



## **Re-evaluating the concentration of water in olivines from the shallow upper mantle with a uniform FTIR protocol and a unique international spectral database: PULI**

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“Water” in the nominally anhydrous minerals (NAMs), especially in olivine being the most abundant constituent of the upper mantle, is considered to play a significant role in determining the rheological, seismic, and melting properties. Both the concentration and the way how water is incorporated is important to understand and formulate the effect of “water” on these properties. The qualitative information appears to be better constrained than the quantitative as the assignment of infrared bands to particular substitution mechanisms is relatively well known for olivine. Our goal is two-fold: 1) To outline a protocol for future quantitative infrared studies of olivine (and NAMs in general) and 2) the application of this protocol to a large number (~700) of recently digitalised olivine infrared spectra comprising part of a complex database for the shallow (<200 km) upper mantle (PULI: Pannon Uniform Lithospheric Infrared spectral database). The digitalised spectra for olivine were all published in leading international journals typically in the last two decades.

Our ultimate aim is to reveal unambiguously the quantitative trends which “water” content in olivine shows with various physical properties such as pressure, temperature and oxygen fugacity.

This is because previous FTIR studies applied different radiations and different analytical protocols which introduced non-systematic errors in the absolute qualitative results, therefore, hampered the recognition of the real trends. The most problematic part of quantitative infrared spectroscopy is the use of both polarized and unpolarized radiations, and the application of mineral-, substitution mechanism- and wavenumber-dependent calibrations for determining absolute concentrations. It has been demonstrated that there is a systematic relationship over a wide range of absorption properties between polarized and unpolarized light, which would make it possible to re-evaluate and, thus, make comparable previous results. It was also shown that wavenumber-dependent calibrations give only a rough first-order approximation on water concentrations, but for more accurate results mineral- and substitution mechanism-dependent calibration should be used. The protocol would give instructions on both the analytical setup (i.e. sample preparation, microscope settings) and data evaluation (i.e. background subtraction, integration and calibration factors), which may facilitate the achievement of more accurate quantitative measurements and direct comparison of quantitative FTIR results in the future.