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# Visible to near-infrared optical properties of pure synthetic olivine across the olivine solid solution

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## 1 Abstract

Olivine exhibits highly diagnostic absorption features across visible to near-infrared (VNIR) wavelengths due to electronic transitions of $Fe^{2+}$ in its crystal structure. The properties of these absorptions vary with composition, enabling compositional analysis of olivine through VNIR spectroscopy, both in the laboratory and through remote sensing. Previous analyses of these trends have relied on natural olivine samples, which are influenced by the presence of minor cations that can affect the diagnostic absorptions. We conduct a systematic analysis of a suite of synthetic (pure Mg/Fe) olivine samples with VNIR (300-2600 nm) reflectance spectroscopy and quantitative spectral deconvolutions. From the full suite of samples described and characterized by Dyar et al. (2009), we identify a small suite of well-characterized and chemically pure olivine samples that demonstrates consistent and reliable spectral reflectance properties across visible to near-infrared wavelengths. This suite covers the stoichiometric olivine solid solution from x = Mg/(Mg+Fe) = 0 to x = 70 ($Fo_0$ to $Fo_{70}$). Because of their tight compositional control, these synthetic samples improve on previous analyses of natural samples. The results of this study provide a new standard for spectral reflectance properties of olivine across visible to near-infrared wavelengths for the compositions present in the suite. We present updated data on the trends in olivine band position as a function of olivine composition, which are the basis for remote compositional evaluation of olivine with visible to near-infrared reflectance spectroscopy. For these reasons, these improved olivine band position trends are of major importance to remote compositional analyses of terrestrial planets.

## 2 Introduction

Olivine is a major component of rocky solar system bodies. It plays a dominant role in planetary mantles, and is common in mafic igneous rocks occurring on or near planetary surfaces. Olivine composition is a valuable means for interpretation of the thermal and chemical evolution of diverse planetary bodies. Because olivine is the first mineral to crystallize from typical mafic melts, it is a common constituent of planetary surfaces and chondritic meteorites. Olivine composition (major element chemistry, typically expressed as Mg#, or molar (Mg/(Mg+Fe)) is an important petrologic indicator for properties such as the body or sampled unit's degree of petrologic evolution and parent melt composition. Furthermore, olivine's VNIR absorption features are sensitive to olivine composition; olivine composition can often be evaluated through remote sensing using techniques that quantify these characteristic olivine absorption features. Thus, determining olivine composition through remote sensing is an important tool for evaluating planetary petrology.

Characterization of the olivine absorption properties using laboratory VNIR spectroscopy for samples with known major element compositions provides the basis for the evaluation of unknown olivines with VNIR spectroscopy. However, pure stoichiometric olivine [$(Mg,Fe)_2SiO_4$] is very rare in natural samples, and the substitution of minor cations like $Mn^{2+}$ (Burns, 1993; Cloutis, 1997), $Ni^{2+}$ (Hu et al., 1990), and $Cr^{2+}$ (Burns, 1975, 1993) can have unexpected effects on olivine's VNIR reflectance properties. Minor cations can introduce additional absorption features in olivine spectra. However, the most significant effects of these minor cations (with respect to compositional evaluation of olivine through analysis of the 1 μm $Fe^{2+}$ feature) largely involve changes to the principal $Fe^{2+}$ crystal field transition absorptions near 1 μm (including changes to band position, relative intensities, and shape). These changes result from changes to the olivine structure resulting from the introduction of cations with different sizes and site occupancy preferences from the stoichiometric cations ($Mg^{2+}$, $Fe^{2+}$). Previous efforts to define olivine's absorption properties across VNIR wavelengths have relied on natural samples covering a compositional range that is as broad as possible (Sunshine and Pieters, 1998). These studies described general trends in olivine's spectral properties across VNIR wavelengths, but the samples studied were not pure stoichiometric olivine of precise compositions because they were natural samples, typically containing minor amounts of non-stoichiometric cations (e.g., $Ca^{2+}$, $Mn^{2+}$, $Cr^{2+}$, $Fe^{3+}$). Furthermore, natural samples cannot sample the full range of olivine compositions with equal levels of sample purity, because certain olivine compositions are not common in natural samples. In particular, pure $Fe^{2+}$-rich olivine samples are relatively rare. For all of these reasons, studies of systematic trends in olivine absorption properties are challenging when relying on natural samples. While it is true that natural samples are unlikely to be completely free from minor cations and thus not perfectly represented by these synthetic samples, the definition of a reference standard is best based on the ideal case, as it represents an unbiased framework in which "real" natural samples can be evaluated.

The present study conducts a systematic survey of olivine's optical properties across the compositional range using synthetic samples, which do not suffer from the complexities and uncertainties resulting from using natural samples. The samples analyzed here are part of a larger suite of synthetic olivine samples described by Dyar et al. (2009) along the solid substitution series between forsterite [Fo, $x = Mg/(Mg+Fe) = 1$] and fayalite [Fa, $x = Mg/(Mg+Fe) = 0$]. The preparation of these samples is discussed by Dyar et al. (2009). Dyar et al. (2009) incorporated a variety of analytical spectroscopic techniques to characterize the properties and systematics of olivine with the high degree of fidelity afforded by the use of synthetic samples. Lane et al. (2011) conducted a systematic survey of the group 1 subset of these samples (subset groups 1 and 2 are defined below) using a variety of spectroscopic techniques at mid-infrared wavelengths. However, the full sample suite is not perfect, and minor levels of contamination and the presence of minor amounts of $Fe^{3+}$ (stoichiometric olivine would contain only $Fe^{2+}$ and $Mg^{2+}$ cations) affect the VNIR spectral properties of some samples significantly. While many of the samples are appropriate for other analysis techniques, those with significant optically active contaminants in the VNIR are excluded because our goal is to produce the definitive characterization of "ideal" olivine's spectral characteristics. Thus the samples used in this study were selected from the larger suite to describe most clearly the systematics of olivine absorptions in the VNIR across the compositional range. We eliminated samples that exhibit obvious and substantial variations from previously identified trends (based on natural samples) in olivine absorption properties (e.g., Burns, 1970, 1974; King and Ridley, 1987; Sunshine and Pieters, 1998). The previous trends are assumed to be generally correct, so the goal of the present work is to refine, rather than redefine, these trends. As such, these previously identified trends are a reasonable standard to use in defining samples to exclude from the present analysis. The remaining high-quality samples are used to refine the trends in olivine absorption properties across VNIR wavelengths. The results should be considered the definitive standard for olivine absorption properties in the VNIR.

