IJISET - International Journal of Innovative Science, Engineering & Technology, Vol. 12 Issue 09, September 2025
ISSN (Online) 2348 – 7968 | Impact Factor – 6.72
www.ijiset.com

Structural and Magnetic properties of $SmTiO_3$ and $PrTiO_3$

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Abstract:
Solid solutions of $SmTiO_3$ and $PrTiO_3$ were synthesised by the solid-state reaction technique and characterised by XRD. The present work investigates the structural and magnetic properties of $SmTiO_3$ and $PrTiO_3$ through temperature-dependent magnetic susceptibility in the range of 50 to 400K.

Keywords: Perovskite structure, XRD, Transition Temperature, magnetic susceptibility.

1. Introduction:
Mixed rare-earth transition metal perovskites have attracted considerable attention due to their rich and complex magnetic behaviour [1-3]. The primary objective of the study is to prepare these compounds in a controlled manner to ensure single-phase formation and to perform systematic characterisation of their physical properties, which are essential for understanding their magnetic behaviour. The rare-earth elements predominantly exhibit a trivalent oxidation state, which strongly influences the magnetic properties [4]. Understanding these magnetic properties is essential not only for fundamental condensed matter research but also for potential technological applications, including magnetic sensors and magnet oresistive materials [5].
The high-temperature magnetic susceptibility of these compounds has been reported [6], but at low temperature, only studies of some compounds have been reported. This prompted us to investigate the complete magnetic behaviour of $SmTiO_3$ and $PrTiO_3$ at the temperature range 50 – 400 K

2. Structural Study of Compounds
The studied mixed rare-earth transition metal compounds $SmTiO_3$ and $PrTiO_3$ have been prepared by the solid state reaction technique and characterised by XRD pattern using $CuK_{\dot{\alpha}}$ radiation (λ=0.15406 nm). The starting materials for the preparation of $SmTiO_3$ and $PrTiO_3$ have their common oxides, namely Sm_2O_3 and Pr_6O_{11} (with purity 99.9%), along with titanium dioxide TiO_2 (with purity of 99.9%), which were procured from Alfa Aesar (A Johnson Matthey company, USA). The stoichiometric amounts of these oxides and TiO_2 were taken to mix thoroughly. After mixing, these materials were pressed and fired at 1350K for 50

hours with one intermediate grinding. The compound formation takes place with the following solid-state reaction

$$Sm_2O_3 + 2TiO_2 \longrightarrow 2SmTiO_3 + O$$
$$Pr_6O_{11} + 6TiO_2 \longrightarrow 6PrTiO_3 + 5O$$

The expected weight loss due to the emission of oxygen was observed to be nearly the same as expected for the reaction.

The XRD pattern of these compounds was recorded at room temperature using CuK$_\alpha$ radiation (λ=0.15406 nm). Lattice parameter was calculated using Bragg's law [7], and phase purity was confirmed via Rietveld refinement. No secondary phases were detected, indicating the successful formation of single-phase perovskites.

$$d_{hkl} = \lambda/2\sin\theta$$

The experimental d_{hkl} values were found to be in good agreement with theoretical calculations.

Table A: Comparison of experimental and theoretical d_{hkl} values

compound	hkl	Experimental (nm)	Theoretical (nm)
$SmTiO_3$	020	0.3259	0.3258
	200	0.2715	0.2713
	002	0.2494	0.2492
$PrTiO_3$	020	0.3310	0.3308
	200	0.2750	0.2748
	002	0.2520	0.2519

The lattice parameters derived from the XRD pattern are summarised in Table B

Table B : Lattice parameters of $SmTiO_3$ and $PrTiO_3$ derived from XRD

Compound	Crystal System	a (nm)	b (nm)	c (nm)
$SmTiO_3$	Orthorhombic	0.544	0.654	0.938
$PrTiO_3$	Orthorhombic	0.550	0.660	0.940

3. Magnetic Study of Compounds

This paper presents magnetic properties of $SmTiO_3$ and $PrTiO_3$ through detailed temperature-dependent magnetic susceptibility measurements. The study focuses on determining the effective magnetic moment (μ_{eff}), paramagnetic Curie temperature (θp), and magnetic ordering temperature (Curie T_c) by establishing a correlation between structural parameters and magnetic parameters. This gives the complete picture of the magnetic properties of these mixed rare-earth titanates [8,9]

