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Application of Raman spectroscopy to quantify trace water concentrations in glasses and garnets

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Abstract

We present a new technique for the quantification of water in glasses down to the parts per million level, using confocal microRaman spectroscopy with the recently developed "Comparator Technique." To test this method, we used a suite of glasses and gemstone-quality garnets with varying chemical compositions. Water contents were independently determined with proton-proton (pp) scattering and infrared (IR) spectroscopy. Moreover, water concentrations obtained for the garnets were compared to data from a study by Maldener et al. (2003) using nuclear reaction analysis (NRA). For each sample, we recorded Raman spectra in the frequency range from 3100 to 3750 cm^{-1} and standardized them using an independently well-characterized glass. In this paper, we demonstrate the usefulness of this technique for quantifying water concentrations in natural and synthetic glass samples and garnets, and verify its adaptability for concentrations from 40 wt ppm up to 40 wt% H_2O. However, in the case of absorbing material (e.g., Fe-bearing samples), the suggested method needs to be modified to overcome problems due to heating and melting of those phases. Furthermore, we propose an integrated molar absorption coefficient for water in quartz glass, $\varepsilon_{itot} = 72\,000 \pm 12\,000$ $Lmol^{-1}_{H_2O}cm^{-2}$, for quantitative IR spectroscopy that is higher than a previously reported value of Paterson (1982) or that predicted by the general calibration trend determined by Libowitzky and Rossman (1997).

Keywords: Raman spectroscopy, glasses, garnet, water determination, proton-proton scattering, FTIR spectroscopy