

VNIR OPTICAL CONSTANT DETERMINATION OF SYNTHETIC JAROSITES FOR QUANTITATIVE ABUNDANCE ANALYSIS OF REMOTE SENSING DATA SETS. E. C. Sklute¹, T. D. Glotch¹ and M. D. Dyar², ¹Department of Geosciences, Stony Brook University, 255 ESS Building, Stony Brook, NY. 11794-2100; elizabeth.sklute@gmail.com, ²Mount Holyoke College, 217 Kendade Hall, South Hadley, MA. 01075; mdayr@mtholyoke.edu.

Introduction: The mineral jarosite, associated with areas of acid mine drainage (AMD) contamination on Earth, and positively identified on Mars [1-3], has been the subject of several spectroscopic studies in recent years [e.g. 4, 5]. Because jarosite can both be used as an indicator of acidification potential of soils on Earth [6] and to constrain environmental conditions at the time of its formation [7], it is of particular interest as a remote sensing target mineral. For both planetary and terrestrial applications, species identification and abundance analysis provide detailed information concerning past and present environmental conditions.

In the visible and near infrared (VNIR) wavelength range (0.35-2.5 μ m), jarosite can be identified through, and differentiated by, several absorption features [4]. Spectral response in this wavelength range is a non-linear function of composition, so direct extraction of mineral abundances through spectral feature matching is not ideal. However, through the determination of optical constants (the real and imaginary indices of refraction n and k), mixture models based on scattering theory can be used to obtain quantitative abundances [8-10]. In this work, we present the preliminary evaluation of select, well-characterized synthetic jarosites and determine their wavelength-dependent optical constant k using a Hapke inversion.

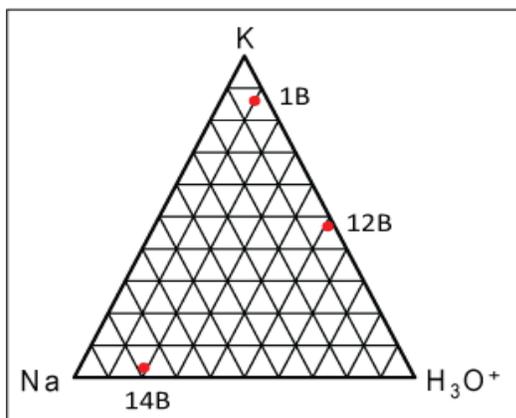


Figure 1: Jarosite sample compositions studied here.

Samples: Powders used in this study are from a suite of jarosites synthesized by G. Brophy at Amherst College in the early 1960's [11]. Samples were prepared by combining 0.05 moles of alkali sulfate with 0.15 moles of Fe₂(SO₄)₃ in 100 mL of 0.2 m H₂SO₄ to

prevent hydrolysis. The samples were reacted for 72 h in an oil bath maintained at 114°C and then air-dried. Because this synthesis method results in excess water being incorporated in the structure, the samples were heated to 120°C for 4 hours. Excess water after heating was considered structural H₃O⁺. Compositions of synthetic jarosites discussed here (1B, 12B, and 14B) are (K_{0.86}Na_{0.04}(H₃O)_{0.10}), (K_{0.47}Na_{0.02}(H₃O)_{0.51}), and (K_{0.03}Na_{0.78}(H₃O)_{0.19}), respectively (Figure 1).

Methods: Samples of three different grain sizes: < 45 μ m, 45-125 μ m, and 125-180 μ m were analyzed with an ASD Fieldspec3 Max spectrometer. Each spectrum consists of 300 scans referenced to a spectralon standard, with incidence and emergence angles of 30° and 0° respectively. Splice-corrected reflectance spectra were processed using a MatLab encoded Hapke inversion following Lucey's 1998 treatment of Hapke's scattering theory to determine the imaginary index of refraction k [8]. For these preliminary calculations, the average refractive index was input for n , the particle phase function $P(g)$ was that empirically derived by Mustard and Pieters [12], the opposition surge, $B(g)$, was assumed to be zero since the phase angle, g , was greater than 15° [13], and grain size was approximated within the known range.

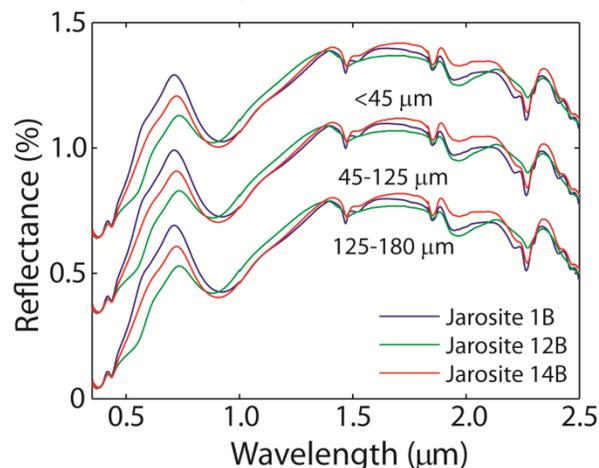


Figure 2: VNIR reflectance spectra of all samples at the three ranges of grain sizes used. Spectra are offset for clarity.

