American Mineralogist, Volume 82, pages 1111–1115, 1997

An IR absorption calibration for water in minerals

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ABSTRACT

Using IR absorption data from polarized measurements on single-crystal minerals with stoichiometric water contents (in the form of H_2O or OH groups in the structure), a linear calibration curve ($r^2 \approx 0.98$) for water in minerals is established in the form: ϵ_i (the integrated molar absorption coefficient in units of cm^{-2} per mol H_2O/L) $= 246.6(3753 - \nu)$ (ν = the mean wavenumber of the OH stretching band [in cm^{-1}]). The investigated minerals include hydrogrossular, analcime, hemimorphite and its dehydrated phase, lawsonite, goethite, diaspore, manganite, mozartite, and pectolite. The influence of hydrogen bonding, leading to increased absorption values with lower OH stretching band energies, is confirmed. It is further shown that only the use of integrated absorbance values (band areas) results in a linear correlation with water content, whereas linear absorption data (peak heights) are not correlated. The calibration agrees with previously published quantitative IR data on staurolite and trace H in pyroxenes. It is also close to the frequently used trend of Paterson (1982). However, some of the previous calibrations of trace H in nominally anhydrous minerals, e.g., kyanite and pyrope, differ appreciably from the correlation derived from stoichiometrically hydrous minerals.