Structural and magnetic characterization of ordered Sr_2LnSbO_6 (Ln=rare earth) perosvkites

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The double perovskites A_2LnMO_6 (A = Sr^{2+} and Ba^{2+}; Ln = trivalent lanthanide cation; M = pentavalent 4d or 5d transition elements) have been widely studied concerning their structure and properties [1]. If the Ln and M cations are ordered within the B-perosvkite sites the symmetry and size of the unit cell change when are compared to the ideal cubic aristotype. Woodward predicted 15 possible space groups for the ordered $A_2BB'O_6$ perovskites when the cation ordering and the octahedral tilting around the pseudo-cubic axes take place simultaneously [2]. The ordered double perovskites A_2LnMO_6 with only one of the two B-sites carrying magnetic moment, namely Ln, show a magnetic sublattice consisting of edge-sharing tetrahedral, which represents a frustrating magnetic geometry in three dimensions. More recently, the structure of double perovskites Sr_2LnSbO_6 (Ln= Dy, Ho, Gd, Y and In) has been investigated, and the monoclinic symmetry of the space group $P2_1/n$, with Ln and Sb elements ordered in the B-sites, was reported [3, 4].

We report the preparation of the whole family of double perovskites Sr_2LnSbO_6 (Ln = La-Lu), which crystallize with the $P2_1/n$ space group, with lattice parameters $a = \sqrt{2}a_p$, $b = \sqrt{2}a_p$ and $c = 2a_p$ (β~90 º), being a_p the lattice parameter of the cubic aristotype. A progressive decreasing was observed in lattice parameters with the increasing of the atomic number of the Ln cation, according with the well-known lanthanide contraction.

Magnetic susceptibility measurements for this family of compounds reveal a paramagnetic behaviour in a very wide temperature range. From experimental spectroscopic data as well as from a semi-empirical estimation (Simple Overlap Model SOM [5]) of the crystal-field parameters corresponding to the point site symmetry of the magnetically active Ln, O_h, and using the wavefunctions associated with the energy levels obtained, the paramagnetic susceptibility and its evolution *vs* temperature is simulated according to the van Vleck formalism. The observed deviation from the Curie–Weiss behaviour at low temperature, very well reproduced in each case, reflects the splitting of the ground state of the corresponding Ln cation under the influence of the crystal field. Thus, magnetic frustration or cooperative interactions do not need to be considered to explain the mentioned low temperature deviation from the linearity of Curie-Weiss plots.

References

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