

Visible - Near Infrared Spectral Indices for Mapping Mineralogy and Chemistry with OSIRIS-REx

Corresponding author: Hannah H. Kaplan (Kaplan@boulder.swri.edu)

Authors:

Hannah Kaplan

Southwest Research Institute, 1050 Walnut St. #300, Boulder, CO 80302

Hamilton, Victoria E.

Southwest Research Institute, 1050 Walnut St. #300, Boulder, CO 80302

Howell, Ellen

Lunar and Planetary Laboratory, University of Arizona, Tucson, AZ 85721

Anderson, F. Scott

Southwest Research Institute, 1050 Walnut St. #300, Boulder, CO 80302

Barrucci, Antonella

LESIA, Observatoire de Paris, PSL Research University, CNRS, Univ. Paris Diderot, Sorbonne Paris Cité, UPMC Univ. Paris 06, Sorbonne Universités, 5 place Jules Janssen, 92195 Meudon, France

Brucato, John

INAF-Astrophysical Observatory of Arcetri, Florence, Italy

Burbine, Tom

Mount Holyoke College, United States

Clark, Beth

Dept. Physics & Astronomy, Ithaca College, Ithaca, NY 14850, US

Cloutis, Ed

University of Winnipeg, Winnipeg, MB R3B 2E9, Canada

Emery, Joshua

Dept. Earth & Planetary Science, University of Tennessee, Knoxville, TN 37996, USA

Fornasier, Sonia

LESIA, Observatoire de Paris, PSL Research University, CNRS, Univ. Paris Diderot, Sorbonne Paris Cité, UPMC Univ. Paris 06, Sorbonne Universités, 5 place Jules Janssen, 92195 Meudon, France

Lantz, Celine

Institut d'Astrophysique Spatiale, CNRS/Université Paris Sud, Orsay, France

Lim, Lucy

NASA Goddard Space Flight Center, Greenbelt, Maryland 20771 USA

Merlin, Frederic

LESIA, Observatoire de Paris, Université PSL, CNRS, Sorbonne Université, Univ. Paris Diderot, Sorbonne Paris Cité, Meudon, France

Praet, Alice

LESIA, Observatoire de Paris, PSL Research University, CNRS, Univ. Paris Diderot, Sorbonne Paris Cité, UPMC Univ. Paris 06, Sorbonne Universités, 5 place Jules Janssen, 92195 Meudon, France

Reuter, Dennis

NASA Goddard Space Flight Center, Greenbelt, Maryland 20771 USA

Sanford, Scott

NASA Ames Research Center, Mountain View, California 94035 USA

Simon, Amy

NASA Goddard Space Flight Center, Greenbelt, Maryland 20771 USA

Takir, Driss

Jacobs/ARES, NASA Johnson Space Center, Houston, TX 77058-3696, USA

Lauretta, Dante

Planetary Laboratory, University of Arizona, Tucson, AZ 85721, USA

Abstract

The primary objective of the Origins, Spectral Interpretation, Resource Identification, Security-Regolith Explorer (OSIRIS-REx) mission is to return to Earth a pristine sample of carbonaceous material from the primitive asteroid (101955) Bennu. To support compositional mapping as part of sample site selection and characterization, we tested 95 spectral parameters on visible to near infrared laboratory reflectance data of minerals and carbonaceous meteorites to find which of these parameters reliably identified spectral features of interest. Most spectral parameters had high positive detection rates when used on spectra of pure, single component materials. The meteorite spectra have fewer and weaker absorption features and, as a result, fewer detections with the spectral parameters. Parameters targeting absorptions at 0.7 and 2.7 – 3 μm , which arise due to hydrated minerals, were most successful for the meteorites. Based on these results, we have identified a set of 17 parameters that are most likely to be useful at Bennu and spectral analogs. These parameters detect olivines, pyroxenes, carbonates, water/OH-bearing minerals, serpentines, ferric minerals, and organics. Particle size and albedo are known to affect band depth but had a negligible impact on parameter accuracy. The effect of instrument-like noise added to the laboratory spectra can result in more false positive detections, but these exhibit large errors. Our study has determined the prioritization of spectral parameters used for OSIRIS-REx spectral analysis and mapping and informs the reliability of all parameter-derived data products.

1. Introduction

Two spectrometers on the Origins, Spectral Interpretation, Resource Identification, and Security-Regolith Explorer (OSIRIS-REx) spacecraft will map (101955) Bennu's (hereafter, Bennu) surface composition and thermophysical properties before the spacecraft collects and returns a sample of the asteroid. One of these instruments, the OSIRIS-REx Visible and Infrared spectrometer (OVIRS), is a point spectrometer that measures reflected light from 0.4 to 4.3 μm , a spectral range that contains features associated with minerals, water, and organics. OVIRS will collect hyperspectral data (resampled to 1393 channels) at spatial resolutions of ~ 20 m during global spectral mapping and ~ 4 m during reconnaissance mapping (Reuter et al. 2018). We will use spectral indices, also called parameters, to reduce the hyperspectral data to single values that direct the science team to regions of interest on Bennu and that can be mapped to evaluate mineral/chemical presence and distribution. These parameters target specific spectral absorptions associated with phases of interest (e.g., organics). The resulting mineral/chemical maps are a major contribution to a science value map that will be considered for sample site selection and will be available in the Planetary Data System (PDS) repository.

