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Hydrous species in feldspars: A reassessment based on FTIR and SIMS

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Abstract

Recent interest in hydrogen incorporation in feldspars has been driven by the potential of this common mineral species to record magmatic water contents. Accurate measurement of H concentrations in feldspars by Fourier transform infrared (FTIR) spectroscopy is hampered by the need to collect polarized spectra in three mutually perpendicular directions, which can be impractical for crystals characterized by small dimensions, polysynthetic twinning, and/or chemical zoning. SIMS is an attractive alternative to FTIR, offering high spatial resolution, high precision, and the feasibility of attaining low detection limits. In this study we compare FTIR and SIMS data for 19 feldspars, including plagioclase, anorthoclase, sanidine, microcline, and orthoclase. We present adjustments to previously published FTIR data on some of these samples. Our new SIMS and FTIR data are well correlated and we demonstrate the feasibility of quantitatively measuring H concentrations as low as 1–2 ppmw H_2O using SIMS. Combination of the new data together with re-evaluation of the NMR calibration of Johnson and Rossman (2003) indicates that the IR absorption coefficients for hydrous species in feldspar increase with decreasing frequency of their O-H absorptions, in accord with theory. We derive new molar integral IR absorption coefficients (I) for feldspars with the following hydrous species as defined by Johnson and Rossman (2003):

Type I and II H_2O (microcline and orthoclase): $I = 120\,470 \pm 11\,360$ L·mol^{-1} H_2O cm^{-2}
Type IIb OH (sanidine): $I = 150\,000 \pm 15\,000$ L·mol^{-1} H_2O cm^{-2}
Type IIa OH (plagioclase and anorthoclase): $I = 202\,600 \pm 20\,260$ L·mol^{-1} H_2O cm^{-2}

These absorption coefficients depend on critical assumptions with regards to SIMS matrix effects. If accurate, one important implication is that the H concentrations of plagioclase crystals estimated in the literature are too high by up to a factor of two, requiring revision of previously estimated plagioclase-melt H partitioning coefficients.

Keywords: FTIR, SIMS, feldspar, calibration, nominally anhydrous minerals, hygrometry, water, crust