American Mineralogist, Volume 95, pages 770–775, 2010

IR absorption coefficients for water in nominally anhydrous high-pressure minerals

Monika Koch-Müller[1,*] and Dieter Rhede[2]

[1]Sektion 3.3, Chemie und Physik der Geomaterialien, Deutsches GeoForschungsZentrum, Telegrafenberg, D-14473 Potsdam, Germany
[2]Sektion 4.2, Anorganische und Isotopengeochemie, Deutsches GeoForschungsZentrum, Telegrafenberg, D-14473 Potsdam, Germany

Abstract

Infrared spectroscopic quantification of traces of OH and H_2O in minerals and glasses is based on the Beer Lambert law $A = \varepsilon \cdot c \cdot t$, where ε is the molar absorption coefficient. Numerous experimental and theoretical studies show 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) that incorporate traces of water in their structures. In this study, we analyze ε-values from literature data and propose that within a polymorphic mineral series of the same composition ε negatively correlates with the molar volume and positively correlates with the density of the respective mineral phase. To test this hypothesis, we determined ε-values for synthetic hydrous ringwoodite samples ranging in composition from $X_{Mg} = 0.0$ 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 but follow the same trend, i.e., they increase with decreasing wavenumbers of the OH bands from 59 000 ± 6000 for the Fe end-member to 85 800 ± 10 000 L/mol(H_2O)/cm^{-2} for the Mg-richest sample. From this relation we can predict an absorption coefficient for the iron-free Mg end-member as 100 000 ± 7000 L/mol(H_2O)/cm^{-2}. This value together with ε-values for forsterite and wadsleyite taken from literature confirm the proposed correlation with the molar volume and 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.

Keywords: Infrared spectroscopy, absorption coefficient, ringwoodite, nominally anhydrous minerals