In advance of OSIRIS-REx's arrival at Bennu, we collected over 100 spectral parameters from the literature, wrote software to apply them to data having OVIRS's spectral resolution, and tested the indices using laboratory spectra of minerals and meteorites. These tests gauge the fidelity and applicability of each spectral index to materials that are relevant to the surface of Bennu.

Here we present a subset of parameters expected to be most useful for science and discuss the conditions under which these indices perform best.

2. Background

Bennu was chosen as the target of the OSIRIS-REx mission for its proximity and regolith properties. Bennu is a near Earth object (NEO) associated with the asteroids in collisional family Polana-Eulalia (Bottke et al. 2015; Campins et al. 2018; de León et al. 2018). Ground-based visible to near infrared (VIS-NIR) spectra of Bennu exhibit a negative (blue) slope and are classified as B-type in the Bus-DeMeo taxonomy (Clark et al. 2011). B-types are thought to be compositionally primitive and volatile rich, and are sometimes observed to have 0.7 μm absorption, which is associated with hydrated minerals. Ground-based spectra of Bennu lack this 0.7 μm absorption. Binzel et al. (2015) observed variation in Bennu's spectral slope with multiple viewings, which they attributed to particle size variation from regolith accumulation at the equatorial ridge.

Comparison of Bennu's ground-based spectrum to a database of laboratory spectra suggests that Bennu is spectrally similar to the carbonaceous (C) chondrites, specifically the aqueously altered CI and CM groups (Clark et al. 2011). The CIs and CMs have low albedos ($< 10\%$ reflectance at VIS-NIR wavelengths) and show great variability in spectral shape, slope, and number of absorptions depending degree of alteration, particle size, and viewing geometry (e.g., Beck et al. 2018; Cloutis et al. 2011a, 2011b; Johnson and Fanale 1973). Absorptions associated with hydration (OH^- , H_2O) or hydrated minerals are prominent in many of the CI and CM meteorite spectra at 0.7 and 2.7 to 3 μm (e.g., Beck et al. 2010; Hiroi et al. 1996), and are also observed in B- and C-Type asteroids (e.g., Clark et al. 2010; Rivkin 2002; Vilas 1994; Vilas and Gaffey 1989). Weaker absorptions due to vibrational modes and overtones in phyllosilicates, carbonates, sulfates, and organics are seen in some laboratory spectra (Cloutis et al. 2011a).

Carbonaceous chondrite mineralogy has been extensively studied (e.g., Bland et al. 2004; Howard et al. 2009, 2015; King et al. 2015; Tomeoka and Buseck 1988; Zolensky et al. 1993) and, along with laboratory spectra, can help inform expectations for Bennu's surface. Briefly, anhydrous silicates, like olivine, pyroxene, and plagioclase, are commonly found in carbonaceous meteorites, with abundances that diminish with progressive aqueous alteration (e.g., Browning et al. 1996; Howard et al. 2015; McSween 1977; Sheng et al. 1991). Phyllosilicates, specifically (Mg, Fe) serpentines and saponite-like clay minerals, are common products of aqueous processing making up 75 – 80% of the volume of some CM and CI meteorites (Howard et al. 2009, 2015; King et al. 2015). Metals (Fe, Ni) and sulfides are also found in C chondrites (e.g., Abreu and Brearley 2010), though they are unlikely to be observed in VIS-NIR spectra due to lack of absorption features. Magnetite, Fe-oxides, and Fe-hydroxides on the other hand, can have a significant effect on albedo and VIS-NIR absorptions even in low abundances (Cloutis et al. 2011a). Organics with up to 5 wt.% C are common in these meteorites (hence carbonaceous), typically in an insoluble form with a varied composition (e.g., Alexander et al. 2007, 2017). Carbon can also reside in carbonates (e.g., Alexander et al. 2015).

Our knowledge of both the composition and spectral features of the C chondrites informs our expectations for the science return from OVIRS. As a result, the following minerals and chemicals were specifically targeted for analysis with spectral parameters: olivine (forsteritic and fayalitic), pyroxene (orthopyroxene and clinopyroxene), serpentine (Mg, Fe), saponite, mixed layered or poorly crystalline Fe-bearing and clay minerals, magnetite, oxides, hydroxides, carbonates, and organic matter. If these a priori assumptions turn out to be incorrect, then parameters may need to be re-evaluated.

