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## Synthesis, structure and magnetic properties of (Tb<sub>1-x</sub>Mn<sub>y</sub>)MnO<sub>3-δ</sub>

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Two samples  $(Tb_{1-x}Mn_v)MnO_3$  (x=0.089, y=0.063 for W1, and x=0.122, y=0.102 for W2) have been synthesized by solid state reactions and characterized using neutron diffraction performed on the C2 High Resolution Powder Diffractometer at Canadian Neutron Beam Centre (Chalk River, Canada) and magnetic measurements. They show similar nuclear crystal structures as TbMnO<sub>3</sub>, which crystallizes in space group *Pnma* at room temperature and Pna21 at low temperature. However, as shown in Figure 1, the Cuire temperatures for W1 ( $T_{c1} \approx 37$ K,  $T_{c2}\approx$ 22K) and W2 ( $T_{c1}\approx$ 42K,  $T_{c2}\approx$ 30K) are different from TbMnO<sub>3</sub> ( $T_{N1}\approx41$ K,  $T_{N2}\approx27$ K). More interesting is that the magnetic ordering of W1 and W2 is different from TbMnO<sub>3</sub>. TbMnO<sub>3</sub> has the sinusoidal antiferromagnetic ordering with two wave vectors  $\mathbf{q}_{Mn}$ = (~0.283, 0, 0) and  $q_{Tb}$ = (~0.415, 0, 0) in the space group  $Pna2_1$  setting below 7K, and the sinusoidal antiferromagnetic ordering

with one wave vector  $\mathbf{q}_{Mn}$ = (0.283~0.290, 0, 0) between 7K and 41K. W1 has the sinusoidal antiferromagnetic ordering with only one wave vector  $\mathbf{q}_{Mn}$ = (0.283~0.290, 0, 0) below 37K as shown in Fig.2. W2 has the sinusoidal antiferromagnetic ordering with one wave vector  $\mathbf{q}_{Mn}$ = (0.283~0.290, 0, 0) and commensurate canted antiferromagnetic ordering below 30 K as shown in Fig.2, and only commensurate canted antiferromagnetic ordering between 30K and 42K. Strong ferromagnetic response is induced by doping more Mn into the Tb site of (Tb<sub>1-x</sub>Mn<sub>y</sub>)MnO<sub>3-δ</sub>. This work was recently published [1].

## Reference

[1] Hao Zhang, Roxana Flacau, Junliang Sun, Guobao Li, Fuhui Liao, and Jianhua Lin Inorg. Chem. 2014, 53, 4535–4540. dx.doi.org/10.1021/ic500222y

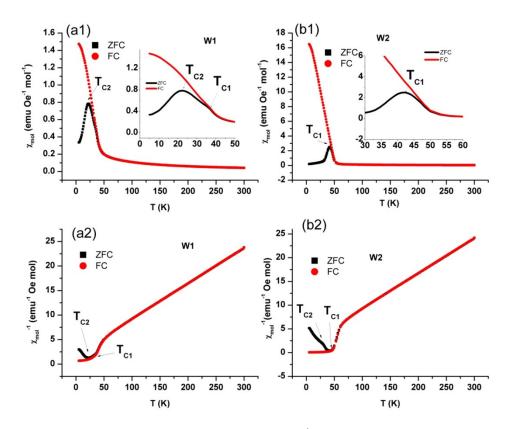


Figure 1 Temperature dependency of  $\chi_{mol}$  and  $\chi_{mol}^{-1}$  for W1 (a1, a2) and W2 (b1, b2).

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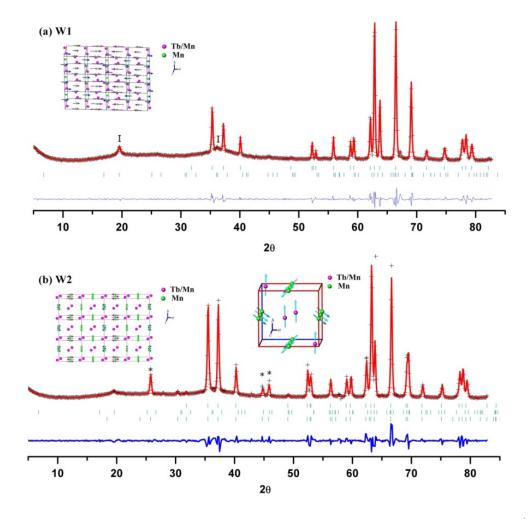


Figure 2 Rietveld plots of the neutron diffraction data for W1 (a) and W2 (b) collected at 3.5K with  $\lambda$ =2.3700Å and analyzed using Fullprof. The symbol + represents the observed pattern, the solid line represents the calculated pattern, the marks below the diffraction patterns are the calculated reflection positions (for (a) the up and down marks are for the nuclear and magnetic diffractions, and for (b) the up, middle, and down marks are for nuclear, incommensurate antiferromagnetic, and commensurate antiferromagnetic diffractions respectively), and the difference curve is shown at the bottom of the figure. Inset is the magnetic structure used for refinement. I indicates the parent reflections caused by incommensurate antiferromagnetic ordering; \* indicates the parent reflections due to commensurate antiferromagnetic ordering.