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Insight into the Stability of Tetragonal and Rhombohedral Phases in Double Perovskites

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The precise structure adopted by double perovskites is known to have a significant influence on the interesting and useful properties these materials adopt such as magnetism, ferroelectricity and colossal magneto-resistance. It is therefore important to understand why apparently similar perovskite systems adopt different symmetry. An example of this is the significantly different structures adopted by members of the series of double perovskites of the type $Ba_2LnB'O_6$ (Ln = lanthanide and B' = Nb^{5+}, Ta^{5+} or Sb^{5+}). It has recently been established that members of the Nb^{5+} series adopt *I*4/*m* tetragonal symmetry while Sb^{5+} adopts rhombohedral symmetry as intermediate phases between the *I*2/*m* monoclinic and the cubic phase [1-3] . The cause of the difference in the intermediate phase adopted in these two similar systems is still not certain.

In order to develop an understanding of why changes to the pentavalent cation influence the symetry of the intermediate phase we have studied the structures of the Ba_2LnTaO_6 series using a combination of synchrotron X-ray and neutron powder diffraction both at, above and below ambient temperature. The majority of oxides exhibited the same tetragonal intermediate phase seen in the niobates. However Ba_2LaTaO_6 adopts the rhombohedral intermediate seen in the antimonates. This prompted us to examine the phase transitions of Ba_2LaNbO_6 using variable temperature diffraction results from which indicate that it exhibits similar behaviour to Ba_2LaTaO_6. That the lanthanum tantalates and niobates exhibit rhombohedral symmetry while other tantalates and niobates exhibit tetragonal symmetry indicates that the factors causing the difference in symmetry adopted are particularly subtle and that the systems are finely balanced between these two possibilities. This paper will examine the results in these and other related compounds and attempt to explain the relative stability of the rhombohedral and tetragonal symmetries in this context.

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