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Single-crystal structure refinement of diaspore at 50 GPa

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Abstract

The crystal structure of diaspore, AlO(OH), has been investigated by in situ single-crystal synchrotron X-ray diffraction at ~50 GPa using the diamond-anvil cell technique. Diaspore is found to retain its structure up to 51.5 GPa at room temperature, which is more than 30 GPa above the transition pressure to δ-AlO(OH) found in quenched high-temperature experiments and derived from density functional theory calculations. The compression is anisotropic and largest for the **a** axis. This can be explained by the fact that the structural response to pressure is mainly due to the shortening of the hydrogen bond, which is oriented nearly parallel to the **a** axis. The hydrogen bond becomes significantly more symmetric with pressure up to 50 GPa.

Keywords: Diaspore, high pressure, crystal structure, synchrotron radiation, single crystal