GAUSSIAN ANALYSIS OF 1μm Fe$^{2+}$ ABSORPTIONS OF MAFFIC MINERALS.

The temperature dependence of characteristic spectral features of mafic minerals has been previously demonstrated(1). Using a portion of these data we have performed a gaussian analysis on Fe$^{2+}$ absorptions located near 1μm. A straight line continuum, chosen for simplicity and consistency, was fitted across the absorption bands and divided out from the data prior to fitting using a non-linear least squares gaussian routine(2). Actual fitting was done to the data in log reflectance versus energy. The results are presented in Figures 1, 2, and 3 for olivine, orthopyroxene, and clinopyroxene respectively. As reported previously(1), the 1μm true band minimum, where the reflectance relative to a continuum is a minimum, remains unchanged for all samples over the temperature range of this study.

OLIVINES Gaussians 2 and 4 correspond to electronic transitions due to Fe$^{2+}$ in the M(1) crystal site, while gaussian 3 corresponds to an electronic transition due to Fe$^{2+}$ in the M(2) crystal site(3). Crystal-field considerations would predict similar behavior for each band as a function of temperature. However, gaussian 2 exhibits anomalous behavior in its center and width trends. X-ray studies of olivine from below to above ambient temperature indicate a preferential expansion of the M(1) site along the x-y plane. The overall symmetry of the site is changed, possibly resulting in the .86μm transition moving to higher energies (gaussian center moving to shorter wavelengths), corresponding to the trend of gaussian 2 in Figure 1. The trends of gaussian 1 do not allow resolution of the source of this band.

PYROXENES The gaussian analysis of the pyroxenes resulted in two consistent gaussians being resolved. We have considered five mechanisms for our consistent 2-gaussian fits: 1) the gaussians represent separate electronic transitions due to Fe$^{2+}$ located solely in the M(2) crystallographic site in these minerals; 2) the gaussians represent electronic transitions due to Fe$^{2+}$ in both the M(1) and M(2) crystallographic sites; 3) the gaussians represent one allowed and one vibronically activated electronic transition; 4) the gaussians represent two discrete mineral phases; and 5) the bands are due to a single crystal field absorption which is intrinsically non-gaussian (asymmetric) in energy space, but which can be well approximated by 2 gaussians.

For orthopyroxene mechanism 1 is eliminated since band 1 would be required to correspond to a much less intense forbidden transition which should increase in intensity with increasing temperature. Mechanism 2 is unlikely since little if any Fe$^{2+}$ is located in M(1)(4). Mechanism 3 is eliminated since the vibronically coupled transition (band 1) should increase in intensity with increasing temperature (although the full nature of this interaction would require a similar study utilizing infrared and/or Raman spectroscopic techniques). Mechanism 4 is eliminated, even though localized calcium-rich zones have been identified in orthopyroxenes, since one would expect the intensity of both bands to behave more similarly.

Mechanism 1 is eliminated for orthopyroxene since for same reasoning as for orthopyroxene. Mechanism 2 is a viable method for resolving 2 individual gaussian absorptions with physical significance, however gaussian analysis applied to a wide range of compositions would be required to verify this. Mechanism 3 is unlikely for reasons outlined above. Mechanism 4 is eliminated since the center position of band 2 is at far too long a wavelength to be attributed to any pyroxene component.

CONCLUSIONS The distinctive olivine spectrum in the 1μm region can be uniquely and consistently modelled with 4 gaussians over a wide range of temperature; the 3 strong band components correspond well with individual crystal-field absorptions(3). Both pyroxenes are uniquely and consistently fit with 2 gaussian components, although a physical mechanism for multiple bands in the 1μm region has not been established. Nevertheless, the consistent behavior of these components over a wide range of temperature-induced changes to the absorption band shape and width(1) argues for the validity, on an empirical level, of these gaussian
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analyses, and their potential utility for quantitative analysis of spectral reflectance data of multimineralic assemblages containing these components.

REFERENCES

![Figure 1-Individual Olivine Gaussian Parameters as a function of Temperature.](image1)

![Figure 2-Individual Orthopyroxene Gaussian Parameters as a function of Temperature.](image2)

![Figure 3-Individual Clinopyroxene Gaussian Parameters as a function of Temperature.](image3)