

VISIBLE AND NEAR INFRARED OPTICAL CONSTANTS OF SYNTHETIC JAROSITES. E. C. Sklute¹, T. D. Glotch¹, and W. Woerner¹, ¹Department of Geosciences, Stony Brook University, 255 ESS Building, Stony Brook, NY. 11794-2100; elizabeth.sklute@gmail.com.

Introduction: The positive identification of jarosite on Mars [1-3], along with its prevalence on Earth in areas contaminated by acidic run-off [4] and hydrothermal alteration [5], make it an interesting target mineral for remote sensing. Since jarosite can be used to constrain environmental conditions at the time of its formation [5] and has been used as an indicator of acidification potential of contaminated soils on Earth [4], identifying jarosite has been helpful in constructing theories of past climate on Mars and targeting cleanup efforts on Earth. However, quantitatively determining abundances of jarosite, and other minerals, from remote sensing data could provide much greater insight about the past and present conditions on the surface of that body.

Many of the relevant remote sensing instruments used to address this problem, such as Casini VIMS, MRO CRISM, and AVIRIS, cover the visible and near-infrared (VNIR; 0.35-2.5 μm). In this wavelength region, spectral response is not a linear function of composition, so direct extraction of quantitative abundances through linear unmixing is not possible. This problem has been dealt with in many ways, most requiring ground truth data [6]. Of the two methods that can be used independently to analyze such data (spectral mixture analysis [7] and radiative transfer theory [8-9]), radiative transfer theory is the only method that takes physical properties of the surface into account [6]. Of the two popular treatments of radiative transfer theory, only Hapke's treatment [8] attempts to relate all variables back to measurable properties of the material, and is therefore the preferred modeling approach for this work.

In order to employ Hapke's treatment of radiative transfer theory to deconvolve remotely sensed spectra, the optical constants (the real and imaginary indices of refraction n and k) of all end member spectra must be known. These can be obtained by inverting the model and applying it to laboratory spectra of pure end members. These optical constants are then used as a kind of scaling factor, along with the linearization technique of converting reflectance to single scattering albedo, so that particulate surfaces can be modeled to mineral mixtures and quantitative mass fractions can be extracted [8].

Since the modeling approach to obtain optical constants relies on minimization of the difference between the calculated and observed spectra, the optical constants, and other parameters, are simply numbers that

create the best fit. Therefore, to ensure a robust solution, multiple grain sizes are used and a single set of optical constants are determined for all grain sizes simultaneously. Since optical constants are grain size independent, this forces the program to adjust other parameters to compensate for the difference in spectral features and overall reflectance.

Methods: Potassium jarosite was synthesized by combining 0.8979 g of K_2SO_4 , 0.405 mL of concentrated H_2SO_4 , and 9.2 mL of DI water in 23 mL par bombs, then adding 0.103 g of 2 mm Fe wire and sealing the bomb under oxygen. The bombs were heated at 203°C for 4 days [10]. The product was then washed and sieved into 3 size fractions: >63 μm , 63-90 μm , and 90-125 μm . Bidirectional reflectance spectra (incidence angle of 30° and emergence angle of 0°, set by goniometer) of each size fraction were acquired with an ASD Fieldspec3 Max spectrometer (3500 scans/spectrum; Spectralon® reference) and an ocean optics HL-2000 light source.

The splice-corrected spectra were smoothed once and processed using a MatLab encoded Hapke inversion that first found an initial value for k with all other parameters fixed [11] and then iteratively (and globally) minimized the difference between the data and modeled spectrum finding values for k , $\langle D \rangle$ (apparent path length of light), b , c (coefficients of the phase function [12]), and s (internal scattering parameter). The first minimization used an average n value to determine k . Then a singly subtractive Kramers Kronig (SSKK) calculation was used to determine a wavelength dependent n [13-14]. This process was iterated until n and k remained constant (3-4 iterations).

Results and Discussion: The imaginary index of refraction, k , for the grain size dependent and grain size independent minimizations is shown in Figure 1. The grain size dependent minimization, which closely follows the inversion methods of Lucey *et al.* [11], assumes knowledge of the grain size (apparent path length of light), phase function, and internal scattering coefficient (set to 0 for this step). The grain size independent minimization only assumes that all features of the absorption coefficient, k , are due to composition rather than grain size and particle properties. It is clear that the grain size independent k is not an average of that for the three grain sizes. Figure 2 shows the data for all three grain sizes overlaid by the modeled spectra using the grain size independent k .