## 3 Background

### 3.1 Olivine structure and VNIR spectroscopy

Olivine structure is discussed by Dyar et al. (2009), but is summarized briefly here. Olivine is an orthosilicate with a nearly hexagonally close-packed structure. It has a general formula of $M1M2SiO_4$, where the cation sites (M1, M2) are six-coordinated (octahedral). The dominant (stoichiometric) divalent cations ($Fe^{2+}$, $Mg^{2+}$) occupy the octahedral cation sites, and the octahedra share edges, creating chains along the *c* axis. The M2 site is the larger and more distorted of the sites, although size effects between the sites are relatively minor (e.g., Bish, 1981). Olivine does not exhibit strong ordering in the cation sites between $Fe^{2+}$ and $Mg^{2+}$, although minor site ordering has been detected using optical absorption spectroscopy (e.g., Taran and Matsyuk, 2013). While $Fe^{2+}$ has a slight preference for the M1 site at relatively low temperatures (below ~600 ± ~100°C, depending on the sample and analytical technique employed), each cation will occupy both sites in pure stoichiometric olivine (Abdu et al., 2008). The geometry of the two M06 octahedral sites is illustrated (for the forsterite endmember) in Figure 1.

The asymmetry of the cation sites (i.e., the irregularity of the M06 octahedra, as illustrated in Figure 1) leads to a splitting in the energy levels of the outer *d* orbitals in $Fe^{2+}$ in the cation sites. This splitting gives rise to the characteristic olivine absorption features near 1 μm. Example olivine spectra are illustrated in Figure 2. The position and shape of the absorption features are controlled by the magnitude of the energy splitting between these orbitals. Cation-ligand (i.e., Fe – O) bond length controls the splitting energy (also termed "crystal field stabilization energy", or Δ), and scales as $\sim r^{-5}$, where *r* is the bond length (Burns, 1993). As incident photons with the proper energy (Δ) interact with the olivine structure, they are absorbed and cause electrons to "jump" between the split energy levels. This photon absorption causes absorption features in the wavelength-resolved optical properties of the mineral.

The characteristic olivine absorption near 1 μm is comprised of three components. Two features (near ~0.85 μm and ~1.25 μm) are caused by $Fe^{2+}$ in the M1 site, and the central absorption by $Fe^{2+}$ in the M2 site (Burns, 1970, 1974). These features shift in relative strength, width, and most substantially, position (energy), as a function of the olivine's relative $Fe^{2+}$ vs. $Mg^{2+}$ content (Mg# or Fo#), largely driven by the changing bond lengths due to the different sizes of the $Fe^{2+}$ and $Mg^{2+}$ cations. The general trend is that with increasing $Fe^{2+}$ content, absorption features shift to longer wavelengths and become slightly broader, while the M1 absorptions become stronger relative to the central M2 absorption (Burns, 1970, 1974; Sunshine and Pieters, 1998).

## 3.2 The Modified Gaussian Model

The reflectance properties of the olivine samples studied are quantified by analysis with the Modified Gaussian Model (MGM). The MGM is a spectral deconvolution routine developed by Sunshine et al. (1990) that has been widely validated as a means for accurately quantifying crystal field absorption features caused by $Fe^{2+}$ in mineral cation sites both in laboratory spectra (e.g., Hiroi and Sasaki, 2001; Isaacson and Pieters, 2010; Sunshine and Pieters, 1993, 1998; Noble et al., 2006; Klima et al., 2007; Mayne et al., 2010; Clénet et al., 2011; Isaacson et al., 2011a) and in remotely-acquired spectra (e.g., Hiroi et al., 1995; Sunshine et al., 2007; Birlan et al., 2011; Farrand et al., 2011; Isaacson et al., 2011b). We note that the scientific literature of research with the MGM is extensive, and we have not attempted a thorough review of it here; the reader is referred to references within those example works we have cited (which emphasize analyses of olivine) for further background. A major strength of the MGM is its ability to quantify absorption features linked to specific transitions in spectra exhibiting multiple overlapping absorptions in a small wavelength region such as olivine and olivine-pyroxene mixtures. The MGM approach is based on the fact that electronic transitions such as those in olivine can accurately be described as “modified” Gaussian distributions in which the fundamental variable is transformed from energy to bond length to better model the properties of real absorption features (Sunshine et al., 1990). MGM deconvolutions are carried out in wavelength and natural log reflectance, in which overlapping features add linearly and thus linear inversions can be used in the deconvolution (Sunshine and Pieters, 1993; Sunshine et al., 1990). The optimization method employed by the MGM is the approach of Tarantola and Valette (1982). The MGM inversion technique is iterative in which the parameters controlling the Gaussians and spectral continuum slope are varied until a pre-defined RMS residual error threshold is met (Sunshine et al., 1990). Additionally, the Tarantola and Valette (1982) and MGM approaches allow the introduction of *a priori* information as constraints on the resulting parameters; for example, Gaussian centers can be prescribed to lie within a specified wavelength range within a certain level of confidence. MGM fits are initiated by a startup file containing initial values for all parameters to be considered in the optimization. By varying the starting parameters, the initial conditions for the run can be changed. MGM results can be sensitive to starting parameters (e.g., Clénet et al., 2011), so the choice of initial parameters is significant. For the results presented here, standard initial conditions roughly consistent with olivine, based on previous work by Sunshine and Pieters (1998), were used for all fits.

## 4 Samples

A full listing of the olivine samples synthesized for an integrated spectroscopic characterization of olivine can be found in the overview publication of Dyar et al. (2009). Two different suites of olivines were described in that publication. The first suite [described here as “Group 1” or “SUNY olivines”, which is the source of most of the olivines evaluated here and of those studied by Lane et al. (2011)] was synthesized by Donald Lindsley at SUNY Stony Brook. The second suite (described here as “Group 2” or “Bristol olivines”) was synthesized by Richard Brooker at Bristol University. Both cover the full range of stoichiometric olivine composition, although the SUNY samples were found to contain fewer impurities due to the different synthesis process employed (the SUNY samples were synthesized with multiple heating/drying steps, while the Bristol samples experienced only a single cycle, leading to less complete reactions in some cases). More complete descriptions of the sample suites, synthesis processes, and quality assessments (including through Mössbauer spectroscopy and X-ray diffraction analyses) are provided by Dyar et al. (2009), and the full listing of samples evaluated is provided in Table 1. Subsequent tables identify the subset of samples used for further analyses.

