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Compression, thermal expansion, structure, and instability of $CaIrO_3$, the structure model of $MgSiO_3$ post-perovskite

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Abstract

Analysis of pressure-temperature dependent monochromatic X-ray powder diffraction data yield the bulk modulus [K_T = 180.2(28) GPa] and thermal expansion coefficients [$\alpha_0 = 2.841(34) \times 10^{-5}$ K^{-1}; $\alpha_1 = 3.37(48) \times 10^{-9}$ K^{-2}] of $CaIrO_3$, the structure model for post-perovskite $MgSiO_3$. $CaIrO_3$ is orthorhombic (*Cmcm*, space group 63, $Z = 4$) with best-fit unit-cell parameters, a = 3.14147(5) Å, b = 9.87515(19), c = 7.29711(11), and V = 226.3754(78) Å^3 at 1 bar and 300 K. The **c**-axis of $CaIrO_3$ has a small compressibility and a large thermal expansion when compared to the other principal axes. Rietveld structure refinement reveals changes in $CaIrO_3$ as a function of temperature in terms of IrO_6 octahedra distortion. Dissociation of $CaIrO_3$ at high temperature has possible implications for the post-perovskite $MgSiO_3$ structure, Earth's lower mantle, and D" layer.

Keywords: Post-perovskite, $CaIrO_3$, pressure, temperature, structure, X-rays, Rietveld refinement, D" layer