

Polarized infrared spectroscopic study of diffusion of water molecules along structure channels in beryl

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ABSTRACT

Incorporation of water in anhydrous synthetic beryl was studied at 500–700 °C and 50–150 MPa of confining water pressure to measure the diffusion of water molecules along the channels in a cyclosilicate. A series of polarized IR spectra series were taken with **E** parallel to the channel direction, which is parallel to the *c*-axis, along a traverse parallel to this axis. Water concentration profiles were determined from absorbance of H₂O peaks. The IR spectra showed that the dominant diffusing species is type I water molecule, whose H-H vector is parallel to the *c*-axis (sharp peak at 3700 cm⁻¹). No pressure dependence on water diffusivity can be recognized under these experimental conditions. The Arrhenius relation gives the activation energy of 133 ± 12 kJ/mol, with a pre-exponential factor of 10^{-2.6} (cm²/s). Diffusion of water is much faster in the beryl channels than volume diffusion in other silicates, but the activation energy and diffusion coefficient values for beryl are similar to the corresponding values previously reported for grain boundary diffusion in quartz aggregates.

Keywords: Water molecule, cyclosilicate, beryl channels, fast diffusion, IR spectroscopy