# 5 Methods

## 5.1 Spectral reflectance measurements

Visible to near-infrared reflectance spectra of all of the synthetic olivine samples were collected over a wavelength range of 300 nm – 2600 nm using the bidirectional reflectance spectrometer in the Brown University RELAB. Reflectance measurements were collected as "bidirectional reflectance", using the standard RELAB viewing geometry of incidence (i) = 30°, emergence (e) = 0° (Pieters, 1983; Pieters and Hiroi, 2004). The samples were in particulate form for these measurements with a standard grain size of <45 μm for all measurements.

## 5.2 Compositional Analyses

All of the samples evaluated in the course of this study were synthesized under carefully controlled conditions, and in general were found to be of high quality and purity based on x-ray diffraction and Mössbauer spectroscopy analyses, although many of the Group 2 samples exhibited higher levels of impurities (likely linked to incomplete synthesis reactions) and higher degrees of compositional variability, manifested in both the abundance of $Fe^{3+}$ and impurities based primarily on Mössbauer spectroscopy analyses (Dyar et al., 2009). However, to ensure that the samples evaluated in this study are consistent with their stated compositions, we performed compositional "spot checks" with electron microprobe (EMP) analysis of grain mounts prepared from selected samples using the Cameca SX-100 at Brown University. Compositional analyses were performed on all six samples that passed the spectral quality assessment (section 5.4).

Many individual analyses were performed on each grain mount, and were averaged to determine mean compositions for the samples. Only analyses that passed quality thresholds were included in these averages. These thresholds were defined based on stoichiometry (moles of cations per four moles of oxygen between 2.98 and 3.02) and oxide weight percent totals (between 98.0% and 102%; the 102% upper cutoff is higher than might typically be used, but the olivine samples tended to have systematically high totals for all analyses).

### 5.3 MGM Modeling

As discussed above, the absorption features in the acquired reflectance spectra were quantified with the Modified Gaussian Model (MGM). Each spectrum was modeled with a series of four standard “fits”, where a “fit” refers to a particular starting condition. Because MGM model results can be sensitive to the initial conditions, as discussed above, we used the same starting conditions for the absorptions in each fit, varying only the constraints on the degree to which the parameters were allowed to vary in optimizing the result. Furthermore, because MGM fits have some uncertainty in predicted band center, we included some fits in which the absorption widths were highly constrained to values consistent with olivine, which generally tended to improve the consistency of the band center results with previously-established trends. Fits were run iteratively until the pre-defined RMS error threshold of $10^{-5}$, consistent with the value employed by Sunshine et al. (1990), was met (when the improvement in RMS residual error between successive iterations was less than this threshold). The continuum used was a first-order polynomial in wavelength (nm) and natural log reflectance units, with an initial offset of 0.8 and a slope of 0.0. The initial parameter values for the absorptions are provided in Table 2. Bands 1-3 are short-wavelength bands required to accommodate short wavelength spectral structure and enable a mathematically valid fit; the ultraviolet (UV) and visible wavelengths are not analyzed thoroughly in this study, and results for these absorptions are not reported. While Gaussians may not be the most accurate of the UV absorptions (which are largely caused by various charge transfer processes), we employ this approach for consistency with previous treatments of olivine spectra concentrating on the electronic transition absorptions that are the focus of this work. Quantitative analysis of charge transfer absorptions in the UV and visible are beyond the scope of this work. The initial values for the principal olivine absorptions (M1-1, M2, M1-2) are intended to be consistent with an intermediate composition (~$Fo_{50}$). The parameter constraints for each fit are listed in Table 3. Note that the other parameters not mentioned explicitly in Table 3 (i.e., Gaussian centers and intensities) were allowed to vary independently during fitting. The same initial offset and slope was used for each fit; the only parameters changed were the constraints imposed on various parameters during fitting. The possibility of a second absorption caused by $Fe^{2+}$ in the M2 site has been raised previously (e.g., Runciman et al., 1974; Hiroi and Takeda, 1992), and there is some support for this idea from analysis of Mg-free orthorhombic olivine-type phosphates where $Fe^{2+}$ is confined to the M2 site (Langer et al., 2006). However, MGM analyses in this work and by previous authors (e.g., Sunshine and Pieters, 1998) do not reveal evidence for this additional band.

### 5.4 Quality assessment and filtering

The “quality” of the resulting fits was determined by analyzing the consistency of the MGM-derived parameters with previously-derived trends (Sunshine and Pieters, 1998). Because the present study is intended to refine the spectral properties of olivine rather than re-define them, we assume that the results of these previous studies represent valid guidelines for the general reflectance properties of olivine spectra. In other words, we used these previous studies to determine which spectra and fits from the present study were most consistent with olivine’s known spectral properties. The criteria used most heavily in filtering the results were the band positions relative to the known composition (Fo#) and the relative band strengths of the M1 absorptions.

We determined the deviation of the M1-1, M2, and M1-2 band positions from previously established trends (Sunshine and Pieters, 1998). Fits with deviations near or above 10 nm for M1-1, 7.5 nm for M2, and 12.5 nm for M1-2 were considered to be of lower quality. Fits with extreme deviations (i.e., deviations far exceeding this "allowable" range) were rejected. While these ranges may seem large, the previous results are only a guide, so we must consider results that deviate from previous results in order not to bias the present study excessively. Previous results indicate that while the strength of the M2 band relative to that of the M1-2 band varies as a function of Fo#, the strength of the M1-1 band relative to the M1-2 band is approximately constant with composition. This is fully consistent with theory, as $Fe^{2+}$ in the same site causes both of these (M1) absorptions. Thus, we rejected any fits in which the strength of the M1-1 band relative to that of the M1-2 band fell beyond a specified range of 0.5 to 0.65. Any fits falling close to the extremes of this range (within ~0.02) were not excluded, but were considered to be lower quality. Examples of excellent, good, mediocre, and poor/rejected results are given in Table 4. The fits described in Table 4 are illustrated in Figure 3. The parameters causing the fit to be downgraded are in boldface type. Quality assessment is according to shading: white / excellent, light grey / good, dark grey / mediocre, and black / rejected. Generally, a deviation indicating reduced quality according to the criteria given above for a single parameter would indicate a "good" result (as opposed to "excellent", which would exhibit no such deviations), while more than one such deviation would indicate a "mediocre" result. In cases where multiple fits produced results of comparable quality (e.g., two "excellent" fits for a single spectrum), we chose the result derived with a flat continuum slope for consistency with previous analyses by Sunshine and Pieters (1998). This situation was only observed for fits 2 and 4 (both with constrained widths, with the only difference being the constraint on continuum slope), so we never were forced to choose between results obtained with the same continuum slope constraint (i.e., fit 1 vs. 2 or 3 vs. 4).

