STRUCTURAL INFORMATION FROM QUANTITATIVE INFRARED SPECTRA OF MINERALS

George R. Rossman California Institute of Technology
Pasadena, Ca. 91125

Infrared spectroscopy of minerals, commonly performed on mineral powders, is capable of providing significantly more information when the anisotropy of single crystals is studied quantitatively. Transmission measurements in the near-infrared region (700 nm - 3000 nm) can be used to determine the oxidation state, site-occupancy and concentration of cations in minerals as well as the spatial distribution of cations in zoned crystals such as pyroxenes. Cations occurring in channels and voids in the structure of beryl and cordierite can be identified in addition to molecular species such as water. The orientation of the channel molecules in beryl, cordierite and milarite is determined from anisotropy studies of both the infrared fundamentals and the near-infrared overtones. X-ray amorphous minerals are also well-suited to infrared study. The disruption of structure in the radiation induced metamictization process produces major changes in the intensity and anisotropy of the infrared spectrum of zircon. Correlations have been established between the anisotropy of the infrared overtones in the spectra of zircon single crystals and the total radiation dose. Quantitative methods applied to powders also allow phase identification to be accomplished with quantitative difference procedures on mixtures of manganese oxides with other phases either too finely divided or too disordered to be identified by powder diffraction techniques. A large range of crystallographic order can be recognized in the infrared spectra of chain, ring and sheet manganese oxides.