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LETTER

Rietveld structure refinement of perovskite and post-perovskite phases of $NaMgF_3$ (Neighborite) at high pressures

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ABSTRACT

Neighborite ($NaMgF_3$) with the perovskite structure, transforms to a post-perovskite (ppv) phase between 27 and 30 GPa. The ppv phase is observed to the highest pressures achieved (56 GPa) at room temperature and transforms to an as yet unknown phase upon heating. Rietveld structure refinement using monochromatic synchrotron X-ray diffraction data provide models for the perovskite and post-perovskite structures at high pressure. The refined models at 27(1) GPa indicate some inter-octahedral F-F distances rival the average intra-octahedral distance, which may cause instability in the perovskite structure and drive the transformation to the post-perovskite phase. The ratio of A-site to B-site volume (V_A/V_B) in perovskite structured $NaMgF_3$ (ABX_3), spans from 5 in the zero-pressure high-temperature cubic perovskite phase to 4 in this high-pressure perovskite phase at 27(1) GPa, matching the V_A/V_B value in post-perovskite $NaMgF_3$. Using Rietveld refinement on post-perovskite structure models, we observe discrepancies in pattern fitting, which may be described in terms of development of sample texture in the diamond-anvil cell, recrystallization, or a change of space group to $Cmc2_1$, a non-isomorphic subgroup of *Cmcm*—the space group describing the structure of $CaIrO_3$.

Keywords: Perovskite, post-perovskite, pressure, diamond anvil cell, X-ray diffraction, Rietveld modeling, structure