As evidenced by Figure 3, the differences between "good" and unacceptable spectra in defining trends for olivine across VNIR wavelengths are difficult to determine from plots of the spectra; all samples and spectra evaluated in this study are olivine with an extraordinarily high purity level. The difference between spectra that pass our defined quality threshold and those classified as unacceptable is likely a small amount of contamination or residual uncrystallized reactants. Because the samples are all of very high purity, we must rely on such quality criteria as those outlined above to identify those samples and spectra that best capture the properties of pure olivine across VNIR wavelengths, and must also assume that those samples not passing the quality test are slightly more affected by minor contamination.

### 5.5 Trends in band position with composition

The band positions derived from MGM analyses (section 5.3) were used along with the compositions determined from EMP analysis (section 5.2) to establish trends in band position with changing olivine composition (Mg#) for each of the three component absorptions. The trends in band position with composition were assumed to vary linearly, as in previous treatments (Burns, 1970; King and Ridley, 1987; Sunshine and Pieters, 1998; Burns et al., 1972). Trend lines were produced for each individual absorption via least squares. In producing our trend lines, we used the mean compositions for each sample determined from EMP analysis rather than the nominal (stated) compositions, and did not use any weighting (e.g., by measurement variance). However, we provide the band position (Table 5) and compositional (Table 6) data that will enable the reader to produce trend lines using alternative approaches.

## 6 Results

The suite of spectra and fits that survived the quality-filtering step are provided in Table 5, along with the MGM results. Compositions for these samples are provided in Table 6; full oxide abundances are provided in the supplemental material. These selected fits are shown graphically in Figure 4. Shading in Table 5 is according to quality of the selected fit, and uses the same scheme as Table 4 (excellent to poor from light to dark). Note that one case, due to moderate deviations from previous trends either in band position or in relative M1 absorption strengths, the best fit is only mediocre [C1DD96/$Fo_{20}$, due to deviations in M1-1 (~9 nm) and M2 (~8 nm) band position]. As the difference between "excellent" and poorer fits is very difficult to determine from plots such as those in Figure 4, the quantitative criteria given in Table 5 are critical for the quality assessment. Note that all results shown in Table 5 were produced from either fit 2 or fit 4; fits 1 and 3 produced significantly poorer results in most parameters. For example, C1DD98, which produced some of the "best" results based on consistency with previously-established trends, exhibited deviations of ~15 nm in band position, up to 70 nm in FWHM, as well as significant variations in relative M1-1 intensity in results from fits 1 and 3, but produced excellent results in the constrained cases (fits 2 and 4). Results from other spectra were often worse in the unconstrained cases, demonstrating the importance of the parameter constraints in producing reliable results.

The suite of spectra and fit results given in Table 5 were used to prepare a series of figures illustrating the reflectance properties of the "surviving" (highest-quality) synthetic olivine compositional range ($Fo_{70}$ – $Fo_{0}$). The following series of plots is labeled by Fo#, with blue colors (Fe-rich) trending to orange and red (Mg-rich). Note that the original suite includes a wider compositional range, in particular more magnesian samples, but those samples did not produce spectra or fits of sufficient quality for these quantitative VNIR analyses. Figure 2 shows reflectance spectra of the synthetic olivine suite. Figure 5 shows the same spectra after continuum removal (a) and after a normalization by band depth (b) that illustrates trends in spectra property without the confusion of variable band strengths, following the approach of Lucey (1998). The continuum slope removed was a straight line, with tangent points at 660 nm and 1960 nm. Band minima and relative strength of the M1-2 (long-wavelength) absorption both increase with increasing Fe content. The $Fo_{30}$ and $Fo_{40}$ spectra deviate slightly from the trend, which is most apparent in Figure 5b, where the $Fo_{30}$ spectrum runs at shorter wavelength than the $Fo_{40}$ spectrum in the M1-2 region. This deviation is discussed further below.

The MGM-derived band positions of the selected subset and fits are illustrated in Figure 6. Results from this study are in heavy lines and symbols, while results from Sunshine and Pieters (1998) are in smaller filled symbols and dashed lines. The trend lines for the present study were calculated with a linear fit to the results for each absorption (section 5.5). A “curve” is observed in the M1-1 absorption at Fe-rich compositions, in which the band positions skew to shorter wavelengths in a curved trend. This curve can be seen most clearly in the M1-1 band centers for the $Fo_{10}$ and $Fo_{20}$ points, which fall at shorter wavelengths than the trend line in Figure 6. A similar effect was observed previously (Sunshine and Pieters, 1998), also apparent in the Sunshine and Pieters points in Figure 6. The slopes of the trend lines in this plot are presented in Tables 7 and 8. Table 7 presents the slopes cast in the form of band positions as a function of composition (Fo#), and Table 8 presents the same slopes cast in the form of Fo#

solved as a function of band position. The values in Table 8 are the bases of equations used to predict olivine composition from MGM-derived band position (e.g., Isaacson et al., 2011b).

The MGM-derived widths and intensities of the selected subset are illustrated in Figure 7, which plots these parameters against MGM-derived band strength. Absorption intensities (in Figure 7b) are shown relative to the M1-2 absorption to eliminate variability resulting from differences in absolute band intensity between the spectra, as overall band intensity is controlled by a number of factors unrelated to the variation with composition that is of primary interest here. As found in previous studies, the central M2 absorption weakens (relative to the M1-2 absorption) with increasing Fe content, whereas the intensity of the M1-1 absorption is roughly constant, weakening slightly (relative to the M1-2 absorption) at Fe-rich compositions. While the overall trend is of increasing M2 relative intensity with decreasing Fe content, the trend is rough, as the $Fo_{10}$ and $Fo_{20}$ points are reversed, as are the $Fo_{30}$ and $Fo_{40}$ points. The absorption widths are relatively constant for the M1-1 and M2 absorptions (they were highly constrained in these fits), although the M1-2 absorption does get slightly wider at more Fe-rich compositions.