2.1 Parameterizing Spectra for Mission Science

Spectral parameters have an established history in planetary science where there is a need to uniformly process and interpret large amounts of returned spacecraft data (Bell et al. 2000; Lucey et al. 1995; Murchie 2000). The aim is to describe a feature or absorption in the spectrum using a single value, which is defined by algorithmically combining spectral data at certain wavelengths (e.g., Pelkey et al. 2007). The spectral parameters (e.g., combination of algorithm and defining wavelengths) for OSIRIS-REx mission science were compiled from the available literature by the team's Spectral Analysis Working Group (SAWG). A reference for each parameter can be found in Table 1.

A comprehensive parameter set was previously created to interpret data from the Compact Reconnaissance Imaging Spectrometer for Mars (CRISM) aboard the Mars Reconnaissance Orbiter (Pelkey et al. 2007; Viviano-Beck et al. 2014), and the resulting mineral maps ("summary products") have been highly influential for highlighting the diversity and distribution of Martian mineralogy (Murchie et al. 2009; Thollot et al. 2012; Wray et al. 2008). Many of the parameters from Pelkey et al. (2007) have been directly adopted for use at Bennu, but because the expected composition of Bennu differs significantly from Mars, a number of those indices were not incorporated, and other sources were used to ensure inclusive mineral/chemical detection. In total, the OSIRIS-REx team collected 107 spectral parameters from the literature for use at Bennu (Table 1). Due to the diversity of sources from which these spectral parameters were collected, the degree to which each of these parameters has been proven reliable differs. For instance, some have been tested broadly on Mars spectral data (e.g., Ody et al. 2013; Pelkey et al. 2007), others were developed for asteroid spectra (e.g., Lebofsky 1980; Vilas 1994), and still others were created and tested using (commonly monomineralic) laboratory spectra (e.g., Cloutis et al. 2004, 2006). Whether these parameters are applicable outside of the specific scenario for which they were created is an open question, and one this study attempts to test.

Reflectance values are known to represent more than just sample composition. The influence of other factors such as particle size (e.g., Mustard and Hays 1997), albedo (e.g., Clark 1983), space weathering (e.g., Lantz et al. 2015, 2017), temperature (e.g., Bishop and Pieters 1995), and the space environment (e.g., vacuum, Takir et al. 2013) on the spectral parameters also may be of great consequence. For instance, significant changes in slope of the Bennu spectrum have been attributed to particle size effects (Binzel et al. 2015). Where possible, the sensitivity of spectral parameters towards each of these factors was tested. However, there are few spectra available measured at low temperatures or under vacuum. In addition, although space weathering has

been studied extensively, its effect on spectra of C chondrites and small bodies like Bennu is complex (Lantz et al. 2017). Therefore, some spectral properties may only be tested and understood with spectral data returned from the mission.

3. Methods

3.1 Spectral Collection

We tested the spectral indices with mineral and meteorite spectra available in the following public spectral databases: Reflectance Experiment Laboratory (RELAB), United States Geological Survey Spectral Library 7 (USGS), and Jet Propulsion Laboratory ECOSystem (JPL) spectral libraries. We also obtained data from the literature and the OSIRIS-REx spectral library (Takir et al. 2013; Donaldson-Hanna et al. 2018). To identify mineral spectra of interest, we performed a keyword search on the entirety of these databases, searching for each of 28 minerals (e.g., olivine minerals: fayalite and forsterite) that are listed in Table 2. We sought meteorite spectra of C chondrites, ordinary (O) chondrites, and ureilites for their high carbon abundances (as graphite, amorphous carbon, and organic compounds), a priority for spectral detection with the OSIRIS-REx mission. These meteorites also span a range of aqueous and thermal alteration scenarios and consequently contain the full range of primary silicate and alteration minerals that our spectral parameters target.

Candidate test spectra were discarded if they: (1) did not show absorptions characteristic of their labeled mineral, (2) appeared to be significantly contaminated by another mineral so that identifying absorptions were obscured, (3) were duplicates or identical repeat measurements of the same sample (e.g., the spliced and unspliced spectra available in RELAB), and/or (4) were physical mixtures or otherwise experimentally altered beyond grinding. Of the original 1340 mineral spectra returned, we found 1149 that met our criteria and we used them to analyze the spectral parameters. The total collected meteorite spectra are as follows: 85 C and O chondrite particulates from RELAB, 60 ureilite particulates from RELAB, 101 C chondrite chips from RELAB, 30 C chondrite particulates measured under vacuum (Takir et al. 2013), and 17 OSIRIS-REx spectral library samples (Donaldson Hanna et al. 2019) (Table 2).

For both meteorites and minerals, we collected metadata on the wavelength range, particle size, and sample information for each spectrum if it was available. Because these laboratory spectra have the typical high signal-to-noise of laboratory instruments, we also created a second library of noise-added spectra with 5% random noise added at all wavelengths, which is in line with expected noise for the OVIRS instrument (Reuter et al. 2018). One thousand random noise profiles were generated and added to each spectrum to determine how noise affects band depths and errors calculated by Spindex.