Results and Discussion: Reflectance spectra for the three samples are shown in Figure 2 with corresponding k values derived from the < 45 μ m size fraction in Figure 3. It is apparent from the reflectance

spectra that the compositional variations of the samples are represented in the spectra and also in k . Of these features, the band close to 1.85 μm is useful as a diagnostic feature for the identification of jarosite group minerals and for differentiating them from other sulfate minerals [4,5]. The combination bands between 2.2 μm and 2.4 μm allow differentiation between Na and K jarosites through both their position and appearance, with increasing K content correlating to a decrease in the wavelength position of the 2.2 μm feature [14]. Hydronium jarosites have an overall more muted spectrum with broad absorptions and a characteristic broad band at 1.9 μm .

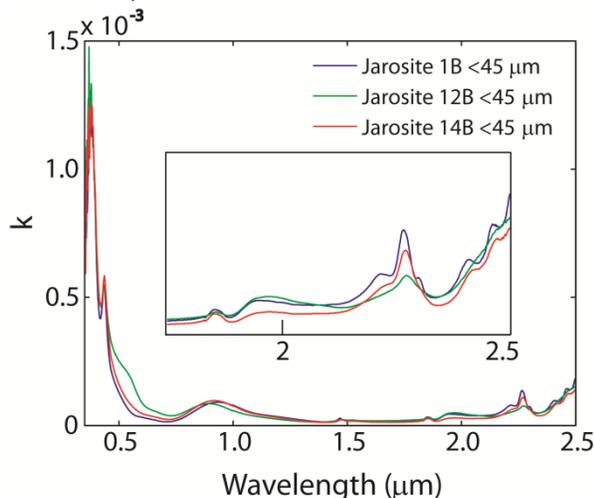


Figure 3: Calculated imaginary index of refraction k vs. wavelength for all three samples at $< 45 \mu\text{m}$ (grain size input of $30 \mu\text{m}$). The insert shows variation in k with composition.

Sulfates in general and jarosite in particular are interesting target minerals for remote sensing studies because their sensitivity to changes in pH, redox, temperature, and relative humidity can indicate the environment in which they were formed. For instance, stoichiometric Na or K jarosites are found associated with hydrothermal deposits and aged supergene deposits on Earth, whereas non-stoichiometric jarosites and hydronium-bearing jarosites are often associated with young or acid-saline deposition conditions [7]. In both cases, natural jarosites are most often intimate mixtures of end-members rather than intermediates in a solid solution [7]. One of our goals will be to determine if these two provenances can be distinguished using scattering theory. Synthetic jarosites, which have high water content, nonstoichiometric formulas, and intermediate compositions, most closely resemble those found naturally in AMD sites [7]; deriving optical constants for these types of samples will be useful in quantifying acidification potential of AMD-affected soils. Like spectral feature mapping, using scattering

theory to analyze remotely sensed spectra is limited by the library of reference materials available as inputs. However, because spectral features can change appearance based upon grain size, and k is, by definition, grain size independent, using nonlinear mixing models and optical constants will allow us to remove uncertainty about grain size-dependent features. In fact, this method can provide fits to remotely sensed spectra that both determine grain size as well as accurately match composition. Most importantly, the use of scattering theory can deliver quantitative abundances within 10% for low resolution data sets [15]. These types of analyses extend the interpretive power of remote sensing data sets so constraints can be placed on formation conditions for the scenes in question. From the standpoint of planetary exploration, quantitative analysis of sulfates can help assess environmental processes that have formed or altered planetary regolith. On Earth, quantifying abundances of sulfates can increase the predictive power of contamination monitoring in areas affected by AMD.

Conclusion and Future Work: Preliminary k values for three compositionally distinct synthetic jarosites were calculated using Lucey's treatment of Hapke scattering theory. This is the first stage in fundamental research on a diverse set of synthetic and natural iron sulfates including r omerite, szomolnokite, rozenite, botryogen, copiapite, paracoquimbite, and melanterite. Future work will include implementation of a Kramers-Kronig transform to determine n , optimization of the scattering theory used to analyze samples, and application of mixture models using these optical constants to the analysis of remote sensing data sets of well-studied localities.

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