

Phase transitions in ϵ -FeOOH at high pressure and ambient temperature

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ABSTRACT

Constraining the accommodation, distribution, and circulation of hydrogen in the Earth's interior is vital to our broader understanding of the deep Earth due to the significant influence of hydrogen on the material and rheological properties of minerals. Recently, a great deal of attention has been paid to the high-pressure polymorphs of FeOOH (space groups $P2_1nm$ and $Pnmm$). These structures potentially form a hydrogen-bearing solid solution with AlOOH and phase H ($MgSiO_4H_2$) that may transport water (OH^-) deep into the Earth's lower mantle. Additionally, the pyrite-type polymorph (space group $Pa\bar{3}$ of FeOOH), and its potential dehydration have been linked to phenomena as diverse as the introduction of hydrogen into the outer core (Nishi et al. 2017), the formation of ultralow-velocity zones (ULVZs) (Liu et al. 2017), and the Great Oxidation Event (Hu et al. 2016). In this study, the high-pressure evolution of FeOOH was re-evaluated up to ~ 75 GPa using a combination of synchrotron-based X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and optical absorption spectroscopy. Based on these measurements, we report three principal findings: (1) pressure-induced changes in hydrogen bonding (proton disordering or hydrogen bond symmetrization) occur at substantially lower pressures in ϵ -FeOOH than previously reported and are unlikely to be linked to the high-spin to low-spin transition; (2) ϵ -FeOOH undergoes a 10% volume collapse coincident with an isostructural $Pnmm \rightarrow Pnmm$ transition at approximately 45 GPa; and (3) a pressure-induced band gap reduction is observed in FeOOH at pressures consistent with the previously reported spin transition (40 to 50 GPa).

Keywords: Phase transitions, infrared-spectroscopy, optical absorption spectroscopy, X-ray diffraction, spin transition; Volatile Elements in Differentiated Planetary Interiors