

Site-specific infrared O-H absorption coefficients for water substitution into olivine

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ABSTRACT

There are four ways by which OH⁻ commonly substitutes into olivine, namely those associated with (1) Si vacancies, (2) Mg vacancies, (3) Ti, or (4) trivalent cations. The four mechanisms, which we label [Si], [Mg], [Ti], and [triv], respectively, may each be fingerprinted by their characteristic O-H stretching modes in the infrared spectrum. We show by comparing the integrated intensities of these characteristic infrared peaks against total water content analyzed by secondary ion mass spectrometry, obtained for a suite of synthetic olivines plus one natural olivine, that the different substitution mechanisms require different absorption coefficients (*k*). For [Ti], we find $k = 0.18 \pm 0.07$, identical to the value previously obtained from natural olivines in which the water was mainly associated with [Ti] defects. Values of *k* for [Si] and [triv] are 0.57 ± 0.04 and 0.18 ± 0.05 , respectively; that for [Mg] is too small to be accurately determined (0.03 ± 0.03). The values of *k* for [Ti] and [Si] defects differ by a factor of three even though their average wavenumbers are virtually the same. The [Ti] and [triv] defects, on the other hand, have very similar absorption coefficients at significantly different wavenumbers. This highlights the inadequacy of using wavenumber-dependent calibrations for olivine and presumably for NAMs in general. Different substitution mechanisms have their own crystallographic environments that determine their absorption coefficients. The large variation in absorption coefficients within a single mineral emphasizes the importance of distinguishing the substitution mechanism if meaningful quantitative results are to be obtained from infrared spectroscopy.

Keywords: Nominally anhydrous minerals, olivine, infrared spectroscopy, secondary ion mass spectrometry, extinction coefficients