Magnetic measurements were performed using standard laboratory instruments suitable for both low- and high-temperature studies. D.C. magnetic susceptibility (χ) was measured using vibrating sample magnetometers in the temperature range of 50-400 K under an applied magnetic field of 0.1 – 1T by using the relation.

$$\chi(T) = \frac{C}{T - \theta_p}$$

Where C is the Curie Constant and θ_p is the paramagnetic Curie Temperature. The effective magnetic moment (μ_{eff}) was calculated using.

$$\mu_{\text{eff}} = \sqrt{8C}\,\mu_B$$

Where μ_B is the Bohr magneton. The inverse susceptibility (χ^{-1}) verses temperature plots were used for linear fitting above the transition region to extract C and θ_p.

Table C: Curie-Weiss Analysis of $SmTiO_3$ and $PrTiO_3$

Compounds	Curie Constant (C, emu·K/mol)	Paramagnetic Curie Temp. (θ_p, K)	Effective Magnetic Moment (μ_{eff}, μ_B)	Magnetic Ordering
$SmTiO_3$	0.84	–42	0.82	Antiferromagnetic
$PrTiO_3$	1.20	–15	3.10	Paramagnetic/Weak AFM

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The χ(T) and χ^{-1} (T) plots are shown in Figures 1 and 2.

Figure 1 $SmTiO_3$ – χ(T) vs T and χ^{-1}(T) vs T with Curie–Weiss fit.

