

Supplementary material for:

Ferrimagnetic and spin glass behavior in the $\text{SrMn}^{2+}_3\text{Ti}^{4+}_{14}M^{3+}_4\text{O}_{38}$ ($M = \text{Ti}$ and Fe) synthetic crichtonites.

José Luis Rosas Huerta,^{*a} Ruiqi Chen,^{a,b} Clemens Ritter,^c Oleg Siidra,^b Marie Colmont^a, Angel M. Arevalo-Lopez^{*a}

^a. Unité de Catalyse et Chimie du Solide (UCCS) - UMR CNRS 8181, Université de Lille - Centrale Lille, Université Artois, ENSCL, Lille, F-59000, France.

^b. Department of Crystallography, Institute of Earth Sciences, St. Petersburg State University, University emb. 7/9, 199034, St. Petersburg, Russia.

^c. Institut Laue-Langevin, BP 156, 38042 Grenoble Cedex, France.

* corresponding author: joseluis.rosashuerta@univ-lille.fr, angel.arevalo-lopez@univ-lille.fr

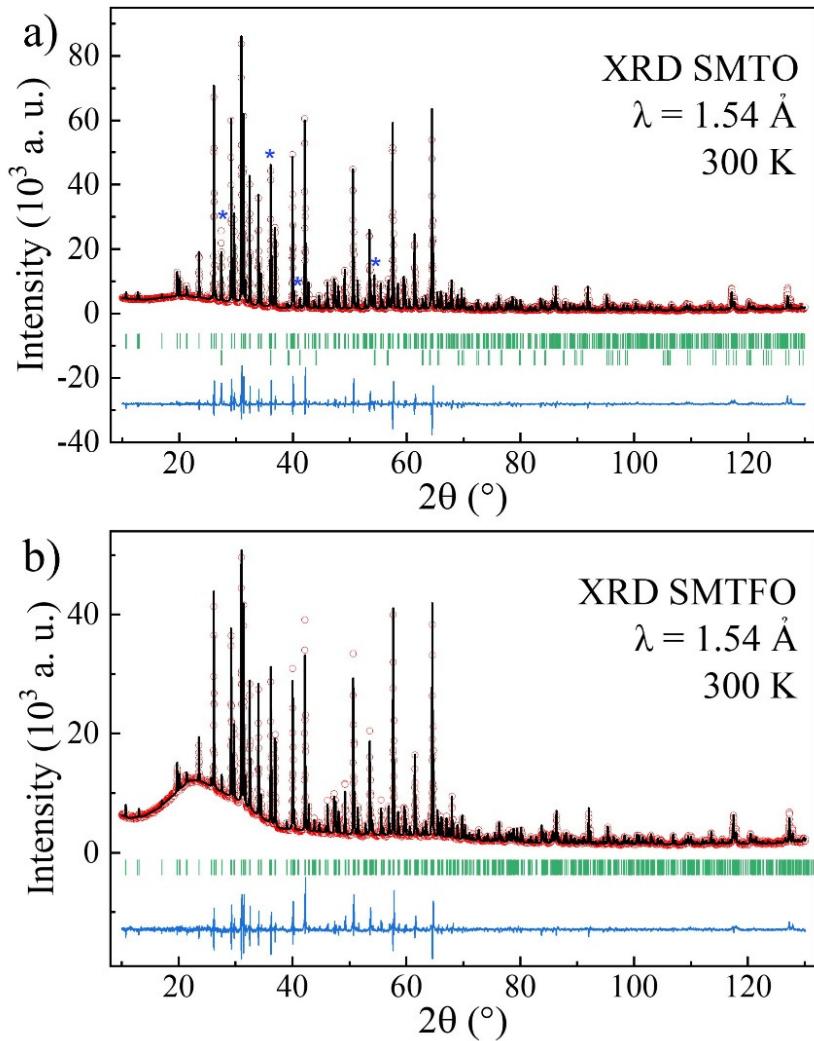


Figure S1. Rietveld refinement to the XRD ($\lambda = 1.54 \text{ \AA}$) at room temperature of a) SMTO and b) SMTFO compounds. The red empty circles, black and blue lines and vertical bars are the observed data, fitted, difference and Bragg reflections, respectively. Blue asterisks in a) SMTO indicate the main peaks of unreacted TiO_2 (7.2(4) % wt). R_{wp} (%) = 10.5 and 6.67; R_{Bragg} (%) = 9.47 and 11.2; R_{exp} (%) = 2.86 and 2.43; χ^2 (%) = 13.4 and 7.5, for SMTO and SMTFO respectively.

