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Quantitative analysis of H-species in anisotropic minerals by unpolarized infrared spectroscopy: An experimental evaluation

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Abstract

Attempts have been made to use unpolarized infrared analyses on unoriented anisotropic crystals of nominally anhydrous minerals to determine H contents, rather than using the more demanding polarized techniques that are more accurate (given that a reliable calibration is available). In this context, different approaches have been either empirically or theoretically proposed for the quantification; however, the involved accuracy has not been systematically documented by experimental work of both polarized and unpolarized analyses. In this study, we present a careful evaluation of experimentally grown, gem-quality OH-bearing olivine, clinopyroxene, and orthopyroxene single crystals. The samples were prepared for polarized and unpolarized infrared analyses, and the obtained spectra were used to estimate the H_2O contents. We show that, regardless of the applied protocol, a single unpolarized determination is inadequate for quantitative analysis and the uncertainty could be up to ~80%. The unpolarized method of Paterson (1982), by considering the linear absorbance intensity either through a single analysis or by averaging the data from multi-grain analyses, commonly underestimates the H_2O content, by a factor of up to ~6. The other unpolarized calibration method by using the averages of integrated absorbances of unoriented grains is in general of good accuracy, mostly within ±25% even for analyses on 2 grains (with perpendicular indicatrix sections), and the accuracy is even better if as many as 10 gains of random orientations are involved, e.g., within ±10%. Therefore, the latter method may be safely applied to quantify H in anisotropic minerals if a reasonable number of randomly oriented grains are chosen for the analyses. However, the uncertainty is non-systematic, and both underestimates and overestimates of H are possible depending upon orientation. These results provide a basis for quantifying H-species in anisotropic minerals and for documenting the quantitative effect of H on the physical properties of the host phases.

Keywords: OH groups, quantitative analysis, unpolarized spectroscopy, infrared spectroscopy, nominally anhydrous minerals; Water in Nominally Hydrous and Anhydrous Minerals