Accurate measurement of H_2O concentration and speciation in silicate glasses using FTIR spectroscopy

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Accurate measurement of H_2O concentration and speciation in silicate glasses is important not only for studies of erupted glasses that use the volatile record to reconstruct eruption processes, but also for studies that use experimental glasses to find e.g. the partition coefficients of other volatiles that partition into H_2O-rich vapour. Fourier Transform Infrared (FTIR) spectroscopy can be used to find not only the overall H_2O concentration (H_2O_t) of silicate glasses, but also the individual concentrations of the two H_2O species: molecular H_2O (H_2O_m), and dissociated hydroxyl groups (OH). Here we discuss key developments and refinements of FTIR methodology with respect to finding the water contents of silicate glasses. Firstly, we demonstrate the importance of using a species-dependent H_2O_t molar absorptivity coefficient when using the 3500 cm^{-1} H_2O_t absorbance peak to find H_2O_t and OH (indirectly as $[OH] = [H_2O_t] - [H_2O_m]$) concentrations, and in particular how this can be used to reconstruct the original H_2O contents of glasses that have since undergone secondary hydration at low temperature. Secondly, we discuss the strong dependence on glass composition of 'silicate peaks' at ~1830 cm^{-1} and ~1600 cm^{-1}, and demonstrate how the 1830 cm^{-1} peak can be used to correct FTIR imaging of H_2O concentrations in samples of varying glass thickness, and how the superposition of the 1630 cm^{-1} H_2O_m and 1600 cm^{-1} silicate peaks may result in overestimation of H_2O_m concentration in thick and/or H_2O_m-poor samples.

Keywords: FTIR spectroscopy, H2O speciation, volcanic glass

