Recently, half-metallic transition metal oxides with ordered double perovskite structure $A_2BB'O_6$ (A is an alkaline-earth ion, and B and B' are transition metals) appear to be promising candidates for magnetoresistive devices due to their remarkable tunneling and inter-grain magnetoresistance (MR) around room temperature. Among the double perovskite compounds synthesized so far, Sr_2FeMoO_6 is the most extensively studied, due to the reported substantial low field magnetoresistance at room temperature and high Curie temperature $T_C \approx 400$ K [1]. Many other double perovskites $A_2B'B''O_6$ with other transition metals (B"= Mo, W, Re…) have been described until now [2]. We are interested in Re and Sb double perovskites; the former have been suggested to present a higher electron density at the Fermi level than the Mo double perovskites and this could increase the Curie temperature. As for the Sb-containing double perovskites, the presence of a p element at the B sublattice favours the long-range ordering and implements interesting magnetic-ordering effects, driven by direct exchange via the empty 5p orbitals of Sb(V).

We prepared the double perovskites A_2MReO_6 (A= Sr, Ca; M = Fe, Co, Ni, Zn) by soft-chemistry procedures; a preliminary XRD study demonstrates that Sr_2MReO_6 perovskites have a tetragonal structure with space group $I4/m$ whereas Ca_2MReO_6 oxides are monoclinic with space group $P2_1/n$ due to the smaller size of Ca^{2+}, leading to a reduction in the tolerance factor. As for the Sb-compounds, we synthesized, for the first time, the oxides A_2MSbO_6 (A= Ca, Sr, Ba; M= Cr, Mn, Fe, Co); preliminary XRD studies demonstrate that the Ba perovskites are hexagonal ($P6_3/mmc$), whereas the Sr and Ca materials are, apparently, tetragonal (I4/m) and monoclinic ($P2_1/n$), respectively. The first objective of this experiment was to investigate the actual symmetry and features of the different materials. The resolution of BM25 permitted us the observation of the extremely weak monoclinic splitting arise in some double perovskites and to accurate determine the tilting of the BO_6 octahedra and the degree of antisite disordering; both parameters are of paramount importance to correctly characterize the crystal structure and thus correlate the structural features with the previously measured magnetic and transport properties.

We collected long patterns with extremely good statistics in suitable capillary sample holders; we needed high resolution and good statistics to determine the subtle symmetry distortions expected for some Sr-double perovskites. In this first part of the experiment our results confirmed the previous findings obtained from neutron powder diffraction data, as far as space group symmetry is concerned. Fig. 1 shows the satisfactory refinement of Sr_2CoSbO_6 in a tetragonal model using the synchrotron x-ray data, which presents the same symmetry as the previously reported using neutron powder diffraction data.

In addition of being interested in precisely determining the room-temperature crystal structure of the new mentioned double perovskites, some of them show evidences to present a structural phase transition above RT, along the sequence monoclinic→orthorhombic→ tetragonal→ cubic. A classical example is Sr_2CoWO_6 [3], which shows two subsequent transitions in the 300-900 K interval. For this part of the

experiment, the sample capillaries were heated in a hot air-flow furnace, allowing us to monitor the structural changes in the 300-800 K temperature interval. We studied the evolution in temperature of the double perovskite Sr_2CoReO_6. Fig. 2 shows the synchrotron x-ray diffraction data of Sr_2CoReO_6 measured at room temperature, 473K and 773K. For the first time we observed a structural phase transition from tetragonal (low temperature, space group I4/m) to cubic (high temperature, space group Fm3m) above 473 K. The onset of Fig. 2 shows the vanishing of the splitting of some peaks when the temperature increases as a consequence of the increment of the symmetry. The publication of these results is in progress.

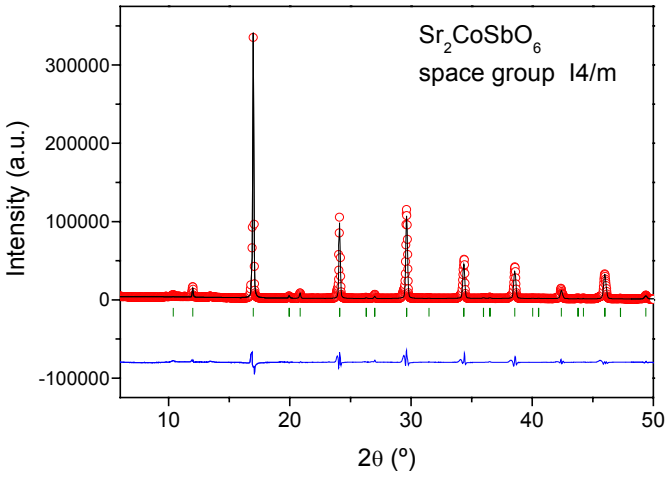

Fig. 1: Rietveld refinement of Sr_2CoSbO_6 from synchrotron x-ray data.

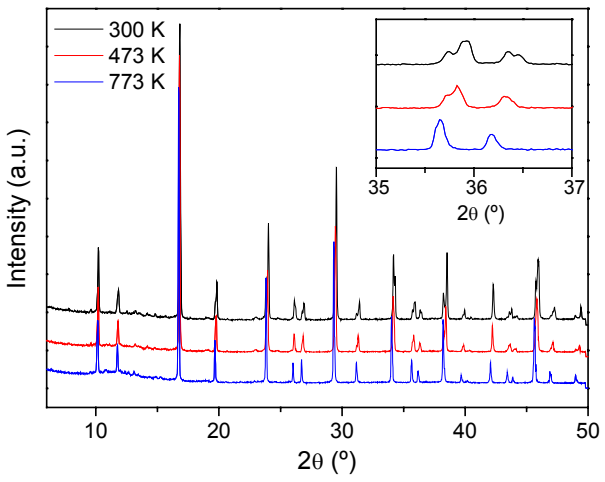

Fig. 2: Synchrotron x-ray diffraction data of Sr_2CoReO_6 measured at room temperature, 473K and 773K.

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