The outliers noted above in Figure 5b are notable outliers in Figure 7a as well. The $Fo_{40}$ and $Fo_{30}$ spectra are widely separated in M2 relative intensity, which likely contributes to their apparent reversal in order in Figure 5b. This apparent reversal in Figure 5b could be caused by a very strong M1-2 absorption relative to the M2 (i.e. a smaller value in Figure 7a) in the $Fo_{40}$ spectrum, which would cause the spectrum to appear at a longer wavelength in the 1250 nm M1-2 region (scaled spectra in Figure 5b) as the scaling approach would tend to over-scale the M1-2 absorption slightly (the scaling factor is determined by the intensity at the band minimum, which is driven primarily by the M2 absorption). Conversely, a weak M1-2 absorption relative to the M2 absorption (as in the $Fo_{30}$ spectrum) would cause the spectrum to appear at shorter wavelengths in the 1250-1300 nm region in Figure 5b). A similar effect to that observed in the $Fo_{30}$ and $Fo_{40}$ spectra is observed in the $Fo_{10}$ and $Fo_{20}$ spectra; they appear reversed in the trends with composition in Figure 7a, and also anomalous in the progression in scaled spectra in Figure 5b (although to a lesser degree than the $Fo_{30}$ and $Fo_{40}$ spectra; the $Fo_{10}$ and $Fo_{20}$ spectra merely plot on top of each other, whereas the $Fo_{30}$ and $Fo_{40}$ spectra appear in the wrong order). Note that this inconsistency between the $Fo_{30}$ vs. $Fo_{40}$ and $Fo_{10}$ vs. $Fo_{20}$ spectra does not mean that the MGM-derived band positions fall in reverse order; as shown in Figure 6, the band centers for these spectra are in the expected trend, with the $Fo_{40}$ and $Fo_{20}$ band centers at shorter wavelengths (relative to the $Fo_{30}$ and $Fo_{10}$ points, respectively). The inconsistency is only observed in apparent band position in the scaled spectra shown in Figure 5b.

## 7 Discussion

### 7.1 Identification of best synthetic olivine spectra

One of the major goals of this study is to identify, from the suite of olivines discussed by Dyar et al. (2009), those spectra that best represent the spectral reflectance properties of olivine across visible to near-infrared wavelengths for the largest compositional range possible. In particular, this study seeks to improve coverage of Fe-rich olivine compositions, for which the data used by Sunshine and Pieters (1998) were of lower purity. The quality of the spectra in the visible to near-infrared is an important consideration, because the quality assessment of Dyar et al. (2009) was based on Mössbauer analyses. While the quality assessments are generally consistent between Mössbauer and VNIR spectroscopy (samples identified as being of poor quality with Mössbauer analyses are unlikely to be good in the VNIR), the correlation is not perfect, and samples that pass the Mössbauer quality test are not necessarily of high quality in the VNIR.

As stated above, our basis for evaluating the "quality" of the VNIR olivine spectra was previous work by Burns (1970; 1974), King and Ridley (1987), Sunshine and Pieters (1998), and Burns et al. (1972). These previous studies represent suitable general guidelines; we assume that these previous studies are not grossly incorrect. Thus, any spectra that were in serious disagreement with results for olivine of similar composition from those previous studies were considered to be of lower quality. The spectra that we consider to be of the best quality from the full suite are listed in Table 5. Note that in order to cover as much of the compositional range as possible, a few spectra of slightly lower quality (e.g., C1DD96/$Fo_{20}$, based on inconsistency in spectral characteristics with previous results) were included in this identified sub-suite. On the flip side, several spectra that would pass the MGM-based quality assessment just based on their spectral characteristics (C1DD92/$Fo_{55}$, C1DD41/$Fo_{50}$) were excluded because of their wide variability in composition based on the EMP analyses.

### *a Trends in band position*

The reflectance properties of our identified sub-suite are remarkably consistent with the results of previous studies (Burns, 1970; Sunshine and Pieters, 1998). However, a few differences are apparent. First, and perhaps most significantly, we observe a flatter slope for the M1-1 absorption relative to the results of Sunshine and Pieters (1998) in the band position vs. composition plot (Figure 6). These slopes can be found in numerical form in Tables 7 and 8. While our M1-1 slope is flatter than that of Sunshine and Pieters (1998), our M1-1 and M1-2 slopes are more similar than those observed by Sunshine and Pieters (1998). The Sunshine and Pieters (1998) study found a steeper M1-1 slope relative to the M1-2 slope. We observe a similar pattern (steeper M1-1), but our values are more similar. In theory, because the same transition causes both absorptions, the slopes for these lines should be similar (Burns, 1970; 1993; Burns et al., 1972). Sunshine and Pieters (1998) used natural samples, which tend to exhibit greater compositional variability than synthetic samples like the ones we analyzed, and this difference could explain minor differences in the band position trends. However, the increased similarity between our M1-1 and M1-2 slopes relative to the results of Sunshine and Pieters (1998) leads us to trust the slope values from the present study.

### *b Outliers in MGM-derived band properties*

We note a few outliers in Figures 4 and 6. More scatter is to be expected in the plots of relative intensity and FWHM (Fig. 7) relative to the band position vs. composition plot (Fig. 6), but insofar as the results can be interpreted directly, the $Fo_{40}$ and $Fo_{10}$ points in particular are inconsistent with the overall trend of decreasing relative M2 strength with increasing Fe content (Fo#), as noted previously in comparison to their close compositional neighbors (the $Fo_{30}$ and $Fo_{20}$ points). Based on that simple trend, the $Fo_{40}$ spectrum appears to have an anomalously low M2 relative intensity, and the $Fo_{10}$ spectrum to have an anomalously high M2 relative intensity. The $Fo_{30}$ fit result (Figure 4) exhibits a slight mismatch in the ~1200 nm region, which may contribute to the anomalous relative absorption intensities. The $Fo_{10}$ spectrum has the most pronounced continuum slope as shown in Figure 4, and both the $Fo_{10}$ and $Fo_{20}$ fits (Figure 4) required sloped continuum slopes, which may contribute to their inconsistency with the other results. The C1DD96/$Fo_{20}$ fit result is more marginal, and was included in the interest of having a more complete compositional series. Additionally, that sample has the highest standard deviation in its composition of any sample included in our suite. While still quite low (1.72 in Mg#, Table 6), this is another possible reason to treat this sample and its results with some caution. Thus, care should be taken in using this spectrum, particularly if conclusions are heavily influenced by these specific spectra or their MGM-derived properties. Overall, it is also important to recall that despite the overall expected trend of relative intensity with composition observed, substantial scatter is expected in the relative intensities based on previous results (Sunshine and Pieters, 1998). This scatter, clearly observed in the results in Figure 7, combined with the relatively small suite of input data points in the present study, caution against over-interpretation of individual data points in the relative intensity results.

