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# Crystal chemistry and high-temperature behavior of Al-bearing stishovite and Al-rich phase D: Implications for water storage in the deep mantle

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## Abstract

High-quality single crystals of Al-bearing stishovite and Al-rich phase D were analyzed using X-ray diffraction, high-temperature Raman, and FTIR spectroscopy. The samples were synthesized in the $MgO$-$SiO_2$-$Al_2O_3$-$H_2O$ system at 25 GPa, 1350–1600 °C. The results demonstrate that Al-bearing $SiO_2$ glass formed by the amorphization of stishovite under high-temperature conditions can incorporate water in the form of hydroxyl groups, with a concentration of at least several hundred ppm $H_2O$ by weight. $Al^{3+}$ prefers to enter the crystal structure of phase D by substituting for $Si^{4+}$ in the M2 site. Since $Al^{3+}$ can be charge-balanced by $H^+$, the Al-rich phase D may have a higher water storage capacity than pure Mg-phase D. Raman and infrared spectral features of Al-rich phase D at ambient temperature can still be observed up to 350 °C. This indicates that, compared to pure Mg-phase D, Al-rich phase D maintains stability at higher temperatures. Al-rich silicate glass formed by the amorphization of phase D under high-temperature conditions can also retain water in the form of hydroxyl groups. In the deep mantle, Al-rich silicate glasses and Al-bearing $SiO_2$ glasses may serve as potential reservoirs of water (hydrogen) in high-temperature regions beyond the ideal stability fields of dense hydrous magnesium silicates and high-pressure $SiO_2$ phases.

**Keywords:** Stishovite, phase D, hydrogen, lower mantle, crystal structure