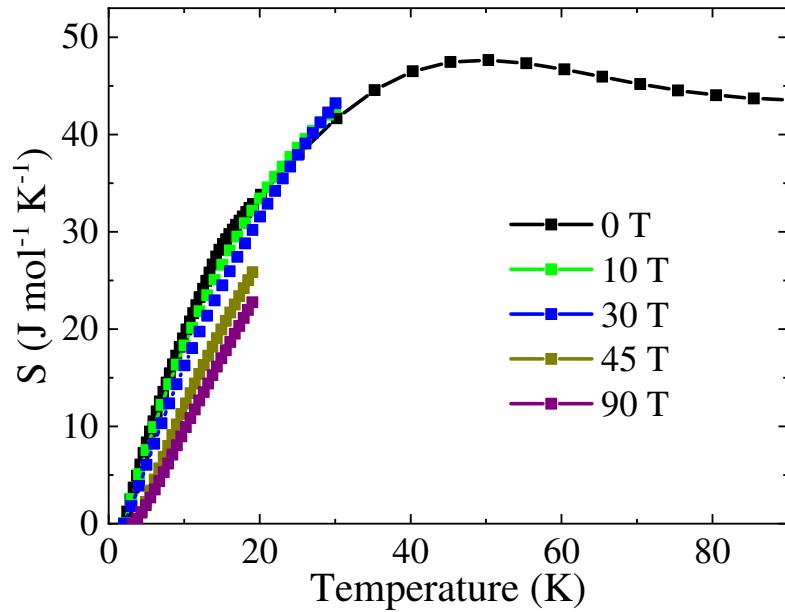


Figure S2. Magnetic entropy contribution in SMTO as function of the applied field. It was obtained by integrating the heat magnetic capacity divided by temperature ($C_m(T)/T$) after remove the phonon entropy contribution (C_p , red line in Fig. 2c). C_p contribution is acquired in the high temperature interval, this was modeled by the Debye and Einstein equation:

$$C_{\text{lat}} = 9C_D N k_B \left(\frac{T}{\theta_D}\right)^3 \int_{\theta_D/T}^0 \frac{x^4 e^x}{(e^x - 1)^2} dx + 3Nk_B C_E \left(\frac{\theta_E}{T}\right)^2 \frac{e^{\theta_E/T}}{(e^{\theta_E/T} - 1)^2}$$

where N is Avogadro's number (6.023×10^{23} mol⁻¹), C_D , θ_D and C_E , θ_E are the weighting factor and Debye/Einstein temperature, respectively, In the fitting performed were found the values $\theta_D=330(2)$ K, $\theta_E=697(3)$ K, $C_D=0.7347$ and $C_E=5$.

