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The concentration and speciation of hydrogen in feldspars using FTIR and ^{1}H MAS NMR spectroscopy

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ABSTRACT

A universal absorption coefficient was determined for quantitative analysis of OH and H_2O in feldspars using infrared spectroscopy. ^{1}H MAS (magic-angle spinning) NMR spectroscopy was used to determine the H concentration in three alkali feldspars, and for the first time, eight plagioclase samples. To accurately measure structural H concentration in samples with low H (<1000 ppm H_2O) it was necessary to eliminate the signal due to adsorbed water in the powdered NMR sample. The pegmatitic and metamorphic albite samples are transparent, but contain variable (40–280 ppm H_2O) concentrations of microscopic to sub-microscopic fluid inclusions. The pegmatitic albites also have sharp bands in the mid-IR similar to the OH bands found in quartz. The other plagioclase samples used in the IR calibration have broad anisotropic bands around 3200 cm^{-1} in the mid-IR and weak combination stretch-bend bands near 4550 cm^{-1} in the near-IR, indicative of structural OH. The OH vector in plagioclase is preferentially aligned parallel to the crystallographic **a** axis. The concentration of structural OH in the plagioclase samples ranges from 210–510 ppm H_2O by weight. The microcline samples contain structural H_2O molecules (1000–1400 ppm H_2O) and the sanidine sample contains structural OH (170 ppm H_2O). An approximately linear trend is produced when the total integrated mid-IR absorbance is plotted vs. the concentration of structural H determined from NMR (OH and H_2O) for plagioclase and alkali feldspars. The integral absorption coefficient for the total mid-IR peak area is 15.3 ± 0.7 $ppm^{-1} \cdot cm^{-2}$ [107000 ± 5000 L/(mol $H_2O \cdot cm^2$)] for natural feldspar samples that contain structural OH or H_2O. Measurements of band areas of unpolarized IR spectra on (001) cleavage fragments provide an estimate of H concentration for alkali feldspars, but this method does not work for most plagioclase samples.