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High-pressure structure and bonding in $CaIrO_3$: The structure model of $MgSiO_3$ post-perovskite investigated with time-of-flight neutron powder diffraction

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Abstract

The structure of $CaIrO_3$ (*Cmcm*) has been refined at high pressure and at low temperature using time-of-flight neutron powder diffraction data. Evidence supporting deviation from space group *Cmcm* to $Cmc2_1$ is inconclusive. As $CaIrO_3$ (*Cmcm*) unit-cell volume changes, refinements indicate deformation of cation-centered coordination polyhedra, rather than tilting. Structure models demonstrate Ca^{2+}-centered polyhedra are an order of magnitude more compressible than Ir^{4+}-centered octahedra. Bond valence sums show significant chemical strain (over-bonding) of calcium and oxygen at ambient conditions. Implications for structure change in $MgSiO_3$ post-perovskite are discussed and a method for predicting the Clapeyron slope between perovskite and post-perovskite phases is proposed based on extrapolation of the volume-ratio between cation-centered polyhedra.

Keywords: Post-perovskite, high pressure, structure, neutron diffraction, Rietveld refinement, bond valence, D" layer, $CaIrO_3$