

Poster Presentation

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High-pressure structural behaviour of CaIrO₃ polymorphs

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The two known polymorphs of CaIrO₃ crystallize into the orthorhombic space groups Pbnm and Cmcm. These compounds have been the focus of much research in the Earth sciences community because they are isostructural with MgSiO₃ perovskite and post-perovskite structures which are likely the most abundant minerals in the Earth's lower mantle. CaIrO₃ post-perovskite is stable at ambient conditions and transforms at 1-3 GPa and at temperatures above 1350 °C to the CaIrO₃ perovskite structure providing an ideal low pressure and low temperature analogue for the MgSiO₃ perovskite to post-perovskite phase transformation which occurs at the extreme conditions of 125 GPa and 2500 K. However, in order to assess whether the CaIrO₃ compounds can be used as analogues of MgSiO₃ phases, a correct knowledge of their atomic structures and their response to changes in pressure and temperature is essential. In this study the structural behavior of both CaIrO₃ polymorphs has been investigated using single-crystal X-ray diffraction at different pressures up to 10 GPa. The orthorhombic distortion of CaIrO₃ perovskite derives from the cubic perovskite aristotype by tilting of the octahedral units. These tilts are very large and their variation with pressure is clearly different from the tilting reported for other Ca-oxide perovskites giving rise to a much stiffer structure. The CaIrO₃ post-perovskite phase has a layered structure consisting of alternating sheets of Ca atoms and distorted IrO₆ octahedra which share edges to form rows running parallel to [100]. With increasing pressure the octahedral tilting remains practically constant and compression of the post-perovskite structure occurs as a result of compression of Ca layers. With increasing temperature, instead, the octahedral tilting increases giving rise to smaller distances between oxygens of adjacent octahedra whose repulsion likely causes the transformation to the CaIrO₃ perovskite structure.

Keywords: High-pressure single-crystal X-ray diffraction, CaIrO₃ perovskite and post-perovskite