Neutron Powder Diffraction in mixed perovskites $LuFe_{1-x}Cr_xO_3$ with x= 0.25;0.45;0.55 and 0.75 to elucidate the magnetic structure and performed MonteCarlo simulations to reproduce the magnetic behavior

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In this work we studied the magnetic structure of the perovskite $LuFe_{1-x}Cr_xO_3$ (x= 0.25;0.45;0.55 and 0.75) family. The structural analysis was carried out by Neutron powder diffraction (NPD) with Rietveld analysis. NPD shown that the magnetic structure of this compound is Γ_4 ($G_xA_yF_z$) (Bertaut Notation) [1] in all the temperatures except the composition x=0.75 in 1K which is Γ_4/ Γ_2. In the Γ_4 structure the moments are oriented mainly in antiferromagnetic (AFM) type-G arrangement along the crystallographic *a*-direction. A ferromagnetic component along *c*-axis (canted configuration) and an AFM type-A arrangement along *b*-axis are allowed by symmetry [2,3]. This canting is responsible to a weak ferromagnetic behavior (WFM) below the Neél temperature. In these compound the WFM can be due to two mechanisms related with two different magnetic interactions: antisymmetric exchange or Dzyaloshinskii–Moriya interaction (DM) and single-ion magnetocrystalline anisotropy. In orthocromites and orthoferrites the WFM is mainly for DM interactions [2]. In the present work we assume a simplified model for the DM interaction consistent with an AFM G_x arrangement and a ferromagnetic canting in the z direction (F_z) only. In our model the DM vectors are all oriented along the *y* direction and staggered in every direction. It is easy to see that such choice of the DM vectors orientations is consistent with the experimentally observed magnetic structure. We model the magnetic behavior of these perovskites using a Hamiltonian of classical Heisenberg spins lying in the nodes of a cubic lattice with *N= (L x L x L)* sites and comparing this results with experimental measurements to magnetic moment vs temperature.

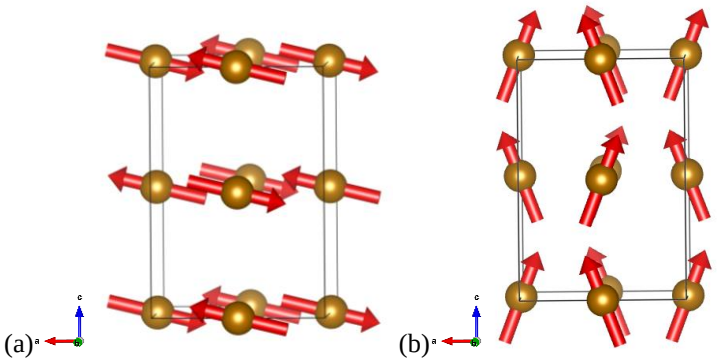

Figure 1. Magnetic structure obtained by NPD of $LuFe_{0.25}Cr_{0.75}O_3$ at 1K (a) and 300K(b).

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