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In-situ high pressure X-ray diffraction of phase E to 15 GPa

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ABSTRACT

In-situ high pressure X-ray diffraction of phase E (free of secondary phases) measured up to 14.5 GPa shows that phase E is stable over this pressure range at room temperature. The pressure dependence of the lattice parameters are $a = 2.967 - 0.011P + 0.0001P^2$ and $c = 13.886 - 0.054P + 0.001P^2$ (P is in GPa). A least-squares fit to third-order of Eulerian strain theory yields a bulk modulus K_{T0} for phase E of 93 (±4) GPa and pressure derivative K'_{T0} of 5 (±1). The bulk modulus obtained by this study is about 10% lower than that obtained by Brillouin scattering. Phase E appears to have the lowest bulk modulus among DMHS. The OH stretching frequency of 3613 cm^{-1} indicates weak, if any, hydrogen bonding. The associated O-O distance of phase E is estimated to be 3.00–3.10 Å.