### *c Features associated with contaminants*

We also note evidence for minor contamination in several of the olivine spectra. In particular, several spectra exhibit weak features at longer wavelengths (e.g., C1DD39/$Fo_{70}$, C1DD97/$Fo_{10}$, C1DD96/$Fo_{20}$). Several spectra also exhibit weak features attributable to $H_2O$/OH contamination are also apparent across this wavelength range (>1500 nm). While these spectral features are attributable to contamination rather than pure stoichiometric olivine (for example, EMP analysis suggested that the $Fo_{70}$ sample in particular appeared to have modally minor (several %) ~$Mg_{70}$ pyroxene), they do not affect the principal olivine absorptions substantially, so they are not a major complication for the results derived from these spectra. This minor pyroxene could, however, explain the very weak absorption in the $C1DD_{39}$/$Fo_{70}$ spectrum just beyond 2000 nm. However, users of these data should not consider the weak absorption features in the spectra beyond ~1500 nm as diagnostic or consistent with pure, ideal olivine.

## 7.2 Choice of continuum slope (fitting approach)

Our default choice of the best fit result was that of fit 4, which was a fit with constrained band widths and an enforced flat continuum slope. This was done to enable the most consistency with previous studies (Sunshine and Pieters, 1998). In practice, this meant choosing between fit 2 and fit 4, where the only difference was that fit 2 allowed the continuum slope to deviate from an enforced “flatness” constraint, because, as mentioned above, valid results were obtained only from the constrained fits (2 and 4). We only obtained two results in which both fits produced equally good results: C1DD98/Fo$_0$ and C1DD42/Fo$_{40}$. In all other cases (for the results shown in Figure 4 and presented in Table 4), the selected fit was clearly the best based on the band positions and relative band strengths. While it would be desirable to have all of the MGM results derive from the exact same starting condition, the goal of using only the best-quality fits is the most important criterion in determining the best results for this study, and we do not believe that the few instances in which a slightly different continuum slope was used impart a major error to our results. For the spectra in which fit 2 was demonstrably superior, the reason was typically that the long-wavelength portion of the spectrum exhibited spectral structure inconsistent with pure olivine (i.e., contamination of some sort). This behavior can be observed in C1DD97/Fo$_{10}$ in Figure 4, in which a positive slope can be observed in the spectrum beyond ~1800 nm. The small sample size (6) of spectra surviving the quality assessment makes it challenging to determine if a systematic effect results from the use of fit 2 vs. fit 4. The two spectra for which fit 2 produced the best results are those for which the Fe-rich “curve” is observed (sections 5, 7.3). However, a more pronounced “curve” for Fe-rich samples was observed by Sunshine and Pieters (1998), and their results were produced using flat continuum slopes for all samples. Thus, we do not believe that the use of fit 2 vs. fit 4 introduces a bias in the results, although the small sample size of our suite of spectra surviving the quality assessment filtering makes this conclusion challenging to test. A more complete suite of olivine compositions with spectra able to pass our strict quality criteria would allow this conclusion to be tested, and would provide additional statistics for refining the trends in olivine spectral properties with changing composition identified in this study.

### 7.3 Re-evaluation of Fe-rich samples

After analysis with the standard series of fits described above, we observed a curve in the M1-1 absorption on the band position vs. composition plot (Figure 6) for the Fe-rich compositions. A similar, albeit more extreme, curve can be observed in the results of Sunshine and Pieters (1998) shown in Figure 6. This trend is suspect, because no comparable curve on this plot is observed for the M1-2 absorption, and transitions in the same cation site control both absorptions. Sunshine and Pieters (1998) attributed this curve to noise in the spectra measured of those compositions. We cannot envision a physical reason (with a basis in mineral physics) that such a trend should be observed in the M1-1 absorption but not in the M1-2 absorption. In an attempt to determine if this "curve" is due to a bias introduced by our use of initial conditions more suited to intermediate compositions, we performed another series of fits using a new starting point for the M1-1 absorption determined by extrapolating a linear trend from the band positions of the more Mg-rich samples ($Fo_{30}$-$Fo_{70}$).

We found that in fits where we allowed the M1-1 position to deviate from its new (extrapolated) initial value, the resulting positions were essentially identical to those obtained from the standard series of fits (the results shown in Figures 3, 5, and 6, in which the curve in M1-1 band positions is observed for the Fe-rich samples). We were not able to obtain satisfactory fit results in which this "curve" in M1-1 band positions was not observed when we allowed the band positions to deviate from these extrapolated initial positions. To obtain a result in which the same "curve" was not observed, we had to constrain the position of the M1-1 absorption to remain at its new initial value. Relying on the constrained results would, in effect, mean that the results for the Fe-rich samples would be determined by the results of the more Mg-rich samples, and would carry an implicit *a priori* assumption that the Fe-rich samples should have similar trends to the Mg-rich samples. While this is a reasonable assumption, some research (using mid-infrared instead of VNIR data) suggests that Mg-rich olivines may behave slightly differently from more intermediate and Fe-rich olivines (Hofmeister and Pitman, 2007; Pitman et al., 2010). However, other mid-infrared studies of olivine [including work by Lane et al. (2011) on some of the same samples studied in this work] did not find a need to define distinct trends for Mg-rich samples (e.g., Koike et al., 2003; Lane et al., 2011). Thus, we do not present alternate trend lines for this new series of fits, and our conclusion is that the best and most testable results are those presented in Figures 5 and 6 and in the “Present Study” rows of Tables 5 and 6. Our tests did not suggest that this curve in the M1-1 band positions for Fe-rich samples could be attributed to bias resulting from our choice of initial conditions. However, we note that the deviation from the trend in the M1-1 band positions for the $Fo_{10}$ and $Fo_{20}$ samples is much less extreme than that observed by Sunshine and Pieters (1998), and might not even be apparent when not compared directly to the Sunshine and Pieters (1998) results. Furthermore, the data point that deviates most strongly from the trend line ($Fo_{20}$) is one of the most suspect points in the study, as discussed previously. We conclude that this slight “curve” in M1-1 band position of the Fe-rich samples is likely an artifact of our fitting procedure and not attributable to a physical property of Fe-rich olivine, effectively consistent with the conclusions of Sunshine and Pieters (1998).

