

Visible-Near Infrared Reflectance Spectroscopy as a Non-Destructive Tool for Quantification of Organic Compounds in Sediments. H. H. Kaplan¹ and R. E. Milliken¹, ¹Brown University, Department of Earth, Environment and Planetary Science, 324 Brook St., Providence, RI 02904 (email: Hannah_Kaplan@Brown.edu)

Introduction: Visible - near-infrared reflectance spectroscopy (i.e., diffuse FTIR) is a powerful tool for analysis of geologic samples. This rapid and non-destructive technique can be used to identify mineralogy and organic compounds [1], and imaging spectrometers provide important spatial context for such phases.

Using the strength of absorption features in reflectance to quantify composition is difficult for intimate mixtures with multiple components [2]. Low albedo, a common characteristic of carbonaceous chondrite meteorites and surfaces of some planetary bodies, is known to have a disproportionate (nonlinear) effect on absorptions in reflectance spectra [3,4]. Water content also plays a role as C-H absorptions fall within broad and strong OH/H₂O absorptions at ~3 μm [Fig. 1].

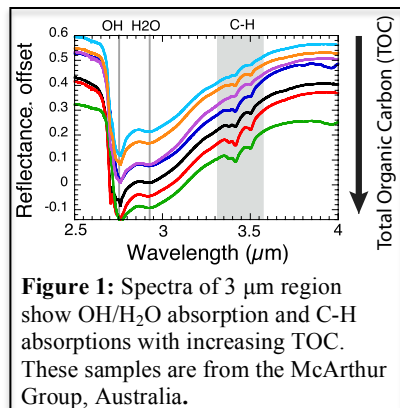


Figure 1: Spectra of 3 μm region show OH/H₂O absorption and C-H absorptions with increasing TOC. These samples are from the McArthur Group, Australia.

The purpose of this study is to build a foundation for the quantification of organic content in sedimentary rocks through analysis of natural samples and synthetic mixtures.

Methods: Reflectance spectra of a range of terrestrial mudstones are measured from ~1.5-25 μm with an FTIR spectrometer. Sample preparation, organic content and geologic setting of the samples has been reported in [5]. Physical mixtures of a solid organic compound (sodium stearate) and clay mineral standards are weighed and mixed by hand. Kaolinite (KGa-1), Illite/Smectite (IsCz-1) and montmorillonite (SAz-1) clays are chosen for their differing amounts of H₂O. Carbon lamp black, which has no absorptions in the VIS-NIR, is added to the samples to control albedo; only a small wt. % is needed to dramatically darken samples [e.g. 4]. Spectral analysis is carried out for all samples, with a focus on band depth (absorption strength) and position of the C-H features as measured in continuum-removed spectra.

Results and Discussion: There is no unifying relationship between total organic carbon (TOC) in a sample and the band depth of organic absorptions for all natural samples. Instead, samples with low albedo or a strong 3 μm H₂O absorption yield a different trendline

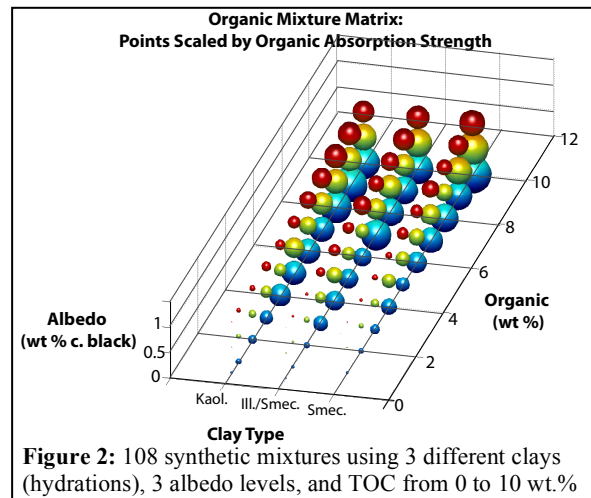


Figure 2: 108 synthetic mixtures using 3 different clays (hydrations), 3 albedo levels, and TOC from 0 to 10 wt. %

than brighter and less hydrated samples. Multiple regression confirms that band depth, albedo, and hydration are significant predictors of TOC.

Because it is impractical to determine the relationship between TOC and band depth for each new geologic setting, we attempt to isolate individual variables that influence the spectra in order to develop robust models for TOC prediction. Spectra of physical mixtures show a clear increase in band depth with TOC [Fig. 2]. For darker samples (more carbon black) the absorptions weaken as expected. Spectra of organics mixed with the less hydrated material (e.g., kaolinite) exhibit stronger absorptions, particularly at low TOC wt. %, than equivalent TOC in more hydrated smectite.

These laboratory mixtures allow us to isolate and quantify the effects of albedo, hydration, and TOC. These trends are then used as baselines to “correct” spectra of natural samples with different hydration and albedo in order to accurately relate observed organic absorption strength to organic content. Results are extrapolated to lower TOC values (< 0.5 wt%) for which it becomes difficult to make homogenous mixtures.

Conclusions: Reflectance spectroscopy can provide remote identification and spatial context of both inorganic (minerals) and organic compounds. The work presented here will help to build a foundation for accurate quantification of organic compounds in complex geologic materials, with implications for laboratory and rover-based analyses.

References: [1] Mustard, J. et al. (2013), *Mars 2020 Science Definition Team*, 154pp. [2] Hapke, B. (1993), *Cambridge University Press*, 455pp. [3] Milliken, R. and Mustard, J. (2007), *Icarus*, 189, 550-573. [4] Clark, R. (1983), *JGR*, 88, 10635-10644. [5] Kaplan, H. et al. (2014) LPS LXXVI, Abstract # 1995.