

## QUANTITATIVE APPLICATIONS OF OPTICAL AND NEAR INFRARED SPECTROSCOPY

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Optical absorption spectroscopy has advanced to the state where it is possible to quantitatively determine the concentration of individual ions in a particular crystallographic site for a variety of minerals (e.g. orthopyroxene, amphibole, cordierite). The calibration data necessary are the wavelengths at which a particular ion absorbs light and the intensity of the absorption as a function of the concentration of the ion. Orthopyroxenes represent one of the best calibrated systems in which site occupancies determined by optical spectra, Mössbauer spectra, and X-ray structure refinements are in excellent agreement. Metal ions in larger, geometrically distorted sites (e.g. orthopyroxene M(2), amphibole M(4) and the channel sites of beryl and cordierite) have the greatest intensities and are the most favorable for quantitative study. The reequilibration of cations in samples quenched from high temperatures is readily determined.  $\text{Fe}^{2+}$  can be identified in both the M(1) and M(2) site of clinopyroxenes. The amount of  $\text{Fe}^{2+}$  in M(2) varies greatly among different samples as does the ratio of  $\text{Fe}^{2+}$  in the two sites. Experimental methods have been developed to study small areas which makes it possible to examine zoned ortho- and clinopyroxenes to determine the site occupancies of the individual zones and chemical zonation of minor elements such as  $\text{Cr}^{3+}$ . The intensities of intervalence absorption bands of  $\text{Fe}^{2+}/\text{Fe}^{3+}$  groupings commonly differ between the zones in amphiboles and pyroxenes suggesting redox zonation. Attempts to quantitatively determine the  $\text{Fe}^{3+}$  concentration in calcic amphiboles from the intensity of the intervalence absorption band are encouraging.