3.2 Parameter Analysis

After collecting our test spectral dataset, we calculated 107 spectral parameters for every spectrum with Spindex, an IDL-based program that was created by the team for calculating the

OSIRIS-REx spectral indices. The test spectral dataset was resampled to the spectral resolution of OVIRS in order to be compatible with Spindex. Of the 107 spectral parameters, 12 were not included in the analysis; these parameters measure slopes or reflectance ratios and will be used to highlight space weathering trends and regional composition at Bennu. For the remaining 95 parameters, Spindex uses 21 different equation types that range from a typical band depth measurement (Clark and Roush 1984) to more complex weighted sums that take into account reflectance values at up to 5 or more different wavelengths (i.e., Ody et al. 2012) (see Supplementary Figure 1). Table 1 contains a full list of these parameters, a reference to the equation used to calculate them, the defining wavelengths, and a threshold value. The threshold is an estimate of the minimum valid band depth value for the parameter, in most cases defined by OVIRS instrument requirements (Reuter et al. 2018; Simon et al. 2018).

Spindex produces a number of data products in relation to each spectrum including band depths, errors on those band depths, band presence (e.g., whether band depth is above or below the designated threshold), and reflectance at 0.5 μm . Although the threshold was an integral part of this analysis, Spindex reports band depth values whether or not they fall above the threshold, and we have attempted to include this information where possible. In addition, we compared the calculated band depths to mineralogy (for the meteorite spectra), particle size, and reflectance at 0.55 μm to determine (a) the relationship between parameter value and composition, if any and (b) the influence of non-compositional variables most likely to affect band depth.

An uncertainty value (band sigma) is computed for every equation type. The adopted uncertainty in the wavelength dimension for spectral band parameter position is 16 nm in each direction from the given value (i.e., 32 nm). In OVIRS spectra short of 2.4 μm , the spectral resolution is 2.5 nm, so the 32 nm range includes 12-13 channels. The root mean square (rms) of these points is taken to be the uncertainty in the spectral value for the calculation. The uncertainties in the calibrated spectra due to read noise, thermal noise, gain, and other instrumental sources, along with the absolute calibration and photometric correction are also included and added to the rms noise in quadrature. For each band calculation, these uncertainties in the input band center and continuum values are propagated according to the band depth formula using a Taylor expansion (Bevington 1969).

To test parameter performance, we visually evaluated every spectrum along with its Spindex output and determined whether the Spindex-identified absorption features were positive, negative, false positive, or false negative. A positive was recorded if the spectral index or parameter identified a spectral feature as being present (i.e., above threshold), and the feature was in fact present. A negative result was recorded if spectral index did not identify the spectral feature, and the feature was not present. A false positive result was recorded if the spectral index identified the spectral feature, but the feature was not present. Finally, a false negative would be recorded when the spectral index did not identify a feature, but that feature was present. However, due to the difficulty of correctly determining the mineral/chemical source of the absorption and estimating whether or not the absorption was stronger than the threshold, false negatives were likely underreported. Due to the high likelihood of inconsistencies, we do

not report the false negative results, though practically speaking, they were helpful in determining gaps and updates needed for Spindex (i.e., new parameters or parameter adjustments). Thus, parameters with high rates of positives and negatives and low rates of false positives were designated as reliable parameters.

4. Results

4.1 Minerals

We tested the parameters on 1149 spectra of 28 different minerals/organics (Table 2) to determine how the parameters perform in the most ideal case, where each spectrum represents a single, pure phase. These tests allowed us to identify parameters that have a high rate of positive identification for the phase of interest and return a low rate of false positives for other minerals/organics. For clarity, we discuss a few examples along with a summary of the overall findings, and all results are presented in Supplementary Tables 1.1 – 1.13.

In the first example, we tested a spectral parameter targeting pyroxene (#47: Pyroxene at 1.9 μm) on spectra of the pyroxene minerals augite, hedenbergite, pigeonite, ferrosilite, and enstatite (Figure 1 a, c). Using this parameter, 83% of the pyroxene spectra have band depths stronger than 5%, so a majority of the pyroxenes are positively identified. If we break these results down by pyroxene mineral, however, we see that the Ca-rich clinopyroxenes (hedenbergite, augite, and pigeonite) typically exhibit weaker band depths, whereas enstatites and ferrosilites almost always exceed the 5% band depth threshold (Figure 1a). Comparing the spectra of the pyroxenes, this discrepancy appears to be due to the longer wavelength position of Ca-rich clinopyroxene 2 μm band, which is not well-captured by the wavelengths defining this parameter (Figure 1c). Ideally, we want parameters that positively identify pyroxene any time it is present in a spectrum, in addition to parameters that can be used to distinguish between low calcium (LCP) and high calcium pyroxenes (HCP).

