Change in compressibility of δ-AlOOH and δ-AlOOD at high pressure: A study of isotope effect and hydrogen-bond symmetrization

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ABSTRACT

The compression behaviors of δ-AlOOH and δ-AlOOD were investigated under quasi-hydrostatic conditions at pressures up to 63.5 and 34.9 GPa, respectively, using results from synchrotron X-ray diffraction experiments conducted at ambient temperature. Because of the geometric isotope effect, at ambient pressure, the a and b axes of δ-AlOOD, which define the plane in which the hydrogen bond lies, are longer than those of δ-AOOH. Under increasing pressure, the a and b axes of δ-AlOOH stiffen at 10 GPa, although the c axis shows no marked change. Identical behavior was found in δ-AlOOD, but the change in compressibility was observed at a slightly higher pressure of 12 GPa. Axial ratios a/c and b/c first decrease rapidly with increasing pressure, then begin to increase at pressures >10 GPa in δ-AlOOH and >12 GPa in δ-AlOOD. At these pressures, the pressure dependence of a/b also changes from increasing to decreasing. The unit-cell volumes of δ-AlOOH and δ-AlOOD become slightly less compressible at high pressures. Assuming $K_0' = 4$, the calculated bulk moduli of δ-AlOOH below and above 10 GPa are 152(2) and 219(3) GPa, respectively. Those of δ-AlOOD below and above 12 GPa are 151(1) and 207(2) GPa, respectively.

Keywords: δ-AlOOH, δ-AlOOD, hydrogen bond, symmetrization, high pressure, isotope effect