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Revealing crystal structure of hexagonal (Fe,Al)OOH$_x$ (HH-phase)

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Hydrous minerals can deliver water into the deep Earth interiors by subduction and store it from the time Earth was formed. Presence of water can have effect on the Earth's mantle electrical conductivity, melting temperature, viscosity *etc.* Many studies were devoted to the revealing a role of iron oxides (like cubic FeO_2) and their hydrous analogs (such as FeO_2H_x) in the Earth's water cycle and formation of the ultra-low velocity zones. Recently, it was reported that at the conditions of the Earth's lower mantle (107–136 GPa and 2400 K) $FeOOH_x$ can incorporate some amount of aluminum forming a new phase [1]. So-called "HH-phase" was suggested to be a potential candidate for water storage in the deep lower mantle.

Despite potential importance of HH-phase for understanding the Earth's deep water cycle, the information about its crystal structure was absent and chemical composition remain ambiguous. We have synthesized HH-phase by thermal decomposition of $(Fe_{0.7}Al_{0.3})OOH$ starting material at 110 GPa and 2300 K. Based on the single-crystal X-ray diffraction in laser-heating diamond anvil cells we managed to solve and refine the crystal structure of HH-phase, identify its chemical composition and measure bulk compressibility on decompression from 110 GPa. Moreover, a phase with the same crystal structure can be obtained by the thermal decomposition of anhydrous oxides such as Fe_3O_4 and Fe_2O_3. At the same pressure, differences between unit cell volumes of HH-phases obtained from various precursors remain insignificant, suggesting minor content or even absence of water in the studied samples.

[1] Zhang, Yuan, Meng & Mao (2018), *PNAS* 115, 2908-2911.