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High-pressure behavior of the polymorphs of FeOOH

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Abstract

The high-pressure structural and electronic behavior of α-, β-, and γ-FeOOH were studied in situ using a combination of synchrotron X-ray diffraction (XRD) and X-ray emission spectroscopy (XES). We monitored α-FeOOH by XES as a function of pressure up to 85 GPa and observed an electronic spin transition that began at approximately 50 GPa, which is consistent with previous results. In the γ-FeOOH sample, we see the initiation of a spin transition at 35 GPa that remains incomplete up to 65 GPa. β-FeOOH does not show any indication of a spin transition up to 65 GPa. Analysis of the high-pressure XRD data shows that neither β-FeOOH nor γ-FeOOH transform to new crystal structures, and both amorphize above 20 GPa. Comparing our EOS results for the β and γ phases with recently published data on the α and ε phases, we found that β-FeOOH exhibits distinct behavior from the other three polymorphs, as it is significantly less compressible and does not undergo a spin transition. A systematic examination of these iron hydroxide polymorphs as a function of pressure can provide insight into the relationship between electronic spin transitions and structural transitions in these OH- and Fe^{3+}-bearing phases that may have implications on our understanding of the water content and oxidation state of the mantle.

Keywords: Spin transitions, high-pressure studies, XES, FeOOH, XRD data