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Intercalibration of FTIR and SIMS for hydrogen measurements in glasses and nominally anhydrous minerals

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Abstract

We present new Fourier Transform Infrared Spectroscopy (FTIR) and ion microprobe/secondary ion mass spectrometry (SIMS) analyses of ^{1}H in 61 natural and experimental geological samples. These samples include 8 basaltic glasses (0.17 to 7.65 wt% H_2O), 11 rhyolitic glasses (0.143 to 6.20 wt% H_2O), 17 olivines (~0 to 910 wt. ppm H_2O), 9 orthopyroxenes (~0 to 263 wt. ppm H_2O), 8 clinopyroxenes (~0 to 490 wt. ppm H_2O), and 8 garnets (~0 to 189 wt. ppm H_2O). By careful attention to vacuum quality, the use a Cs^+ primary beam, and a resin-free mounting technique, we routinely achieve hydrogen backgrounds equivalent to less than 5 ppm by weight H_2O in olivine. Compared to previous efforts, the new calibration extends to a wider range of H_2O contents for the minerals and is more reliable owing to a larger number of standards and to characterization of anisotropic minerals by polarized FTIR on oriented crystals. When observed, discrepancies between FTIR and SIMS measurements are attributable to inclusions of hydrous minerals or fluid inclusions in the crystals. Inclusions more commonly interfere with FTIR analyses than with SIMS, owing to the much larger volume sampled by the former. Plots of H_2O determined by FTIR vs. $(^{1}H/^{30}Si) \times (SiO_2)$, determined by SIMS and electron microprobe (EMP) yield linear arrays and for each phase appear to be insensitive to bulk composition. For example, basalt and rhyolite calibration slopes cannot be distinguished. On the other hand, calibration slopes of different phases vary by up to a factor of 4. This reflects either phase-specific behavior of $^{1}H/^{30}Si$ secondary ion ratios excited by Cs^+ ion beams or discrepancies between phase-specific FTIR absorption coefficient schemes.

Keywords: Spectroscopy, infrared, water, mantle, ion microprobe