High-Pressure Synthesis of Novel Polyhydrides of Zr and Hf with Th₄H₁₅-type Structure

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Figure S1. Energy-dispersive X-ray diffraction patterns of Zr hydrides (shifted vertically for clarity) in a hydrogen atmosphere measured during compression in a DAC in run 1. The peaks at E < 19 keV are fluorescence emission lines from zirconium; other peaks are of a diffraction origin. The scattering angle $2\theta = 12.19^{\circ}$, corresponding to $E^*d = 58.4$ keV*Å. The black ticks indicate the calculated peak positions for ZrH₂ at ambient pressure (ThH₂-type with a = 3.52 Å, c = 4.46 Å). The magenta ticks show the calculated positions of the peaks from new zirconium hydride Zr₄H₁₅ at P = 16.2 GPa (cI16-type with a = 7.86 Å). The orange curve labeled "Re gasket" shows a diffraction pattern from the strongly textured rhenium gasket measured at 11GPa.