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Structure change of $Ca_{1-x}Sr_xTiO_3$ perovskite with composition and pressure

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ABSTRACT

Structure refinements of solid solutions of $(Ca_{1-x}Sr_x)TiO_3$ (x = 0.0, 0.25, 0.5, 0.6, 0.65, and 1.0) were undertaken using single crystals at ambient conditions. Their lattice constants, c/a axial ratios, and cell volumes indicate continuous changes from orthorhombic to cubic through a tetragonal phase. The orthorhombic structure is continuous between x = 0.0 and x = 0.6, and a phase at x = 0.65 shows a tetragonal structure with space group $I4/mcm$. With increasing Sr substitution, the symmetry changes to cubic with $Pm\bar{3}m$ space group. A-O and B-O distances in ABO_3 perovskite were determined as a function of the composition of the A cation (Ca and Sr). Tilting and rotation angles of the TiO_6 octahedral linkage with x of $(Ca_{1-x}Sr_x)TiO_3$ were also evaluated. Single-crystal structure refinements of $Ca_{0.35}Sr_{0.65}TiO_3$ perovskite at 3.5, 4.1, and 7.0 GPa at 300 K were carried out using a diamond anvil cell. The tetragonal phase transforms to an orthorhombic structure with space group $Pbnm$ at 3.5 GPa. The polymorphic transition of $^{VIII}A^{2+VI}B^{4+}O_3$ perovskites under compression is discussed.