We are equally interested in how a spectral parameter deals with spectra of minerals that are not targeted by that parameter. For example, when the pyroxene parameter above is tested on all 1149 mineral spectra it returns a false positive 18% of the time (i.e., positively detects pyroxene where a visual inspection reveals that there is no pyroxene). An example of the positive, negative, and false positive results for six different parameters is shown in Figure 2, with the results tabulated by mineral type. In some cases where there are overlapping absorption features (e.g., pyroxene and olivine at 1 μm) we expect a higher rate of false positives, so results broken down by mineral allow for a fuller assessment of parameter performance (Figure 2, Supplementary Table 1.1-1.13).

These tests demonstrate that most parameters work as expected for pure mineral spectra. For instance, an olivine parameter defined in Pelkey et al. (2007) (#48: olivine @ 1.05 – 1.47 μm) positively identifies the 1 μm feature in both fayalitic ($\text{Fo} < 50$) and forsteritic ($\text{Fo} > 50$) olivine (Figure 2a). However, this parameter also generates false positives for a number of the other mineral types, usually as a result of a non-olivine iron absorption near 1 μm . In another example,

a serpentine parameter (#66: Mg-OH at 2.32 μm) also performs well for the targeted serpentine minerals (antigorite, chrysotile, cronstedtite, and lizardite), but likewise returns many false positives for carbonates, organics, and clays due to their absorption features in the 2.2 – 2.5 μm region (Figure 2b). Parameters #89 and #107, targeting aliphatic organics at 3.42 μm and carbonate at 3.95 μm , respectively, are two examples that perform well (> 75% positive detections) for their target chemical/mineral groups and have false positives concentrated in specific mineral groups (Figure 2c, d). The aliphatic organics absorption at 3.4 μm overlaps with a carbonate absorption at that same wavelength, so this parameter returns false positives specifically for the carbonate minerals calcite, dolomite, and magnesite.

In a small number of cases, parameters perform poorly even on their target minerals. Figure 2(e, f) shows two extreme examples: parameters #13 (NH @ 3.43 μm) and #42 (olivine @ 1.25 μm). Parameters that return only false positives, but never any positive results, are concerning due to the likelihood of misinterpretation when mapping Bennu and have been labeled “Do Not Use (DNU)”. Most of these parameters target absorption features that overlap with the strong OH/H₂O absorption at 3 μm . These parameters are likely to be useful for many applications including the one for which they were designed but may be unsuitable for application to Bennu if a 3 μm absorption is present.

4.2 Organics

Organics are one of the key phases targeted by OVIRS observations. Absorptions due to aromatic CH at 3.28 μm (#105) and aliphatic CH at 3.42 μm (#89) were chosen as the most likely features to be seen on Bennu based on the carbonaceous chondrites (e.g., Alexander et al. 2017; Kebukawa et al. 2011; Orthous-Daunay et al. 2013; Schmitt-Kopplin et al. 2010). This expectation is consistent with previous remote detections (e.g., Campins et al. 2010; Cataldo et al. 2013; Chiar et al. 2013; Dartois et al. 2004; Pendleton and Allamandola 2002; Rivkin and Emery 2010). Previous work has shown that band depth at 3.42 μm is strongly correlated with hydrogen to carbon ratio (H/C) in pure, insoluble organics extracted from meteorites and sedimentary rocks (Kaplan and Milliken 2018; Kaplan et al. 2018). Because insoluble organic matter (IOM) constitutes the majority of the organic matter in C chondrites (Alexander et al. 2017), IOM spectra were used as the most reliable test of the organic spectral parameters. We find that the IOM with the highest H/C values have aliphatic absorption features (#89) greater than the 5% threshold, but there are no aromatic absorptions greater than 5%.

In laboratory spectra of meteorites, the aliphatic organic absorption is rarely detected at > 5% band depths and aromatic absorptions are no longer seen (Kaplan et al. 2019 – in review). However, if we change the threshold for detection of the aliphatic absorption to 4%, we find that there are 30% more positive organic detections in the meteorites and still <4% false positives (e.g. these are real detections in the meteorite spectra). If the threshold is 3%, there are 95% more positive organic detections for the meteorite spectra and the false positive detection rate increases to 8%. It may be necessary, therefore, to lower the threshold of valid band depths for

this parameter in order to detect organics on Bennu and tests on the meteorite spectra show this can be done without greatly increasing the number of false positive detections.

