Water Diffusion into Synthetic Beryl Channel at 500-700C, 50-100MPa

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Beryl (Be3Al2Si6O18) is a typical cycrosilicate found in pegmatite. The crystal structure of beryl is characterized by rings of six SiO4 tetrahedrons. The rings are connected with BeO4 tetrahedron and AlO6 octahedron, stacks along the c axis, and makes a long cavities. The cavity is often called channel. Many studies on extra molecules in the channel of natural beryl, such as H2O, CO2 and alkali ions have been reported by many spectroscopy and X ray, neutron diffraction. Alkali ions in the channel are introduced to compensate charge balance by the replacement of Be2+ or Al3+ with other ions. Depending on temperature, pressure and H2O fugacity during beryl growth, the number of H2O molecules varies in beryl channel. Cordierite, which is commonly found in contact and regionally metamorphosed rocks, has similar structure to beryl.

Two types of H2O molecules have been recognized by the difference of direction. H2O which locates its H-H direction parallel to the c axis in the channel is labelled as TypeI. H2O which locates its H-H direction perpendicular to the c axis is TypeII. The rotation of the direction of H2O molecules is attained by the attraction of alkali ion close to it.

To investigate the H2O contents in beryl channel under various temperature and pressure, we observed diffusion of H2O into the beryl channel. First, we synthesized unhydrous single crystal beryl of about 1mm as a starting material by flux method using MoO3-Li2CO3. No water in a thin section of synthetic beryl was confirmed by no peaks around 3000-4000cm-1. The synthetic beryls were used for diffusing water into beryl channel. A few beryls and water about 5-15 micro liters enclosed in gold capsule, were kept 36-360h, 500-700C, 50-150MPa in hydrothermal reactor.The recovered samples were made into polished thin sections parallel to the c axis. Two peaks around 3700cm-1 and 3603cm-1 were observed in the recovered samples. They are assigned to TypeI and TypeII H2O respectively. TypeII H2O results from alkali ion in the channel. Li+ is a candidate of alkali ion in the channel since Li2CO3 used as flux for synthesizing beryl. Polarized IR spectra were measured along c axis from rim to core every 100 micro meters. H2O contents were maximum at rim and decreased toward the core of crystal. IR measurements perpendicular to c axis results in almost the same absorption peaks. This indicates that H2O molecules diffuse into the beryl structure along the channel direction. Along the c axis from rim to core, line profiles of absorption due to the H2O molecular vibration in 3000-4000cm-1 were measured. Total amounts of H2O molecules diffused into beryl channel were estimated from normalized absorbance due to TypeI and II. Diffusion coefficient and activation energy, under some temperature and pressure were calculated from the line profiles.