

American Geophysical Union

Washington, D.C.

Dec 9-13, 2024

V41C-3151 Hydride incorporation in Ti perovskites

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**Abstract**

Studies of nominally anhydrous minerals (NAMs) in the mantle have long focused on the hydroxyl group (OH<sup>-</sup>) as the primary hydrogen species of interest. However, titanate perovskites in the (Ca,Sr,Ba)TiO<sub>3</sub> composition range demonstrate the ability to incorporate high concentrations of an alternate hydrogen species – the hydride (H<sup>-</sup>) ion. Considering the high solubility of Ti in Ca perovskites like davemaoite (CaSiO<sub>3</sub>), this presents the intriguing possibility of an unaccounted-for hydrogen reservoir in earth's mantle. Even so, questions remain surrounding hydride incorporation in mantle perovskites, including: How is H<sup>-</sup> solubility constrained by pressure, temperature and fO<sub>2</sub>? How would H<sup>-</sup> partition between perovskite and Fe<sup>0</sup> or FeH<sub>x</sub> phases? Identifying and characterizing H<sup>-</sup> in these materials, which carries unique technical challenges, will be critical for such future studies. Here, we present our efforts to characterize hydride-doped Ti perovskites primarily via infrared and <sup>1</sup>H nuclear magnetic resonance spectroscopies. These efforts encompass both naturally derived and synthetic materials, with particular focus on the SrTiO<sub>3</sub> and CaTiO<sub>3</sub> members of the titanate perovskite family. Density functional theory (DFT) calculations are crucial for interpreting spectroscopic measurements and provide a pathway to analyze hydride's possible coupling to the CaTiO<sub>3</sub> component of davemaoite. This work represents the first steps towards contextualizing the role of hydride in earth's mantle, and possibly the interiors of other planets.