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A Protocol, a standard and a (PULI) database for quantitative micro-FTIR measurements of water in nominally anhydrous minerals: an update

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'Water' (H_2O, OH and H+) in the nominally anhydrous minerals (NAMs) of the upper mantle play a key role in determining its geochemical and geophysical properties. Both the concentration and the substitution mechanism of water are important to formulate its effect on material properties. Fourier-transform infrared (FTIR) spectrometry can provide both qualitative and quantitative information on the substitution of water into NAMs, therefore, it is a widely used analytical technique. The quantitative evaluation of micro-FTIR mineral spectra, however, seems to be still rather ambiguous. This is because there are several different – sometimes controversial – ways to measure or estimate the total polarized integrated absorbance (Atot). Furthermore, there are mineral-, substitution mechanism- and wavenumber-dependent calibrations factors available to convert Atot to the absolute concentration of water (usually given in ppm wt.%). No wonder that very different absolute water concentrations may be obtained from the very same IR spectrum. Thus, there is certainly a need for an evaluation protocol which would reduce these uncertainties giving clear instructions how Atot should be obtained and what calibrations factors should be used. This will be introduced in our study.

Inter laboratory differences were monitored by analysing the some unoriented grains of the Pakistani olivine standard using different brands of infrared microscopes in several different countries and laboratories worldwide. During these measurements optimal measurement settings for the IR analysis of NAMs were constrained. The results show that the inter laboratory deviations are typically less than 10%. To put constraints on the micro-scale (<50 microns) distribution of water in the Pakistani olivine standard high resolution infrared maps were recorded using a synchrotron light source. The hyper spectral images revealed small-scale heterogeneities within the crystals which otherwise could not have been observed with the aperture size of routine micro-FTIR analysis.

Over the last decades several papers and books, dealing with various aspects of water in NAMs reported numerous infrared spectra. To keep up with this rising numbers of infrared spectra an electronic spectral database would be desirable. This was the motivation why we have constructed the Pannon Uniform Lithosheric Infrared (PULI) spectral database (puli.mfgi.hu), which by now include over a 1000 spectra of olivine and pyroxenes from the shallow upper mantle. The spectra were collected in uniform electronic formats (txt or xls) which will facilitate the comparison and quantitative re-evaluation.