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Variation of hydrogen bonded O···O distances in goethite at high pressure

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ABSTRACT

In-situ synchrotron X-ray powder diffraction experiments on goethite were performed up to 24.5 GPa using a diamond-anvil cell at BL-18C in the Photon Factory, Japan. The compression behavior of goethite is anisotropic: the **a** axis, which is close to the direction of the hydrogen bond, is almost twice as compressible as the **b** and **c** axes. A second-order Birch-Murnaghan fit ($K' = 4$) to the unit-cell volumes and pressures up to 24 GPa gave a bulk modulus $K_0 = 111(2)$ GPa. The pressure medium apparently affects the compression behavior of goethite, as a sudden strain broadening occurs above 11 GPa, where solidification of the 4:1 methanol:ethanol pressure medium occurs. The crystal structure of goethite was refined by means of the Rietveld method at several pressures below 10 GPa. The main compression occurs in the "vacant channels" in the crystal structure, where the O-H···O bridges are located. The hydrogen-bonded O···O distance shortens with increasing pressure at the rate of about -0.023 Å/GPa and reaches 2.60(1) Å at 9 GPa.