

LETTER

HP-PdF₂-type FeCl₂ as a potential Cl-carrier in the deep Earth

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ABSTRACT

We report for the first time the formation of a HP-PdF₂-type FeCl₂ phase (space group $Pa\bar{3}$), through high pressure-temperature (P - T) reactions in the hydrous systems (Mg_{0.6}Fe_{0.4})SiO₃-H₂O-NaCl and FeO₂H-NaCl in a laser-heated diamond-anvil cell up to 108 GPa and 2000 K. Applying single-crystal X-ray diffraction (XRD) analysis to individual submicrometer-sized grains, we have successfully determined the crystal structure of the as-synthesized FeCl₂ phase, in agreement with our theoretical structure search results. In situ high P - T XRD data revealed the substitution of Cl for OH(O) in such a cubic $Pa\bar{3}$ structure, demonstrating that this topology is a potential host for both H and Cl in the deep Earth. The chemical analysis of the recovered sample showed that the post-perovskite phase contains considerable amounts of Na₂O and Fe₂O₃. The coexistence of the cubic FeCl₂ phase and post-perovskite suggests that the lowermost mantle could be a potential reservoir of Cl. The possible presence of volatiles such as H and Cl in the deep lower mantle would impact the composition and iron valence state of the post-perovskite phase.

Keywords: Iron chloride, multigrain X-ray diffraction, lower mantle, hydrogen and chlorine cycle, post-perovskite; Physics and Chemistry of Earth's Deep Mantle and Core