



IR-based Water Quantification in Nominally Anhydrous High-Pressure Minerals

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Infrared spectroscopy is a powerful tool to determine traces of OH and H₂O in minerals and glasses. The application is based on the Beer Lambert law $A = \varepsilon \cdot c \cdot t$, where A is the absorbance, ε the absorption coefficient, e.g. in $\text{L mol}^{-1} \text{H}_2\text{O cm}^{-2}$, c the concentration in mol/L and t the thickness in cm. It has been shown in numerous experimental and theoretical studies, i.e. Paterson (1982) and Libowitzky and Rossman (1997) that ε generally increases with decreasing wavenumbers. However, this general trend seems to be valid only for hydrous minerals and glasses and should not be applied to water quantification in nominally anhydrous minerals (NAMs) which incorporate traces of water in their structures (e.g. Rossman 2006, Thomas et al. 2009). For example, Bell et al. (2003) showed that if the general IR calibration of Paterson (1982) is adopted, the water concentration of olivine is underestimated by about 25 %. A similar result has been obtained by Deon et al. (2010) for Mg-wadsleyite. Thomas et al. (2009) evidenced using a large variety of analytical methods that not using mineral-specific IR-calibrations for the OH quantification in NAMs (e.g. SiO₂ polymorphs and olivine) leads to either underestimation as for olivine or overestimation of the water content as for stishovite and coesite. Thus, to quantify the water content of NAMs mineral specific absorption coefficients are needed but unfortunately only for a few minerals available.

In this study we propose that within a polymorphic mineral series of the same composition ε positively correlates with the density and negatively with the molar volume of the respective mineral phase. To prove this hypothesis we determined ε -values for synthetic hydrous ringwoodite samples ranging in composition from $x_{\text{Mg}} = 0.0$ to 0.6 by combining results of FTIR-spectroscopy with those of Secondary Ion Mass Spectrometry. The ε -values plot well below the general calibration curves of Paterson (1982) and Libowitzky and Rossman (1997) but follow the same trend, i.e. they increase with decreasing wavenumbers of the OH bands from 59000 ± 6000 for the Fe-endmember to $85800 \pm 10000 \text{ L mol}^{-1} \text{H}_2\text{O cm}^{-2}$ for the Mg-richest sample. From these data we can predict an absorption coefficient for the iron-free Mg-endmember as $100000 \pm 7000 \text{ L mol}^{-1} \text{H}_2\text{O cm}^{-2}$. This value together with ε -values for forsterite (Thomas et al. 2009) and wadsleyite (Deon et al. 2010) confirm the negative correlation with the molar volume and positive correlation with the density within this polymorphic series. This allows us to predict absorption coefficients for some minerals, where coefficients for one or better two of their polymorphs, either high- or low-pressure, are available.

References

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