4.3. Meteorites

The meteorite test spectra help establish how well the parameters work on heterogeneous materials that are our current closest approximation to Bennu's surface. The C chondrite spectra have lower overall reflectance and fewer absorption features (particularly features with > 5% depth) than the pure mineral spectra. Prominent features in the meteorite spectra include Fe-related absorptions from 0.5 – 1.2 μm and the OH/H₂O absorptions from 2.7 – 3 μm (Cloutis et al. 2011b, 2011a). Many of the carbonaceous chondrites also have spectral features associated with organics and carbonate (3.4 and 4 μm). Although some carbonaceous chondrites have weak pyroxene and olivine absorption features (1 and 2 μm), only the ureilites, rare stony meteorites with high carbon content (e.g., Berkley et al. 1980), routinely have olivine and pyroxene absorptions with >5% band depths (Figure 1b,d).

Parameters tested on the C chondrite spectra calculate weaker band depths, resulting in fewer positive detections and fewer false positive detections than for the mineral spectra. Parameters applied to the meteorite spectra have, on average, ~2% false positives compared to the 9% average false positive returns for the pure mineral spectra. Only half of the 95 parameters are ever observed above their threshold value and, of these positive detections, more than 80% are due to the 4 parameters that measure the 3 μm region.

Absorptions associated with hydrated minerals at 0.7 and 2.7 – 3 μm are of particular interest for the OSIRIS-REx mission (Lauretta et al. 2015). Parameter #7 targeting OH @ 2.7 μm results in band depths surpassing the 5% threshold in 62% of meteorite spectra. This absorption feature is least prominent in the pristine ureilites and more prominent in aqueously altered CH, CK, CI, CR, and CM chondrites (Figure 3a). In fact, the band depth of this 2.7- μm absorption becomes weaker with increasing petrologic type (i.e., Beck et al. 2014; Garenne et al. 2016), which corresponds to decreasing aqueous alteration and increasing thermal processing (Figure 3b). Other parameters associated with the 3 μm region (#3, #4, and #52) showed comparable results, but may be more strongly influenced by adsorbed terrestrial water in spectra measured under ambient conditions. The 0.7- μm band is positively identified in fewer meteorite spectra (15%) and is even more specifically associated with spectra of aqueously altered C chondrites as it is only observed in the CM and C-ungrouped meteorites (Figure 3 c, d). All of the meteorites with a 0.7- μm absorption are petrologic type 1 or 2, or the most aqueously altered of the meteorites.

A small portion of the meteorite spectra used in this study (30 out of 293 total spectra) were measured under vacuum, and all of these are C chondrites. Takir et al. (2013) demonstrate that the vacuum environment reduces the strength of the 3 μm H₂O absorption in these spectra by removing adsorbed terrestrial water. However, even with the adsorbed water absent, we detect a 3 μm absorption (#3, H₂O/OH @ 3 μm) in 78% of these vacuum spectra. By comparison, this absorption is detected in 99% of the C chondrite particulates measured under ambient

conditions and in 94% of the C chondrite chip spectra, which are also measured under ambient conditions but are expected to be less affected by adsorbed water than the particulates (Supplementary Figure 2). Given the predominance of ambient spectra in our collection, the positive detection rates and band depths at 3 μm are overestimates, though the vacuum spectra confirm that this feature is still likely to be observed with our parameters for asteroids and other space observations.

4.4 Summary of Mineral, Organic, and Meteorite Tests

Using a combination of the meteorite test results (Supplementary Table 1.13) and the mineral/organic test results (Supplementary Tables 1.1-1.12), we identified the 17 parameters that are most likely to perform well for carbonaceous meteorites, Bennu, and similar asteroid surface mapping (Table 3). These results were guided by the expected mineralogy/chemistry of bodies like Bennu as described in the background section (e.g., minerals/chemicals we want to be able to detect) and the results of the mineral and meteorite parameter tests (e.g., how good we are at actually detecting them) with more weight given to the meteorite test results. This subset of parameters targets olivines, pyroxenes, phyllosilicates, ferrous minerals, carbonates, and organics. Most of these parameters yield positive detections in >80% of cases for the pure minerals, and those that result in a lower fraction of successful cases were chosen specifically because they worked well for meteorites or filled a needed niche (e.g., aromatic organics).

5. Composition, Albedo, Particle Size, and Simulated Instrument Noise

5.1. Composition

We collected 17 well-characterized meteorite and analog mineral mixture spectra as part of preparation for the OSIRIS-REx spectral measurements with OVIRS and the thermal emission spectrometer (OTES) (Christensen et al. 2018). The dataset consists of particulate samples measured under ambient conditions at the OVIRS and OTES wavelengths without added noise. Donaldson Hanna et al. (2018) report the team's spectral interpretation of those samples, focusing on the OTES wavelengths. We compared mineral abundances and band depths for the OSIRIS-REx spectral library samples to understand the relationship, if any, between parameter strength and composition (Figure 4). We collected the meteorite mineral abundances from literature (Howard et al. 2015) and measured them directly (Donaldson-Hanna, 2018), but the meteorites are known to be heterogeneous and there is no guarantee that the sample aliquots measured spectrally are identical in mineralogy to the ones in the literature or even the thin sections of our own samples.

