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Intercalibration of FTIR and SIMS for Hydrogen Measurements in Garnets

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The importance of understanding the hydrogen incorporated in nominally anhydrous minerals (NAMs) that influences their physical and chemical properties significantly is well accepted, however, quantitatively experimental constraints between hydrogen concentration and physical and chemical properties are only meaningful if hydrogen concentration can be accurately determined. Fourier Transform Infrared Spectroscopy (FTIR) may be the most powerful technique since it provides information about both bulk concentration and local bonding environments, while Secondary Ion Mass Spectrometry (SIMS) has held promise as an ideal method for hydrogen analyses for its advantages of high spatial resolution and insensitivity to crystal orientation. Great efforts have been made to establish experimental standards for these two techniques since they have no rigorous self-calibration. We here present new Fourier Transform Infrared Spectroscopy (FTIR) and Secondary Ion Mass Spectrometry (SIMS) analyses of 1H in 11 natural garnets (grossular, spessartite and pyrope). This set of garnets extends to a wider range of H₂O contents (~4 to 6790 wt. ppm H₂O) than previous studies and can be more reliable if more garnets can be investigated. We routinely achieve a less than 5 ppm by weight H₂O with high vacuum quality, the use of a Cs⁺ primary beam, and carefully prepared samples using a resin-free mounting technique (described in Aubaud C. et al., 2007).

Intercalibration of FTIR and SIMS for hydrogen measurements in glasses and nominally anhydrous minerals. *American Mineralogist*, 92, 811-828). Although some scatter is observed, the straight line with a slope of 0.0722 defined by all garnets in a plot of (H)FTIR vs. (H+/Si+)SIMS* (SiO₂)EMP suggests small matrix effects, while some previous efforts demonstrated the existence of such matrix effects. Discrepancies between FTIR and SIMS measurements can be partially distributed to the impurities, which have different hydrogen concentration as the host crystals, because much larger volume is sampled by FTIR than SIMS.
