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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