We find multiple parameters that are correlated with mineral abundance. Fit using a linear regression, the relationships reported here have r^2 values > 0.6, and in some cases as high as 0.82. First, pyroxene abundance is correlated with three parameters (#25, #56, and #71) that measure band depth near 0.9 μm . However, the pyroxene band depths are all below the 5% detection threshold. Given how weak many of the meteorite absorption features are, it may be important to map and assess band depths below the threshold at Bennu. Phyllosilicate

abundance is correlated with parameters (#3, #4, #7, and #52) that measure the 3 μm feature between 2.7 μm (OH) and 3 μm (OH/H₂O) (Figure 4). The 3- μm absorption band depths are greater than the 5% threshold, though the strength of this feature may be artificially increased due to the presence of adsorbed terrestrial water (Takir et al. 2013), which likely explains why some samples with 0 vol.% phyllosilicates have band depths that exceed zero. Garenne et al. (2016) also demonstrate a linear relationship between 2.8 μm band depth and H wt.% for C chondrite spectra measured under vacuum ($r^2 = 0.66$), where H wt.% is a proxy for phyllosilicate abundance, suggesting that a relationship exists whether or not adsorbed water is present. Ultimately, a larger number of samples with coordinated spectral and compositional measurements (e.g. X-Ray Diffraction, microprobe) is needed to provide further evidence for band depth-compositional relationships in meteorites.

5.2 Albedo and Particle Size

Because the spectra collected for this study were measured for many purposes, the variable measurement conditions allow us to test the effects of sample and spectral properties on the Spindex parameters. In particular, it is important to know how these parameters respond to spectra of natural surfaces with variable particle size and albedo. For most minerals and the meteorites, we have enough spectra (Table 2) that a wide range of albedos is represented by the dataset (e.g., see Figure 5 for range of reflectance at 0.55 μm for serpentines and meteorites). In addition, the dataset includes spectra of both optically thick slabs (referred to here as chips) and particulates, with particulate size fractions ranging from <10 μm to >1000 μm , with <45 μm being the most common particle size.

We compared the reflectance at 0.55 μm to band depth for each of the parameters and found no correlations. Reflectance at 0.55 μm was used because it corresponds to the V passband (e.g. filter centered at 0.55 μm used in broad-band photometry) and is the most common wavelength for reporting geometric albedo or normal reflectance of asteroids. Band depths weaken as albedo decreases (Clark 1983; Milliken and Mustard 2007; Nash and Conel 1974), so if an albedo effect is present, we would expect to see a positive correlation between reflectance at 0.55 μm and the band depth returned by each parameter. Figure 5 (a, b) shows one such comparison for parameter #50 (Fe²⁺-Fe³⁺ @ 0.7 μm in serpentine) for both serpentine mineral spectra and meteorite spectra. In this case, the parameter appears to have the strongest band depth at the lowest reflectance values. This association between albedo and band depth is likely a result of this absorption feature arising in only the most aqueously altered C chondrites, which are also the lowest albedo samples.

As with albedo, there is no observed particle size effect in these data. In VIS-NIR spectra, samples with the smallest (<10 μm) and largest (> 500 μm) particle sizes have the weakest band depths due to dominance of surface scattering and absorption respectively over volume scattering (e.g., Hapke 1993; McGuire and Hapke 1995; Mustard and Hays 1997). Laboratory spectra are commonly measured on powders ground to an intermediate particle size of < 45 μm to maximize volume scattering. We analyzed the meteorite spectra with an 0.7- μm absorption and found that this absorption is observed at all particle sizes, including for chips. There are as many detections

as non-detections (above and below threshold) at all particle sizes for this spectral parameter (Figure 5c, d). The mean, mode, or distribution of particle sizes in the samples is rarely reported, so it is possible that the maximum particle size, which is used here, does not accurately represent sample particle size. Interestingly, within the meteorite spectra, a greater proportion of the chips have a 0.7- μm feature than the particulates. Again, this difference is likely a result of compositional variability between the two groups; the chip samples are primarily CM-group C chondrites, which are likely to have a 0.7- μm absorption, whereas the particulate sample group also includes ureilites, ordinary chondrites, and thermally processed C chondrites that typically do not have this absorption feature. All other parameters also lack a relationship with particle size.

5.3 Noise

We see systematic differences in Spindex results when $\pm 5\%$ random noise is added to every spectrum (e.g., Figure 6). Spindex calculations account for noisy data by averaging 3 or more channels for every wavelength calculation, so small, single channel spikes should not disproportionately affect the calculation. There is a possibility of removing real absorption features or adding spurious ones when noise is present. We consider four different outcomes of added noise: (1) there is no change in absorption features detected, (2) a previously detected absorption feature is no longer observed when noise is added, (3) a previously detected false positive is no longer observed when noise is added, and (4) added noise creates a new feature that was not previously detected. We find that all four outcomes routinely happen for our noise-added laboratory spectra (Figure 6).