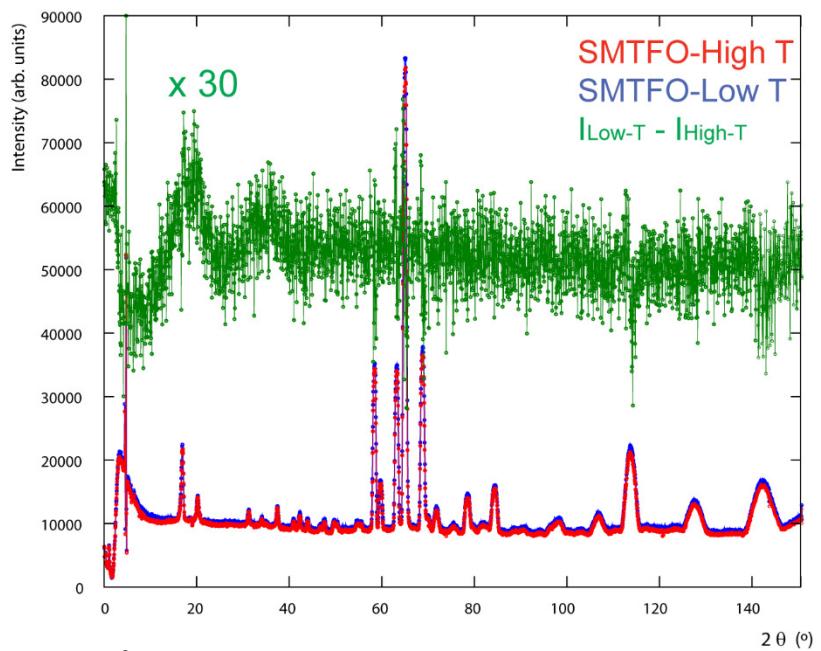


Figure S3. HR ($\lambda = 2.41 \text{ \AA}$) NPD at high (red line) and low (blue line) temperature for the SMTFO compound. The difference is shown multiplied by 30 in green line.

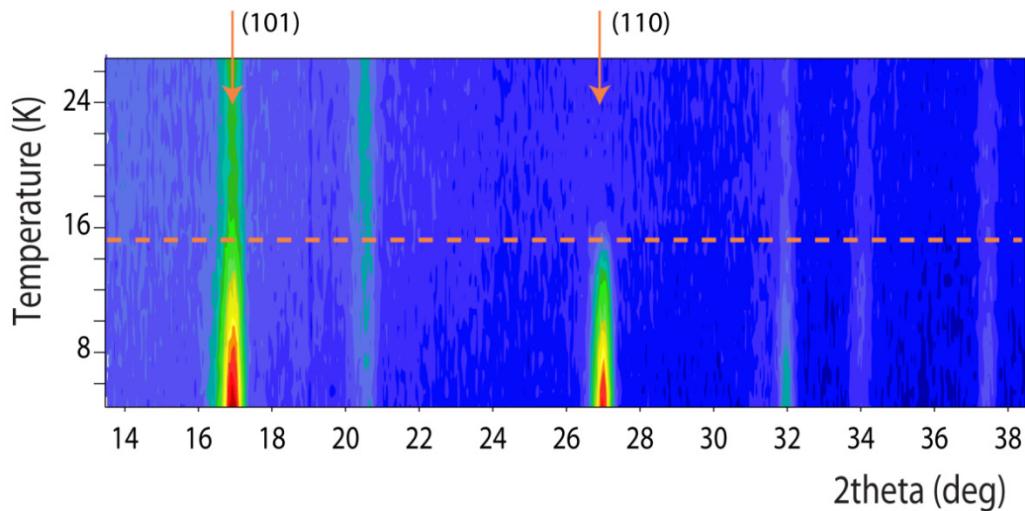


Figure S4. Thermal NPD at low temperature of (101) and (110) main reflections for the difference between 1.5 and 50 K intensities in the SMTFO compound.

Table S1. Bond lengths obtained from the Rietveld fitting made to the NPD ($\lambda = 1.36 \text{ \AA}$) patterns for SMTO and SMTFO compounds at 300 K.

Bond lengths (\AA)	SMTO	SMTFO
Mn1 – O1 (x6)	2.224 (4)	2.200 (6)
Mn2 – O2 (x1)	2.092 (11)	2.088 (14)
Mn2 – O3 (x3)	2.016 (4)	1.971 (7)
Ti1 -O1	1.872 (9)	1.871 (13)
Ti1 -O3	1.101 (7)	2.177 (11)
Ti1 -O3	1.984 (7)	2.049 (11)
Ti1 -O4	1.861 (6)	1.829 (10)
Ti1 -O5	1.964 (9)	1.902 (15)
Ti1 -O6	2.017 (9)	2.012 (14)
Ti2 -O1	1.941 (9)	2.009 (14)
Ti2 -O3	2.022 (7)	2.055 (11)
Ti2 -O5	1.961 (8)	2.005 (13)
Ti2 -O6	2.020 (8)	1.928 (13)
Ti2 -O6	2.034 (8)	2.047 (14)
Ti2 -O7	1.876 (6)	1.849 (19)
Ti3 -O2	2.031 (8)	1.977 (17)
Ti3 -O4	2.023 (7)	2.018 (16)
Ti3 -O4	1.963 (9)	1.965 (18)
Ti3 -O5	1.976 (7)	2.008 (13)
Ti3 -O7	2.057 (7)	2.085 (14)
Ti3 -O7	2.031 (9)	2.004 (17)