

Formation of hydrous stishovite from coesite in high-pressure hydrothermal environments

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ABSTRACT

In low-temperature, high-pressure hydrothermal environments coesite transforms into hydrous forms of stishovite. We studied hydrous stishovite produced from hydrothermal treatment of silica glass as initial SiO₂ source at temperatures of 350–550 °C and pressures around 10 GPa. The *P-T* quenched samples were analyzed by powder X-ray diffraction (PXRD), scanning electron microscopy (SEM), thermal analysis, and IR and magic-angle spinning (MAS) NMR spectroscopy. The presence of significant amounts of H₂O (ranging from 0.5 to 3 wt%) is shown from thermogravimetric measurements. PXRD reveals that at temperatures below 400 °C, hydrous stishovite is obtained as two distinct phases that may relate to the solid ice-VII environment present at prevailing *P-T* conditions. Initially formed hydrous stishovite is metastable and dehydrates over time in the low-temperature, high-pressure hydrothermal environment. The primary mechanism of H incorporation in stishovite is a direct substitution of 4H⁺ for Si⁴⁺ yielding unique octahedral hydrogarnet defects. In IR spectra this defect manifests itself by two broad but distinct bands at 2650 and 2900 cm⁻¹, indicating strong hydrogen bonding. These bands are shifted in the deuteride to 2029 and 2163 cm⁻¹, respectively. Protons of the octahedral hydrogarnet defect produce ¹H MAS NMR signals in the 9–12 ppm region. The presence of multiple resonances suggests that the octahedral defect is associated with various proton arrangements. At elevated temperatures, the NMR signals narrow considerably because of proton dynamics.

Keywords: Coesite-stishovite transition, hydrous minerals, octahedral defects, high-pressure hydrothermal environments