We find that 5% noise can strongly affect the interpretation of absorption features in the spectrum, and in some cases the noise disproportionately increases or decreases band depth by over 100% (Figure 6 b, c). For instance, our original, noise-free spectrum of the Murchison meteorite does not have a 3.42 μm organic absorption feature and, appropriately, when parameter #89 (CH @ 3.42 μm – aliphatic organics) is calculated on that spectrum, band depth is close to zero. However, when this parameter is calculated on 1000 Murchison spectra with added noise, the 3.42 μm band depth varies from -1 to 0.8 (80%) and a large portion of the noise-added spectra have band depths greater than the 5% threshold. Thus, the added noise is creating a new feature that was not previously detected. Alternatively, parameter #7 (OH @ 2.7 μm) was originally above the threshold value, but in some of the noise-added spectra, that absorption no longer has a band depth > 5%.

Error analysis can reduce false interpretations from noise. Band depth is highly correlated with the error value on that band depth (e.g., $r^2 = 0.96$ for parameter #89 calculated on Murchison), in such a way that error is minimized when band depth is closest to the true (noise-free) band depth (Figure 6 b, c). The largest, spurious band depths also have the largest errors, which means they are more likely to be identified and removed during spectral analysis and mapping.

6. Caveats

Spectral parameters are a useful method for collapsing hyperspectral data into a single data point, which enables rapid assessment of spectra and provides a straightforward value for mapping, but there are important caveats to consider when using parameter values instead of full spectra. The first is that abundance and band depth are not necessarily correlated. Although a small number of parameters appear to have increasing band depths with mineral abundance (Figure 4 b, c), for others this correlation does not exist or there is not enough mineral/chemical data to test for a relationship. VIS-NIR absorption strength is expected to be non-linearly related to composition (e.g., Hapke 1993; Hulst 1981) and only a few other studies have looked at absorption strength and composition for comparable materials (Garenne et al. 2016; Kaplan et al. 2019-in review). In all likelihood, obtaining more than relative abundances from the mineral/chemical maps produced from these parameters will be a non-trivial task.

The potential also exists for low signal to noise data or spikes at specific wavelengths to influence the Spindex band depths (and specifically band depths above the determined threshold value). For some parameters (e.g., organics and other weaker features) absorptions may only be detected below the given threshold value and individual spectra will need to be visually inspected to distinguish between noise and spectral features at these low values. Similarly, absorption features in regions where there are multiple similar absorptions (e.g., the 1 μm feature in both olivine and pyroxene) will be difficult to distinguish with spectral parameters and combinations of bands (e.g., checking whether or not the 2 μm band is present to potentially distinguish pyroxene from olivine) may be needed to positively detect these phases. We recommend that any important or unusual identifications, and especially any band depths with high uncertainty values, should be validated manually in the original spectral data prior to inclusion or exclusion from maps.

Although we attempt to create a comprehensive set of spectral parameters, both asteroid and instrument conditions may require additional parameters or adjustment of existing ones. The laboratory spectra used to test the parameters typically were measured under ambient conditions that may lead to the observation of hydration features that are not indigenous to the sample. Space weathering may also change spectral features in ways that are not readily testable with unweathered samples. Therefore, some parameters that do not work well in our test scenarios may turn out to be useful for Bennu. Additionally, parameters that are deemed inappropriate for C chondrites or carbonaceous asteroids may be highly useful for other applications.

7. Conclusions

From an original list of 95 spectral parameters derived from the literature, we describe the 17 that are most likely to capture the mineral and chemical diversity on Bennu and in C chondrite meteorites (Table 3). These parameters were tested on 1149 mineral spectra and 293 meteorite spectra and they: a) identify absorption features that we expect to be present on Bennu, and b) rarely falsely identify absorptions that are not present in the spectrum. In the course of finding the best parameters, we have also identified parameters that routinely return negative and/or false results, which require extra caution when applied to asteroid or meteorite spectra. These

results will provide guidelines for mineral/chemical mapping on Bennu given expected asteroid and instrument conditions. Although the laboratory spectra do not show systematic relationships between albedo or particle size and band depth, we anticipate that differences in albedo, particle size, viewing geometry, and space weathering could have a discernable effect on the spectra gathered at Bennu.

Analysis of laboratory spectra with the spectral parameters intended to be used during the OSIRIS-REx mission informs our expectations and procedures for spectral mapping of features in OVIRS data. The positive and false positive detection rates calculated for various mineral types and meteorite groups will be useful for estimating errors on the mineral/chemical maps. These maps will be an integral part of sample site selection for OSIRIS-REx and will be available in the PDS for use by the scientific community.

Acknowledgments

This material is based upon work supported by NASA under Contract NNM10AA11C issued through the New Frontiers Program.

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