A study of the crystal structures and the phase transitions of the ordered double perovskites Sr2ScSbO6 and Ca2ScSbO6

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Abstract

The crystal structures and phase transitions of the two ordered double perovskites Sr2ScSbO6 and Ca2ScSbO6 were studied using conventional X-ray and neutron powder-diffraction methods. The crystal structures of both compounds have the P21/n space group symmetry at room temperature, resulting from Sc/Sb ordering. The evolution with temperature of the structure of the Sr containing compound shows the presence of three phase transitions with the following sequence: P21/n → I2/m → I4/m → Fm’3m, at about 400, 560 and 650 K, respectively. The smaller size of Ca cation, with respect to that of Sr cation, leads to a large distortion of Ca2ScSbO6 at room temperature. This fact in turn causes that the Ca containing compound shows only the first phase transition from P21/n to I2/m at high temperature at about 1440 K. The analysis of the phase transitions and the refinements have done using the symmetry adapted modes and the tools of the Bilbao Crystallographic Server.

Key words: Double Perovskite, X-Ray and neutron powder diffraction, Crystal structure, Phase transitions, Symmetry adopted modes PACS: 61.10.Nz, 61.50.Ks, 61.66.Fu, 64.70.Kb