}_3$ in the paramagnetic state at $T = 130$ K. No corrections for strain effects were used. The tick marks indicate Bragg peak positions of the crystal structure. Resultant R and χ^2 values with and without strain corrections are given.



Supplementary Fig. S2. Temperature dependence of specific heat C_p/T of $(\text{Er}_{0.7}\text{Mn}_{0.3})\text{MnO}_3$ measured on cooling (filled symbols) and heating (empty symbols) at magnetic fields $H = 0$ Oe and $H = 70$ kOe. The vertical dashed lines indicate the FiM phase transition at $T_{\text{C}} = 104$ K and the Spin-reorientation temperature at $T_{\text{SR}} = 11$ K at zero field.



Supplementary Fig. S3. Temperature dependence of the ordered Mn and Er moments of (Er_{0.7}Mn_{0.3})MnO₃ based on Model #2. The vertical dashed lines indicate the FiM phase transition at $T_C = 104$ K and the Spin-reorientation temperature at $T_{SR} = 11$ K.



Supplementary Fig. S4. Field dependence of the single-ion magnetization in an external magnetic field applied along the a -, b - and c -axes for Er^{3+} in $(\text{Er}_{0.7}\text{Mn}_{0.3})\text{MnO}_3$ (a) and $(\text{Er}_{0.8}\text{Mn}_{0.2})\text{MnO}_3$ (b) at $T = 1$ K calculated by McPhase.