

# An FTIR Calibration for Structural Hydrogen in Feldspars Using $^1\text{H}$ MAS NMR

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## Abstract

It is important to know how to determine the speciation and concentration of H in feldspars because this information could be used to determine primary magmatic water activity or to estimate the degree of hydrothermal alteration in igneous rocks. FTIR spectroscopy is sensitive to changes in speciation of hydrogen, and can be calibrated for quantitative determination of H concentration using  $^1\text{H}$  MAS (magic-angle spinning) NMR spectroscopy. Three pegmatitic albites, one metamorphic albite, three volcanic plagioclases (albite, andesine, and anorthite) and one pegmatite oligoclase were used in this study to provide a range of plagioclase compositions. Two pegmatitic microclines and one sanidine were also studied. Polarized infrared spectra were obtained in the three principal optical directions for each specimen. Samples were prepared for  $^1\text{H}$  MAS NMR experiments at 12 kHz spinning speed in a dry box, without the use of a liquid grinding aid. A spectrum from anhydrous synthetic corundum was used as a baseline for feldspar NMR spectra. The pegmatitic and metamorphic albites are transparent, but contain submicroscopic fluid inclusions as evidenced by a broad band at  $3400\text{ cm}^{-1}$  and an asymmetric band at  $5200\text{ cm}^{-1}$  in the IR spectra that shift to bands characteristic of ice upon cooling to 77 K. These albites have a very sharp band at 4.7 ppm (relative to TMS) in their NMR spectra consistent with fluid inclusion water. In addition to the broad fluid inclusion band, the pegmatitic albites have sharp bands in the mid-IR similar the OH bands found in quartz. All other plagioclases have broad, anisotropic bands around  $3200\text{ cm}^{-1}$  in the mid-IR and MOH combination stretch-bend bands near  $4500\text{ cm}^{-1}$  in the near-IR, indicative of structural OH. The NMR spectra of these plagioclases have a broad band at 4.7 to 4.9 ppm TMS. The OH vector in plagioclases is preferentially aligned parallel to the *a* crystallographic axis. The concentration of structural OH in the plagioclases ranges from 50-200 ppm  $\text{H}_2\text{O}$  by weight. The microclines contain structural  $\text{H}_2\text{O}$  molecules (1000-1400 ppm  $\text{H}_2\text{O}$ ) and sanidine contains structural OH (170 ppm  $\text{H}_2\text{O}$ ). Plots of the total integrated mid-IR absorbance and total mid-IR peak height vs. concentration of structural H in plagioclase and alkali feldspars produce linear trends. Therefore, it is sufficient to use one absorption coefficient for both types of structural H (OH and  $\text{H}_2\text{O}$ ) in all feldspar compositions. The integral absorption coefficient for total mid-IR peak area is  $16\text{ ppm}^{-1}\cdot\text{cm}^{-2}$  or  $114000\text{ L}\cdot(\text{mol H}_2\text{O})^{-1}\cdot\text{cm}^{-2}$ . The absorption coefficient for total mid-IR peak

height is  $0.06 \text{ ppm}^{-1} \cdot \text{cm}^{-1}$  or  $418 \text{ L} \cdot (\text{mol H}_2\text{O})^{-1} \cdot \text{cm}^{-2}$ . Since most of the mid-IR band intensity occurs with  $E\|a$  in plagioclase, it may be possible to determine H concentration in plagioclase using a single polarized spectrum with  $E\|a$ , facilitating the measurement of H concentration in fine-grained or twinned natural feldspars.