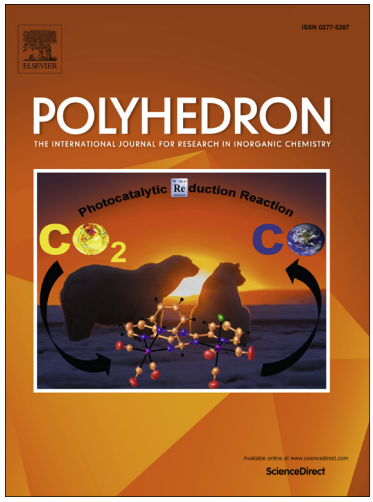

Effect of the M^{3+} cation size on the structural and high temperature phase transitions in Sr_2 $MSbO_6$ (M = *Ln*, Y) double perovskites

B. Orayech, A. Faik, J.M. Igartua

PII: S0277-5387(16)30653-2
DOI: http://dx.doi.org/10.1016/j.poly.2016.09.066
Reference: POLY 12360

To appear in: *Polyhedron*

Received Date: 25 April 2016
Accepted Date: 13 September 2016

Please cite this article as: B. Orayech, A. Faik, J.M. Igartua, Effect of the M^{3+} cation size on the structural and high temperature phase transitions in Sr_2 $MSbO_6$ (M = *Ln*, Y) double perovskites, *Polyhedron* (2016), doi: http://dx.doi.org/10.1016/j.poly.2016.09.066

Effect of the M^{3+} cation size on the structural and high temperature phase transitions in Sr_2MSbO_6 (M = *Ln*, Y) double perovskites

B. Orayech [a,b], A. Faik [a] and J. M. Igartua [c]

[a] *CIC energigune, Albert Einstein 48, 01510 Miñano, Alava, Spain*

[b] *Departamento de Física de la Materia Condensada, Facultad de Ciencia y Tecnología, Universidad del País Vasco, P.O.Box 644, Bilbao 48080, Spain*

[c] *Fisika Aplikatua II Saila, Zientzia eta Teknologia Fakultatea, Euskal Herriko Unibertsitatea, P.O.Box 644, Bilbao 48080, Spain*

Abstract

In the present work, synchrotron X-ray powder-diffraction measurements at room temperature and laboratory X-ray powder-diffraction measurements at high temperatures of nine members of the antimony family Sr_2MSbO_6 M = Ln (Nd, Eu, Gd, Dy, Ho, Er, Tm, Yb) and Y ; are reported. Six of them are synthesized for the first time in this work. The crystal structures at room temperature of these compounds are determined and their symmetries are described in the $P2_1/n$ ($a^-a^-b^+$) space group (No. 14, non-standard setting). The materials have double perovskite structure with 1:1 ordered arrangement of the B sites. The high-temperature measurements show the existence of two temperature driven phase-transitions: a discontinuous one, from the RT symmetry to $R\bar{3}$ ($a^-a^-a^-$) and a continuous one from the latter symmetry to the highest one, the cubic $Fm\bar{3}m$ ($a^0a^0a^0$). The phase transition temperatures are correlated to the M^{3+} cation size. The analysis of the phase transitions and the structural refinements have done using the symmetry-adapted modes. A step forward in these analysis is performed: parametrization of the refinements by fixing a selected common direction in the sub-space spanned by X_5^+ , tri-linearly coupled to the order parameters of the cubic to monoclinic first order phase transition.

Key words: Double Perovskite, Symmetry mode analysis, Crystal structure, Phase transitions, Synchrotron X-ray diffraction.

1 Introduction

The structure of double perovskite is very simple, the B and B' cations form octahedra and are connected alternary each to other via vertices. The A-atoms