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Polarized IR study of water speciation in Nominally Anhydrous Minerals: danburite

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The crystal structure of Anhydrous silicate minerals, which composed of mantle and crust, can be included a few hundreds ppm water content, as H_2O molecule and hydroxyl. In generally, these anhydrous minerals are called Nominally Anhydrous Minerals (NAMs).
NAMs are studied especially mantle minerals (ex, pyroxene, olivine, garnet, kyanite, rutile, coesite, spinel,zircon). Because of amount of water in deep earth can not be explained by hydrous minerals supplied by subduction zone, NAMs are thought play an important role in reserve and carry of water.
Water in NAMs will affect physical properties of mantle rocks such as melting temperatures, electro-conductivity, rheology, plutonism, volcanism and convection.
On the other hand almost crustal minerals are grouped into NAMs (ex, quartz, feldspar, pyroxene). These minerals are used to know thermodynamic properties and fluid evolution, water activity and oxidation state in the lower crust.
Danburite is a borosilicate mineral and has frame work structure, which composed of $BO_4$and SiO_4 tetrahedron in the structure.
This mineral is a one of the typical skarn mineral containing boron.
Beran(1987) discovered 0.04wt% water in crystal structure of danburite.
Danburite should be grouped into NAMs.
In this study, FT-IR observation and Chemical analysis using EPMA(EDS, WDS) were conducted to clarify hydrogen position, concentration of hydrogen in danburite structure and its relation to H^+ and the trace element such as Al, Na and major element B.
Four OH bands (3325, 3422, 3456 and 3577cm^{-1}) were confirmed in the crystal from the FT-IR spectra. The polarized FT-IR observation of four peaks showed that each peaks are absorbed at the specific directions. This polarized FT-IR results suggested OH dipoles in danburite structure would be oriented to specific directions.
>From the analysis based on the 3 restrictions, [1] Angles of OH in the crystal, [2] Bond-Valence Sum and [3] Distances between oxygens of hydrogen bridge. Hydrogen would be located between O3-O1, O1-O4, O1-O1, O5-O4.
Moreover, these positions are in the channel enclosed by Si and B tetrahedron in the structure.
According to the chemical composition analysis by EPMA (EDS and WDS) a decrease of Si content and an increase of B content were confirmed in the Hydrogen concentrated region.
Hydrogen should be incorporated in the mineral not only by the replacement of $Si^{4+}$and Al^{3+}+H^+but also by $Si^{4+}$and B^{3+}+H^+.

Keywords: Nominally anhydrous minerals, Danburite, Polarized FT-IR spectroscopy