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Letter

HP-PdF_2-type $FeCl_2$ 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-PdF_2-type $FeCl_2$ phase (space group $Pa\bar{3}$), through high pressure-temperature (*P-T*) reactions in the hydrous systems $(Mg_{0.6}Fe_{0.4})SiO_3$–H_2O–NaCl and FeO_2H–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 $FeCl_2$ 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 Na_2O and Fe_2O_3. The coexistence of the cubic $FeCl_2$ 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