present the results of accurate structure determinations at several temperatures between 160 and 293K by single-crystal x-ray diffraction, in order to characterize the low temperature phase. To further clarify the structural changes as a function of temperature we have analyzed the diffraction data by the Maximum Entropy Method (MEM) [3] in a small temperature range close to the phase transition.

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Keywords: manganites, CMR, MEM

P.11.11.3
Comparison of $Ba_{0.05}Sr_{0.95}RuO_3$ and $Ca_{0.05}Sr_{0.95}RuO_3$ Structures
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$SrRuO_3$, which has a nearly ideal perovskite structure, is a rare example of a 4d transition metal oxide that is metallic and ferromagnetic [1]. Its saturation moment is smaller than expected and it is usually considered an example of an itinerant ferromagnetism, however the nature of magnetism is not yet fully understood [2]. In spite of the structure of perovskite $SrRuO_3$ is described in the literature as orthorhombic, we have found this compound possesses a space group $P112_1/m$. This space group may be the clue to understand the low temperature magnetic behaviour.

In this work we have studied both solid solution $Ba_{0.05}Sr_{0.95}RuO_3$ and $Ca_{0.05}Sr_{0.95}RuO_3$ by powder X-ray diffraction at room temperature and at higher temperatures. In both compounds, weak observed reflections were not well refined in orthorhombic space group, like in pure $SrRuO_3$. In the monoclinic structure, bond distances, angles and a bond valence sum study shows that, when cation Sr is replaced by Ba it is over-bonded, contrasting to the replacement by Ca. In order to diminish this valence sum, RuO_6 rigid groups tilt along the three cubic axes (in the Pnma space group, this is not possible with different angles). In order to detect the phase transition $P112_1/m$ –Pnma, a reexamination of the sequence of high-temperature phases in both compounds has been performed.

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Keywords: powder X-ray diffraction, perovskites, ferromagnetics

P.11.11.4
Verwey Transition in a Perovskite-Type Structure
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Above Verwey transition at 120 K, magnetite (Fe_3O_4) is a spin-polarized conductor, feasible for applications in spin computing. Owing to continuing controversy about charge order in the complex low-temperature phase, Verwey transition in magnetite remains a mystery. Double-cell perovskites of the $YBaFe_2O_5$ type contain iron in the average oxidation state +2.5 and exhibit all symptoms of the Verwey transition. The charge-ordered superstructures are simple and the refined iron–oxygen bond distances suggest a 70 to 80% of long-range charge separation into di- and trivalent iron, likely to mean a 100% charge separation on the local scale. The charge order violates Coulombic minimization of point charges, implying orbital ordering. The associated orthorhombic distortion identifies the doubly-occupied d_{xz} orbital of Fe^{2+}. Magnetic interactions define the orientation of the orthorhombic distortion, but the charge order occurs independently of any specific spin coupling. Magnetostriction opens for an incipient partial charge ordering that occurs before the Verwey transition itself distorts the structure under continued cooling. Replacing Y with Sm and Nd shows that when the size of this seemingly uninvolved atom becomes unfavorable (a large projected ΔV at the transition), orbital ordering continues at a cost of symmetry lowering. Oxygen nonstoichiometry decreases Verwey-transition entropies ΔS and

transition temperatures T_V in a manner that corresponds to an ideal solution of $YBaFe_2O_6$ in the $YBaFe_2O_5$ solvent. Verwey transition is a klassengleich switch from a valence-mixed halfmetal into a valence-ordered semiconductor, achieved via orbital ordering of one single, singly or doubly occupied d orbital of t_{2g} symmetry.
Keywords: mixed valence oxides, phase transition, superstructure

P.11.11.5
Nanostructural Effects at $KNbO_3$ Synthesis
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It was recently established that ferroelectric properties of oxides with perovskite-type structures (for example, $BaTiO_3$ and $PbTiO_3$) in nanocrystalic states were been reduced [1,2]. The nature of ferroelectricity at nanoscal, such as critical size dependent suppression in particles, is much debated in the literature.

Attempts to understand further the finite size effect in ferroelectric oxides led us to studies of $KNbO_3$ synthesis process from K_2CO_3 and Nb_2O_5 stoichiometric mixture at different temperatures using X-ray diffractometer.

Special attention is paid to changes in symmetry, lattice parameters and dimensions of coherent scattering areas in synthesis and stabilization processes of $KNbO_3$ perovskite structure. It is found that there are correlations between microscopic (atomic parameters and lattice constants) and mesoscopic (dimensions of coherent scattering areas) characteristics of $KNbO_3$ structure which provide an opportunity to describe not only nanostructural effects but some physical parameters of $KNbO_3$ in dependence from nano-sizes of crystal phases.

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Keywords: perovskites, synthesis, nano-size effects

P.11.11.6
Crystal Structure of the Layered Compound $Sr_3NdFe_3O_9$
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This compound belongs to the series $Sr_3LnFe_3O_9$ (Ln = La − Sm). An original feature of the latter ones is the rapid reaction with ambient moisture to transform into hydrated oxyhydroxide $Sr_3LnFe_3O_8(OH)_2$ H_2O. [1] Previous electron microscopy and X-ray diffraction studies of $Sr_3NdFe_3O_9$, [1] revealed an orthorhombic lattice with parameters $a_p\sqrt{2} \times a_p\sqrt{2} \times 28$ Å (a_p: lattice parameter of the perovskite). In a first time, the structure was considered as an oxygen deficient n = 3 Rp-Member $Sr_3NdFe_3O_9$. Powder neutron diffraction experiments at RT and 673 K were then carried out and show that the structure can be described as a stacking of blocks formed by two external slabs of FeO_6 octahedra and a central slab of FeO_4 tetrahedral. To this point of view this structure result of the intergrowth of Brownmillerite type blocks $Sr_{3/2}Nd_{1/2}Fe2O5$ with K_2NiF_4 type blocks $Sr_{3/2}Nd_{1/2}FeO_4$ instead of triple perovskite type blocks with adjacent NaCl type layers of SrO.

Powder Neutron diffraction data at Room temperature and susceptibility measurement although shows that this compound although present an antiferromagnetic transition at ~500 K

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Keywords: powder structure resolution, layered compound, magnetic properties