### 7.4 Implications: Definitive standard for olivine optical properties in the VNIR

Our analyses suggest that the results of this study can be considered the new standard in the optical properties of olivine across VNIR wavelengths. Our results build on and refine previous attempts to define these properties. In particular, we have refined the state-of-the-art in understanding of the position and characteristics of the three diagnostic olivine absorption features near 1 μm over the compositional range from $Fo_0$ to $Fo_{70}$. In the process of quantifying these properties, we have identified a suite of synthetic olivine samples that can be considered the best examples of the optical properties of pure stoichiometric olivine across these wavelengths. These samples and their reflectance spectra represent the best examples of pure olivine unaffected by the inclusion of minor cations, particularly across the critical 1 μm region. While natural olivines are unlikely to be entirely pure and thus may not exhibit identical properties to these samples, our results represent the behavior of the most "ideal" olivines, and thus they are a standard to which natural samples can be compared that is not biased by minor cations. However, the suite of olivine samples used to define these important trend lines is small due to our strict quality criteria. A sample suite with a broader range of compositions (particularly at intermediate and Mg-rich compositions) and spectra able to meet these quality criteria would improve on the results of this study and should be a goal for future research. Nevertheless, the synthesis of our results, captured in Tables 7 and 8, can be used to evaluate the composition of olivine on planetary surfaces with VNIR reflectance spectroscopy.

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# 1 Figure Captions

Figure 1: Illustration of geometry of the M1O6 and M2O6 octahedral sites in olivine. These illustrations are viewed down the *a* axis. The specific geometries (i.e., sizes, bond lengths, and deviation of the MO6 symmetry from a regular octahedron) are shown for the forsterite [x = Mg/(Mg+Fe) = 1] endmember. The illustration is based on data reported by Brown (1970).

Figure 2: Bidirectional reflectance spectra of synthetic olivine subset suite. The geometry for the bidirectional reflectance measurements is discussed in the text. Legend is labeled by Fo# [x =Mg/(Mg+Fe)]. The principal olivine absorption near 1000 nm is composed of three overlapping absorptions, caused by $Fe^{2+}$ ions in the M1 (external absorptions) and M2 (central absorption) sites. The component absorptions are labeled as referred to throughout the paper. The Fe-rich samples ($Fo_0$ – $Fo_{30}$) are from Group 1, and the Mg-rich samples ($Fo_{40}$, $Fo_{70}$) are from Group 2.

Figure 3: Examples of MGM fits to synthetic olivine spectra. Fits correspond to the spectra described in Table 4. Note the differing Y-axis scales between the plots, used to maximize the contrast visible in each plot. The residual error in the fits (between model and spectrum) are captured in the dotted RMS lines. Parts a-d are ordered by decreasing “quality” of the spectrum/fit result, with (a) being excellent and (d) being poor. In order, the plots are C1DD98 ($Fo_0$) Fit 4, C1DD95 ($Fo_{30}$) Fit 2, C1DD96 ($Fo_{20}$) Fit 2, and C1DD115 ($Fo_{70}$) Fit 2. Note the sloped continuum in b-d; these fits were produced with the Fit 2 setup, in which the slope is allowed to deviate from the flat initial value. Part a was produced from Fit 4, which forces the continuum slope to remain flat in optimizing the fit. The fit in part d is considered poor and would be rejected from the final analysis for the parameters flagged in bold-face in Table 4 (the M1-1 absorption is too strong, and the M1-2 band position deviates too much from previously-

established trends). The problems with the fit in part d are difficult to see on the plot, which emphasizes the importance of quantitative quality threshold criteria.

Figure 4: MGM fit results for the identified sub-suite of spectra passing our quality criteria. The results shown are presented numerically in Table 5. Note the differing Y-axis scales between the plots, used to maximize the contrast visible in each plot. The residual error in the fits (between model and spectrum) are captured in the dotted RMS lines. The fits are to the spectra illustrated in Figures 2 and 5 and listed in Tables 5 and 6.

Figure 5: Reflectance spectra of the synthetic olivine subset suite after continuum removal (a) by straight line tangent at 660 nm and 1960 nm and normalization to maximum band depth (b). Legend is labeled by Fo#. The spectra are the same as those shown in Figures 2 and 4.

Figure 6: MGM-derived band position vs. composition for synthetic olivine subset, compared to the results of Sunshine and Pieters (1998). Our results are in heavy open black symbols, whereas the Sunshine and Pieters results are in small blue symbols. The trend lines calculated from the results of this study are in heavy black lines, and the trend lines from Sunshine and Pieters (1998) are in the dashed grey lines. Error bars are ± 1 standard deviation ($\sigma$) in measured olivine composition (Table 6). The parameters for these trend lines are presented in Tables 7 and 8. Our results suggest a slightly shallower slope in the M1-1 position with composition, and we observe a curve in the M1-1 position for Fe-rich compositions, similar (but lesser in magnitude) to that observed by Sunshine and Pieters (1998). Note that the $Fo_{20}$ band positions (which deviated slightly from the best-fit trend line) are determined from a more marginal fit (Table 5).

Figure 7: MGM-derived parameters for synthetic olivine subset, based on the fits shown in Figure 4. (a) Relative absorption intensity (relative to the M1-2 absorption) vs. band position. (b) Full width at half maximum intensity (FWHM) vs. band position. Points are labeled by Fo#/10, using the same color scheme used for Figures 2 and 4. The overall trends are consistent with those identified by previous studies, in which the M2 absorption weakens relative to the M1-2 with increasing olivine Fe content, and the M1-1 stay relatively constant (weakening slightly at very Fe-rich compositions). The widths stay relatively constant, except for a slight increase in the M1-2 feature's FWHM at very Fe-rich compositions.

