Near-infrared (0.67-4.7 μm) Optical Constants Estimated for Montmorillonite. T.L. Roush, NASA Ames Research Center, MS 245-3, Moffett Field, CA 94035-1000, troush@mail.arc.nasa.gov.

Introduction: Various models of the reflectance from particulate surfaces [e.g. 1-2] are used for interpretation of remote sensing data of solar system objects [e.g. 3-4]. These models rely upon the real (n) and imaginary (k) refractive indices of the materials. Such values are limited for commonly encountered silicates at visual and near-infrared wavelengths (λ, 0.4-5 μm). Availability of optical constants for candidate materials allows more thorough modeling of the observations obtained by Earth-based telescopes and space craft.

Two approaches for determining the absorption coefficient ($\alpha=2\pi k/\lambda$) from reflectance measurements of particulates have been described; one relies upon Kubelka-Munk theory [5] and the other Hapke theory [6-7]. Both have been applied to estimate α and k for various materials [e.g. 6-10]. Neither enables determination of the wavelength dependence of n, $n=f(\lambda)$. Thus, a mechanism providing this ability is desirable.

Using Hapke-theory to estimate k from reflectance measurements requires two additional quantities be known or assumed: 1) $n=f(\lambda)$ and 2) d, the sample particle diameter. Typically n is assumed constant (c) or modestly varying with λ [9-10]; referred to here as n_0. Assuming n_0, at each λ an estimate of k is used to calculate the reflectance and is iteratively adjusted until the difference between the model and measured reflectance is minimized. The estimated k's (k_1) are the final results, and this concludes the typical analysis [9-10].

Analytical Approach: The approach described here combines Hapke theory with subtractive Kramers-Kronig (sK-K) analysis [11]. Hapke theory is used to determine k_1 and the next step applies a sK-K analysis to yield n_1, where $n_1=f(\lambda)$. These steps are repeated until no significant change in n and k occurs.

Experimental: The montmorillonite used here (SWy-1) is from the Clay Minerals Society and is originally from Wyoming. The <38- and 38-45 μm grain size fractions were separated via dry sieving. Reflectance spectra were measured with incident and reflected beams at 8° and 6°, respectively.

Results: Using d of each sieve fraction, derived via SEM (3.38- and 3.03-μm), and assuming $n=1.405$ [12], k_1's were derived (figure 1a). Although the k values agree well, there is a difference of ~100 between these and the results of [12].

Reevaluation of the SEM image analyses suggest d's are biased to smaller values as large grains were excluded because they either had small grains adhering to them, or were aggregates of small grains.

An approach in derivation of k that initially relies upon the median particle size of a sieve fraction has been described [10]. Addressing the observed discrepancy at the longer λ's, the analyses were repeated using the median values (19- and 41.5 μm). The resulting k values are shown in Figure 1a. Although these are a factor ~2-3 different from each other, they are closer to the data of [12].

[10] also described adjusting median particle d's to force k's derived from different sieve fractions into agreement. Using this approach d's of 26 μm for both sieve fractions produces k values in agreement with those of [12, figure 1b]. In the iterative approach described above, d of 26 μm is used.

Figure 1c shows the difference between successive values derived for n (Δn). Going from $n=c$ to $n=f(\lambda)$, i.e. n_1-n_0, the greatest Δn is produced, ~0.015 (gray dashed line). Subsequent iterations, n_2-n_1 and n_3-n_2, show a decreasing Δn until it is zero. Similar trends are seen in Figure 1d for the difference in derived k values (Δk). The procedure quickly reaches a solution and further iterations are unnecessary.

One additional effort was motivated by the desire to estimate the optical constants of montmorillonite for the broadest wavelength range. It involved combining the k's derived here with those of [12] for the same sample (figure 1f). These k values were used in the sK-K analysis to provide $n=f(\lambda)$ (figure 1e).

Comparison with previous data: [8] reported α for one Wyoming montmorillonite (sample #25). To compare α's figure 3 of [8] was digitized independently six times. A linear interpolation was used to create: 1) a common λ scale, from 0.4 to 2.5 μm with a sampling of 0.01 μm; and 2) associated α's. From these interpolated values, the average and standard deviation were calculated (figure 2).

It is only feasible to provide a semi-quantitative comparison of the α's derived by the two different techniques. This is due to the difference in the spectral resolution of the instruments used to obtain the data of [8] (see [5]) and the measurements of SWy-1.