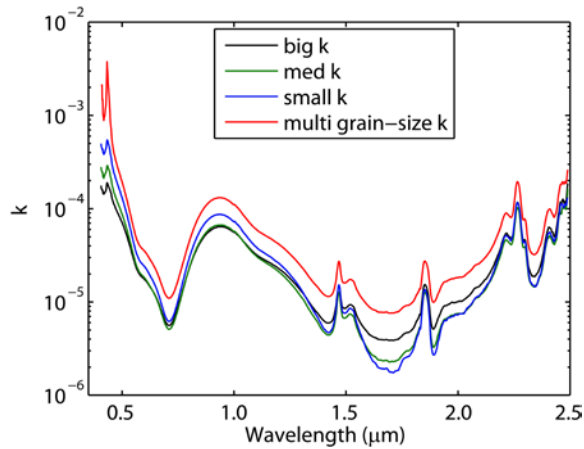


Figure 1: Absorption coefficient, k , for synthetic potassium jarosite.

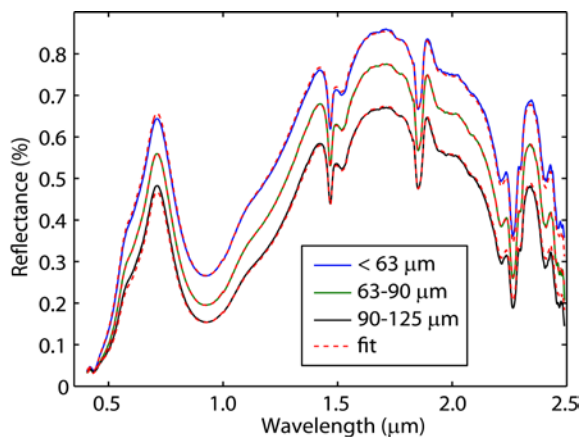


Figure 2: Synthetic jarosite VNIR spectra overlaid by modeled radiance coefficients determined using a grain size independent k .

The wavelength dependent real index of refraction, n , determined using a SSKK calculation, was first determined using only VNIR k data for jarosite. Since the SSKK is known to converge faster than a standard Kramers Kronig calculation [14], it was assumed that the n data acquired in this way would be similar to those where a greater wavelength range was considered. However, it was found that this assumption is not valid. Therefore, additional reflectance data (out to 100 μm) for jarosite were obtained using a pressed pellet and a Nicolet 6700 FTIR spectrometer (gold reference). Dispersion analysis was used to estimate k at longer wavelengths [15], and the extended range was used for all further n determinations. Figure 3 shows the change in n using gradually longer data sets along with the constant n value used for the first iteration and n determined by extrapolating k to shorter and longer wavelengths based solely on the VNIR spectral features.

It is clear that the shape of the n curve changes appreciably with extended data sets up to 50 μm , and then the shape (in the VNIR) seems to stabilize. Ex-

tending the data set down to zero through extrapolation also produces notable changes to the shape of n . Without knowledge of spectral behavior in this region, it is difficult to substantiate such effects [14].

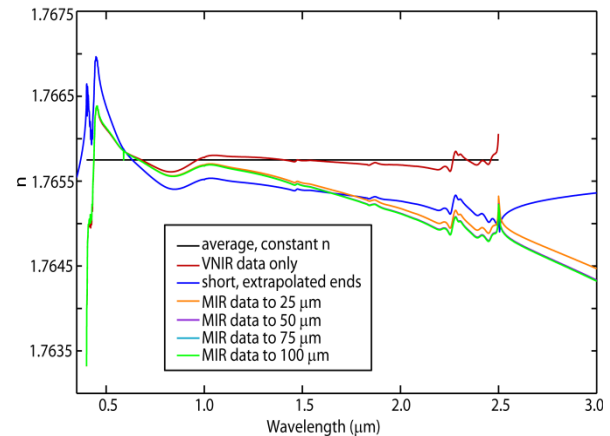


Figure 3: Real index of refraction, n , for synthetic potassium jarosite calculated using data sets that span VNIR only through FIR.

Conclusion and Future Work: A coarse-grained synthetic potassium jarosite was synthesized and the grain size independent VNIR optical constants were iteratively determined using Hapke's treatment of radiative transfer theory and an SSKK calculation. These values can now be used in modeling intimate mixtures on Earth, Mars, and other bodies to extract quantitative abundance information from remote sensing spectra. Future work will include synthesizing natrojarosite, hydronium jarosite, and intermediate compositions and determination of the optical constants for each. In addition, reflectance spectra of these minerals will be taken at additional geometries and phase functions will be determined for each mineral to further constrain modeling. Additional extensions of Hapke's treatment of radiative transfer equation to account for anisotropic scattering and other particle shapes will be explored.

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