# Tables

Table 1: List of samples and compositions evaluated in this study

| Sample | Nominal Composition (Fo#) | Suite (1/2) |
|---|---|---|
| C1DD37 | 90 | 2 |
| C1DD38 | 80 | 2 |
| C1DD39 | 70 | 2 |
| C1DD40 | 60 | 2 |
| C1DD41 | 50 | 2 |
| C1DD42 | 40 | 2 |
| C1DD43 | 30 | 2 |
| C1DD44 | 20 | 2 |
| C1DD45 | 10 | 2 |
| C1DD46 | 90 | 2 |
| C1DD85 | 100 | 1 |
| C1DD86 | 89.5 | 1 |
| C1DD87 | 80 | 1 |
| C1DD88 | 75 | 1 |
| C1DD89 | 70 | 1 |
| C1DD90 | 65 | 1 |
| C1DD91 | 60 | 1 |
| C1DD92 | 55 | 1 |
| C1DD93 | 50 | 1 |
| C1DD94 | 40 | 1 |
| C1DD95 | 30 | 1 |
| C1DD96 | 20 | 1 |
| C1DD97 | 10 | 1 |
| C1DD98 | 0 | 1 |
| C1DD115 | 70 | 1 |
| C1DD116 | 89.5 | 1 |

Table 2: Initial values for individual bands used in MGM fits.

| Absorption | Position (nm) | FWHM* (nm) | Intensity (ln reflectance) |
|---|---|---|---|
| 1 | 300 | 375 | -0.5 |
| 2 | 650 | 115 | -0.01 |
| 3 | 750 | 115 | -0.01 |
| M1-1 | 879 | 228 | -0.15 |
| M2 | 1054 | 176 | -0.13 |
| M1-2 | 1254 | 424 | -0.25 |

*Full width at half maximum strength.

Table 3: MGM model starting conditions

| Fit Number | Offset Constraint | Slope Constraint | Width constraint |
|---|---|---|---|
| 1 | Free | Free | Free |
| 2 | Free | Free | Constrained[*] |
| 3 | Free | Fixed Flat | Free |
| 4 | Free | Fixed Flat | Constrained[*] |

[*] Principal olivine bands (M1-1, M2, M1-2) allowed to vary slightly in width, but were highly constrained to the relations determined by previous analyses (Sunshine and Pieters, 1998).

Table 4: Example evaluations of MGM fit results illustrated in Figure 4

| Sample/Fit | M1-1 Rel. Str.[*] | M2 Rel. Str. | M1-1 Deviation[**] | M2 Deviation | M1-2 Deviation |
|---|---|---|---|---|---|
| C1DD98 / 4 | 0.55 | 0.47 | 3.81 | -4.93 | -6.67 |
| C1DD95 / 2 | **0.65** | 0.63 | 3.06 | -0.42 | 9.40 |
| C1DD96 / 2 | 0.54 | 0.48 | **-9.29** | **-7.97** | -6.67 |
| C1DD115 / 2 | **0.71** | 0.80 | -7.35 | -7.20 | **-25.36** |
| Quality criterion | 0.5-0.65 | | ±10 | ±7.5 | ±12.5 |

Shading indicates the quality assessment: white / excellent, light grey / good, dark grey / mediocre, and black / rejected.

[*] Intensity of absorption (natural log reflectance) divided by intensity of M1-2 absorption

[**] Difference between projected band position at the composition of that sample from trends of Sunshine &and Pieters (1998) and MGM-derived band position. This quantity is effectively the deviation of the result from the trend lines derived by Sunshine and Pieters (1998).

Table 5: Results of best MGM fits for spectra with MGM results passing the quality tests

| Spectrum / Fit | Fo# | Position (nm) | | | FWHM (nm) | | | Intensity (ln reflectance) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | M1-1 | M2 | M1-2 | M1-1 | M2 | M1-2 | M1-1 | M2 | M1-2 |
| C1DD98 /4 | 0 | 917.1 | 1073.7 | 1289.2 | 228.4 | 177.7 | 507.9 | -0.49 | -0.41 | -0.89 |
| C1DD97 / 2 | 10 | 899.6 | 1068.4 | 1287.2 | 228.5 | 178.0 | 493.8 | -0.41 | -0.39 | -0.72 |
| C1DD96 / 2 | 20 | 887.6 | 1061.6 | 1269.8 | 228.6 | 178.6 | 529.1 | -0.48 | -0.42 | -0.88 |
| C1DD95 / 4 | 30 | 889.2 | 1062.8 | 1268.1 | 228.3 | 177.5 | 478.1 | -0.35 | -0.33 | -0.57 |
| C1DD42 / 4 | 40 | 876.7 | 1056.0 | 1245.7 | 228.5 | 178.3 | 523.6 | -0.53 | -0.45 | -0.97 |
| C1DD39 / 4 | 70 | 854.8 | 1044.7 | 1232.3 | 228.2 | 177.7 | 493.1 | -0.43 | -0.42 | -0.73 |

Table 6: Compositional data for samples passing the quality tests

| Name | RELAB ID | Nominal Mg# | Measured Mg# | Mg# Standard Deviation | # Analyses (n)[2] |
|---|---|---|---|---|---|
| C1DD98 | DD-MDD-098 | 0 | 0.01 | 0.02 | 7 |
| C1DD97 | DD-MDD-097 | 10 | 10.47 | 0.19 | 8 |
| C1DD96 | DD-MDD-096 | 20 | 21.44 | 1.72 | 15 |
| C1DD95 | DD-MDD-095 | 30 | 30.40 | 0.29 | 13 |
| C1DD42 | DD-MDD-042 | 40 | 41.52 | 0.26 | 4 |
| C1DD39 | DD-MDD-039 | 70 | 65.42 | 1.42 | 14 |

[1] RELAB ID's are unique identifiers for these samples in the Brown University RELAB database.

[2] Analyses reported only if they meet quality criteria (moles of cations per 4 moles oxygen between 2.98 and 3.02, oxide weight percent totals between 98.0% and 102.0%).

Table 7: Linear trend data for band position vs. Fo; Band position(Fo)

| Sample Suite | Fo Range for Slope | Absorption | Slope | Offset |
|---|---|---|---|---|
| Sunshine & Pieters | 01 - 90 | M1-1 | -0.64 | 900.9 |
| | | M2 | -0.44 | 1076.4 |
| | | M1-2 | -0.89 | 1290.5 |
| Present study | 0 - 70 | M1-1 | -0.89 | 912.4 |
| | | M2 | -0.43 | 1073.2 |
| | | M1-2 | -0.95 | 1292.1 |

Table 8: Linear trend data for band position vs. Fo; Fo(Band position)

| Sample Suite | Fo Range for Slope | Absorption | Slope | Offset |
|---|---|---|---|---|
| Sunshine & Pieters | 01 - 90 | M1-1 | -1.23 | 1139.9 |
| | | M2 | -2.18 | 2347.8 |
| | | M1-2 | -1.06 | 1376.2 |
| Present study | 0 - 70 | M1-1 | -1.09 | 993.8 |
| | | M2 | -2.28 | 2442.9 |
| | | M1-2 | -1.01 | 1305.6 |