Inspection of Figure 2 shows agreement is good for the highest α's within the region of λ overlap of the two data sets, with values of about 7- and 15-cm^{-1} near 1.4- and 1.9-μm, respectively. In λ regions outside these higher values, α's agree to a factor of ~2, except at the longest wavelengths, where the measurements of [8] are only qualitative. The local maximum at ~2.2 μm in the SWy-1 data corresponds to a hydroxylated silicate spectral feature [13].
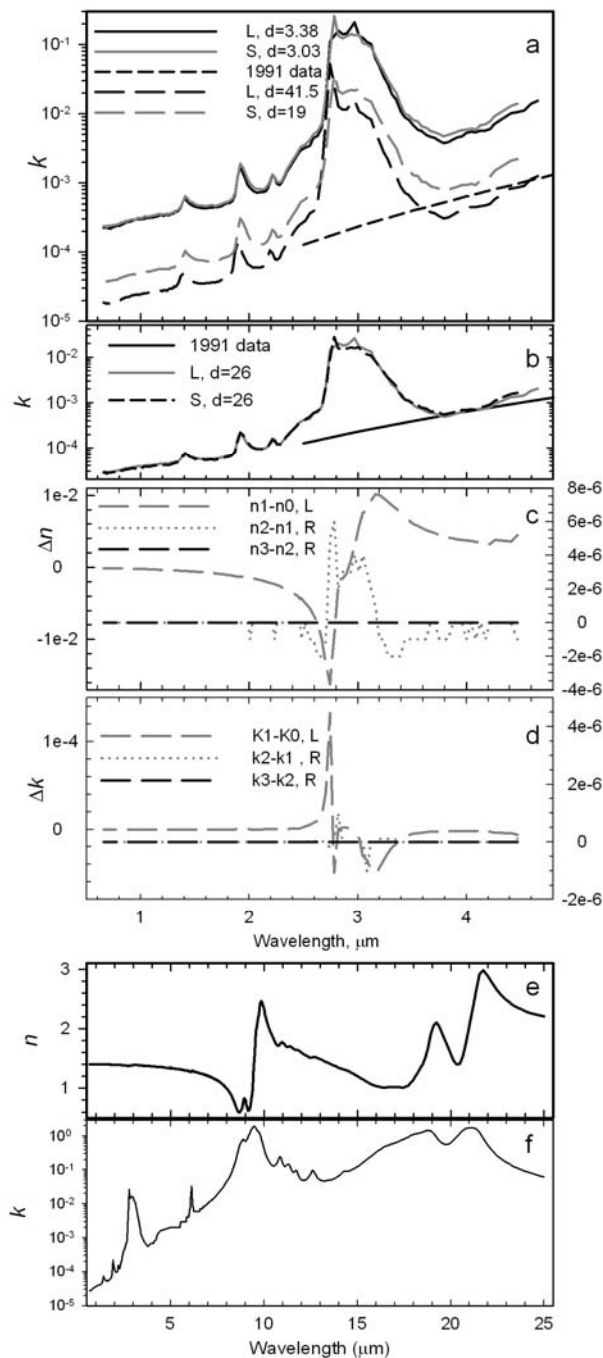
Figure 1. (a) k values of SWy-1 derived using: 1) d determined via SEM (solid lines); 2) median of each sieve fraction (long dashed lines), for the large (L) and small (S) sieve fractions, and values from [12] (short dashed line). (b) k values derived with $d=26$ μm, for large (L) and small (S) sieve fractions, are comparable to the values of [12]. (c) Δn for successive iterations. L and R refer to the ordinate axis. (d) same as c, but for Δk. (e) n via sK-K analysis of k shown in panel f. (f) k's derived and combined with those of [12].
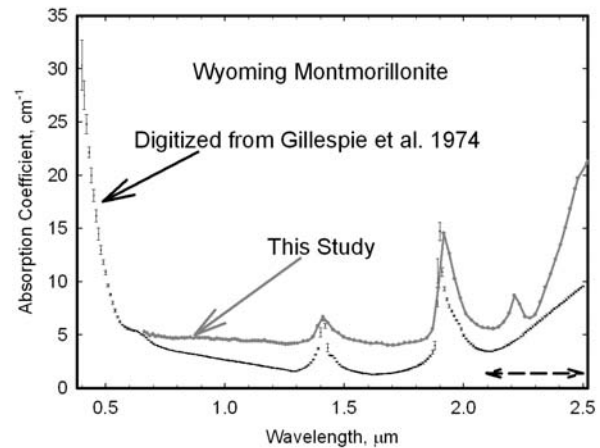

Figure 2. Comparisons of the absorption coefficients derived in this study for montmorillonite (gray points and line) to those determined by [8] (black points with error bars). The dashed arrow indicates estimated values shown by [8].

The discrepancy between the wavelength positions of the local α maxima at ~1.9 μm may be due to the difference in the intrinsic instrumental resolutions. Alternatively, it may be due to differences in the composition or hydration state of the samples. Cationic substitution and hydration state influence the position, width, and asymmetry of the montmorillonite 1.9 μm band [14-15].

Summary: Procedures described here provide the ability to estimate the wavelength dependence of both n and k from reflectance spectra in the visible and near-infrared. The resulting α's compare favorably with those previously reported for montmorillonite [8].

References: [1] B. Hapke, *Theory of Reflectance and Emittance Spectroscopy*, Cambridge U. Press 1993 **[2]** Y. Shkuratov et al., *Icarus:137*, 235, 1999 **[3]** T. Roush, *JGR:106*, 33315 2001 **[4]** D. Cruikshank et al., *Comptes-Rendus Physique:4*, 783, 2003 **[5]** J. Lindberg and D. Snyder, *Appl. Opt:12*, 573, 1973 **[6]** B. Hapke and E. Wells, *JGR:96*, 3055, 1981 **[7]** R. Clark and T. Roush, *JGR:89*, 6329, 1984 **[8]** J. Gillespie et al., *Am. Mineral:59*, 1113, 1974 **[9]** T. Roush et al., *Icarus:86*, 355, 1990 **[10]** P. Lucey, *JGR:103*, 1703, 1998 **[11]** S. Warren, *Appl. Opt.:23*, 1206, 1984 **[12]** T. Roush et al., *Icarus:94*, 191, 1991 **[13]** R. Clark, et al., *JGR:95*, 12653, 1999 **[14]** E. Bruckenthal, MS thesis, U. Hawaii, 1987 **[15]** J. Bishop et al., *Clays Clay Minerals:43*, 702, 1994