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OLIVINE COMPOSITION AND REFLECTANCE SPECTROSCOPY RELATIONSHIP REVISITED.

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Introduction: We revisit the behavior of the three primary olivine absorptions near 1 μm (referred to as M1-1, M2, M1-2) and their interrelationships by means of an advanced version of MGM analysis [1, 2]. We build on previous works carried out [e.g., 3, 4] to document at best the compositional variation of olivine from diagnostic absorption features across the visible and near-infrared wavelengths due to electronic transitions of Fe²⁺ in the crystal structure.

Olivine synthetic samples and spectral processing : MGM inverse modeling provides with band center, band width and band depth estimates. Band centers are used to determine trend line equations for each individual absorption band M1-1, M2, M1-2, with an assessment on the regression performance (*rms* spectral distance between band center estimate from MGM and the one from the trend line). The olivine composition (Molar Forsterite *Fo#*) is then predicted based on minimizing the deviations in band centers from the established trends for the three absorptions simultaneously, using the integrated *rms* spectral distance to trend quantity (*sdt*).

Two suites of synthetic olivine samples, with small grain size (<45micron), are available and span the full range of stoichiometric olivine composition along the forsterite-fayalite solid solution series. The first suite is referred to as 'SUNY' (for State University of New York) and comprises 15 samples. The second suite includes 10 samples, prepared at Bristol University and referred to as 'BRISTOL' olivines.

A logical step is to implement our MGM deconvolution on each synthetic suite. While for the band widths and strengths, no obvious differences are noticed between the two suites, two trends are clearly found for the band centers, with a band center scattering significantly more pronounced for the Bristol suite. For both suites, the scattering associated with the 850nm band center prevails over the 1050 and 1250 band centers ones. Some samples markedly depart, in both suites, from the overall trends and call for caution. We also note that some Bristol samples tend to agree with the Suny trend.

Based on these results, and on previous experimental analyses [5], it appears that the Suny suite should be taken as the master list, and possibly completed by Bristol samples to reinforce the robustness of the trend line variations as a function of composition.

However, as shown above, in both suites some samples depart from the overall trend.

Accordingly, a series of tests is performed on various subsets selected from both Suny and Bristol suites. For each subset of samples, a systematic testing of the coherency is performed to assess the performance of the regression, on the basis of the quantity *sdt* (more precisely, *rsdt*: real spectral quadratic distance to trend, associated with *Fo#*; *psdt*: predicted spectral quadratic distance to trend, associated with *Fô#*) and on the standard deviation (*rms*) associated with the *Fo#* estimates.

A suite composed of 12 samples (9 Suny, 3 Bristol), which entirely spans the olivine composition domain from *Fo#*0 to *Fo#*90, is found to have the best consistency, in terms of *rsdt*, *psdt* and *Fo#* estimates (*rsdt*: 6.01nm, *psdt*: 4.94nm, *rms* "*Fo#-Fô#*":**0.046**). The regression so defined is significantly more robust than either the Bristol (*rsdt*:15.5nm, *psdt*:10.9nm, *rms* "*Fo#-Fô#*":**0.110**) or Suny (*rsdt*:8.5nm, *psdt*:5.8nm, *rms* "*Fo#-Fô#*":**0.087**) one considered separately.

This way we assess and mitigate, through the statistical consistency of the considered subset, the impact of the 'poor' quality of any given sample/spectrum [4,5] in the regression set to define the trend lines equations. With the addition for a few spectra of a couple of bands (2000, 2500nm) in the MGM modeling to handle minor contaminations, the same regression gives then very consistent results for 19 Suny-Bristol spectra (*rsdt*:6.12nm, *psdt*:5.49nm, *rms* "*Fo#-Fô#*":**0.036**).

Conclusions: The trend lines equations derived from the current MGM modeling are more robust than previous solutions [3, 4, 6]. The band center positions of the three primary olivine absorptions (M1-1, M2, M1-2) are used simultaneously to produce a constrained prediction across an extended range *Fo#[0-90]* of olivine composition with synthetic or natural samples.

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