

# Synthesis and characterization of mullite-type NdMnTiO<sub>5</sub>: Structural, spectroscopic, thermal and magnetic properties analyses

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Members of the multiferroic  $RMn_2O_5$  ( $R = Y, Bi$  and rare earth elements) family are well known for their concomitant presence of more than one order parameters at a given temperature [1]. Due to centrosymmetric structure of the mullite-type  $BiMn_2O_5$  compound the microscopic origin of the multiferroicity was explained in terms of complex interplay between spin-ordering, highly polarizable  $Bi^{3+}$  with stereo-chemically active lone electron pair,  $Mn^{3+}/Mn^{4+}$  charge-ordering and geometric distortions of the  $MnO_6$  coordination polyhedra. A cooperative antiferromagnetic (AFM) ordering between  $M^{3+}$  and  $Nd^{3+}$  was also observed for  $NdCrTiO_5$  [2] and  $NdFeTiO_5$  [3,4]. Below the respective  $T_N$  the  $M^{3+}$  cations become AFM and turn the  $Nd^{3+}$  cations into AFM along the  $ab$  plane through exchange coupling [2]. The collinearly ordered  $M^{3+}$  cations along the octahedral chain directing  $c$ -axis gives rise to magnetostriction, leading to multiferroicity in this compound [2]. In search of novel multiferroic, we report the synthesis and characterization of the mullite-type O10 phase isostructural  $NdMnTiO_5$  compound. The crystal structural features are described using Neutron powder diffraction (NPD) and Powder X-ray diffraction data (PXRD) Rietveld refinements (Fig. 1).  $NdMnTiO_5$  crystallizes in the orthorhombic space group  $Pbam$  with metric parameter  $a = 755.20(1)$  pm,  $b = 869.91(1)$  pm,  $c = 582.42(1)$  pm and  $V = 382.62(1)$   $10^6$  pm<sup>3</sup>. The  $Mn^{3+}$  and  $Ti^{4+}$  cations are observed to be located in the octahedral and pyramidal site, respectively. The vibrational features in these polyhedral sites are characterized by Raman and Fourier transform infrared spectroscopes. The higher decomposition temperature of  $NdMnTiO_5$ , compared to other  $RMn_2O_5$  phases, is explained in terms of higher bond strength of Ti-O bonds than those of Mn-O bonds. Temperature-dependent DC magnetic susceptibility suggests a paramagnetic to antiferromagnetic phase transition ( $T_N$ ) at 43(1) K. Inverse susceptibility in the paramagnetic region above 120 K follows the Curie-Weiss law, resulting in a magnetic moment of 6.33(1)  $\mu_B$  per formula unit. Neutron diffraction data collected at 7.5 K reveal that the magnetic moments of  $Nd^{3+}$  and  $Mn^{3+}$  in  $NdMnTiO_5$  are incommensurately ordered with a propagation vector  $\mathbf{k} = (0, 0.238, 0.117)$ .

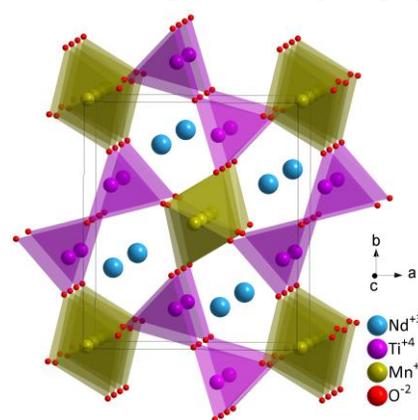


Fig. 1: Crystal structure of  $NdMnTiO_5$

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