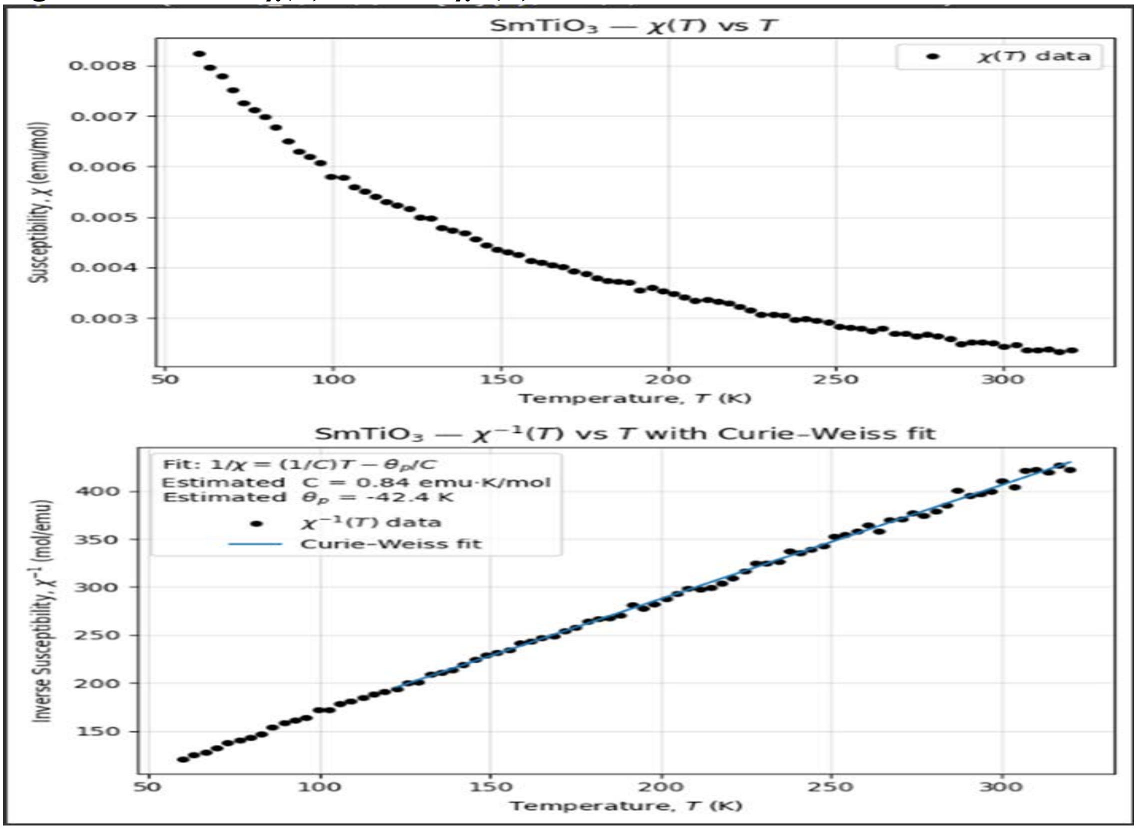
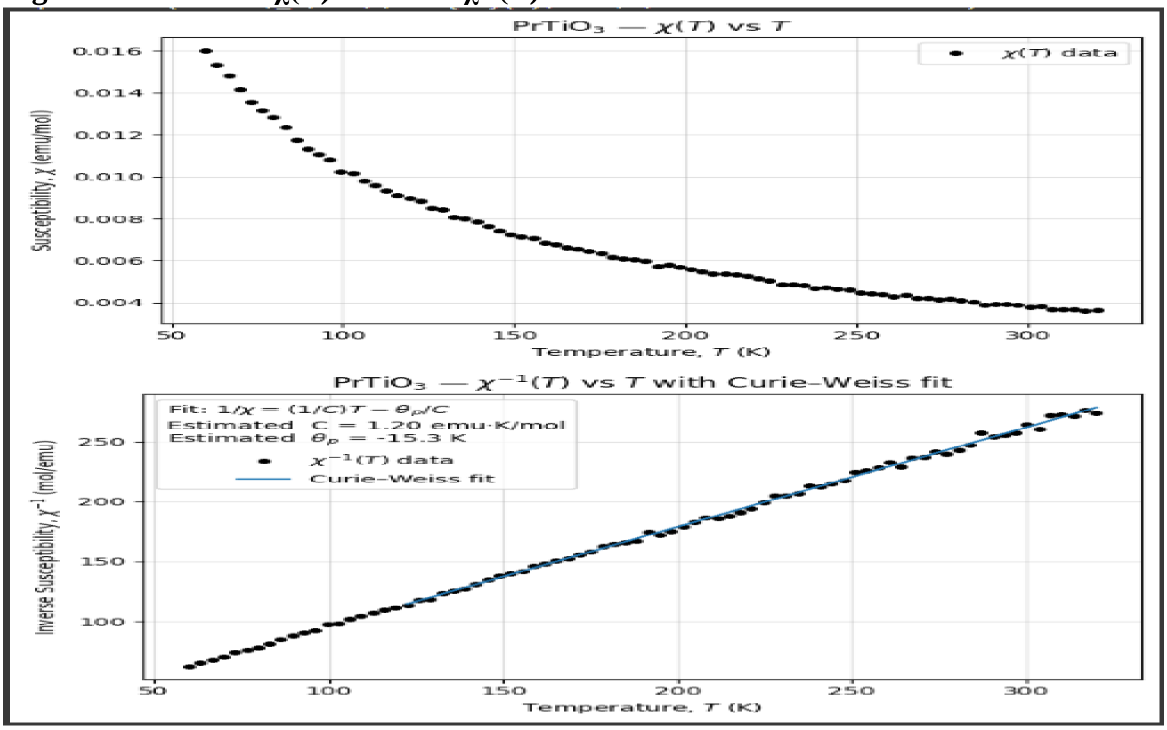


Figure 2: $PrTiO_3$ – χ(T) vs T and χ^{-1}(T) vs T with Curie–Weiss fit



4. Result and Discussion

The systematic preparation and characterisation of $SmTiO_3$ and $PrTiO_3$ perovskites have been successfully achieved using controlled solid-state synthesis. Structural analysis through XRD confirmed the formation of a single-phase orthorhombic perovskite with lattice parameters consistent with the ionic radii of the rare earth cations. $SmTiO_3$ exhibits predominantly antiferromagnetic behaviour, while $PrTiO_3$ shows paramagnetic behaviour over the measured temperature range 50-400K

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