Earth and Space Science

Supporting Information for

TANAGER: Design and Validation of an Automated Spectrogoniometer for Bidirectional Reflectance Studies of Natural Rock Surfaces

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Introduction

Here we present details of the characterization of the Three-Axis N-sample Automated Goniometer for Evaluating Reflectance (TANAGER) instrument upon delivery to Western Washington University (WWU) in Spring 2021. These characterization data (Text S1-S5) were collected to evaluate TANAGER's performance requirements (Table 1 in the main text), and later to reevaluate them after ~300 hours of instrument use (Table S1). From these assessments we have developed recommendations for long-term TANAGER operations (Text S6).

Text S1. Sample Heating Characterization

Incident light sources can gradually raise the temperature of illuminated portion of samples, which may cause signal drift (change in spectral shape and reflectance over time), loss of adsorbed water (especially for particulate samples) and/or phase changes for some minerals. To quantify these effects, we measured sample temperature and spectral changes over one hour of exposure to the TANAGER light source for solid and particulate targets with a range of albedos: Spectralon® white reference target (Labsphere Inc.; Sutton, New Hampshire), Gray70 color standard (70% white, Lucideon Inc.), Gray33 color standard (33% white, Lucideon Inc.), Black color standard (Lucideon Inc.), basalt sand (Columbia River Flood Basalts, Grand Ronde; 125-250 µm), and powdered kieserite (Sigma-Aldrich).

The temperature of each target was collected just before exposure to incident light and then at regular intervals over the next hour using an infrared laser thermometer with +/- 0.1°C accuracy. Spectralon® and Lucideon Black were also exposed to the incident light source of a Malvern Panalytical Contact Probe for comparison. The distance from light source to target is not equivalent for TANAGER (22 cm) and the Contact Probe (3.5 cm), nor are the illumination sources (the Contact Probe uses a halogen bulb and TANAGER uses a stabilized broadband tungsten-halogen light source), but given that the Contact Probe is an industry standard for geologic sample characterization, it provides a useful point of comparison.

We evaluated target temperatures after two, ten, and 60 minutes of exposure to the incident light source as typical illumination durations during TANAGER data collection (two minutes is the duration each sample remains under the illuminated spot during an automated run). All samples heated rapidly immediately after exposure to incident light. Beyond ten minutes, samples continued heating at a slower rate until a maximum temperature was reached over the next hour (Figure S2). Targets increased by 2-4°C after two minutes of exposure to the TANAGER light source and up to 16°C after an hour, except for Spectralon®, which heated negligibly (0.4°C). These temperature increases are not insignificant, but they are a noticeable improvement over those from the Contact Probe (Figure 22). We observed no changes to the reflectance spectra for any targets over the duration of the experiment.

Text S2. Heating and Dehydration Characterization

We exposed crushed anhydrite ($CaSO_4$, also known as drierite, powdered to < 106 µm) to the TANAGER light source and monitored spectral changes as a test for whether enough heating would occur to drive off adsorbed water. We ran one experiment for 30 minutes of intermittent light exposure (in 2-3 minute cycles, which simulates normal use of TANAGER), and another for 30 minutes of continuous exposure (which simulates maximum exposure during TANGER setup). During both tests, we collected spectra every

2-3 minutes, and temperature of the anhydrite was collected with an infrared thermometer immediately following spectra acquisition.

We observed minimal changes to the temperature of the anhydrite under intermittent and continuous exposure to incident light. Under intermittent exposure, the temperature increased by a maximum of 0.7°C from baseline. Under continuous exposure, the temperature increased by 2.4°C in the first 5 minutes, and an additional 0.7°C after the full 30 minutes of the experiment. These continuous exposure results are consistent with our other heating experiments (Text S1).

We also observed negligible spectral changes during both experiments (Figure S3). The spectra of powdered anhydrite are bright and largely featureless, except for the hydration features at ~1400 nm and ~1900 nm. The smaller features near 1750 nm and 2210 nm indicate that minor gypsum ($CaSO_4 \cdot 2H_2O$) is present in the sample, and therefore some component of the hydration features is attributable to structural water; however, most of the band depths near 1400 nm and 1900 nm are attributable to adsorbed water molecules on the mineral grains.

We measured band depths beneath a continuum (Clark & Roush, 1984) for the absorptions at 1420 nm and 1910 nm during exposure to TANAGER's light source (Figure S4). Band changes negligible during both the intermittent (less than 0.0005 over 30 minutes) and continuous exposure experiments (<0.006 for both bands, with ~90% of the change occurring within the first 10 minutes). These results suggest very minor changes to the amount of adsorbed water on the powered samples, which gives us confidence that heating due to TANAGER's light source will not drive off significant adsorbed water from mineral grains or otherwise dehydrate samples during normal operations.

Overall, we assess that the TANAGER light source is low risk for inducing spectral changes, but we still recommend caution where appropriate. Continuous exposure can be limited by taking care to keep the incident light on the Spectralon® puck (which has negligible temperature effects; Figure S2) or a blank sample slot, instead of a target sample, during set up and between data collection runs. Additionally, during height finding (which usually occurs under the incident light), the light source can be turned off.

Text S3. Detector Spot Size Characterization

We determined TANAGER's detector spot size by collecting spectra of a series of black paper disks with central openings of increasing diameter layered over white paper. The disks were 7 cm in diameter and had apertures that ranged from 1 to 5 cm. We made disks with apertures at intervals of 0.2 cm from 1.0 to 3.0 cm, and 0.5 cm from 3.0 to 5.0

cm. We collected spectra at e = 0°, 15°, 30°, 50°, and 70°; and i = 0° (except for e = 0°, where we instead used i = 30°).

We evaluated spectra between 635 nm and 1395 nm (where the black paper has a steep positive slope, and the white paper has a near-zero slope) using two metrics: slope and root mean square error (RMSE), a statistical comparison of similarity between series. RMSE is calculated using the following formula:

$$\boldsymbol{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(\boldsymbol{P}-\boldsymbol{O})^2}{\boldsymbol{n}}}$$

where *P* is the predicted value (or reflectance of the white paper) and *O* is the observed value (or reflectance of the disk). Disks with neutral slopes and low RMSE indicate a lack of influence from the black paper and an aperture size larger than the detector spot size.

A high and a low confidence threshold were used to provide a range of slope and RMSE values considered similar to white paper based on the natural variation in 4 spectra of the white paper. The high confidence threshold was determined by:

$$MAX_{\text{white paper}} + (MAX_{\text{white paper}} - MIN_{\text{white paper}})$$

where MAX white paper is the maximum slope or RMSE value from the 4 white paper spectra and MIN white paper is the minimum slope or RMSE value. The low confidence threshold is similarly calculated by:

$$MAX_{\text{white paper}} + [5*(MAX_{\text{white paper}} - MIN_{\text{white paper}})]$$

Spectra of disks that yield RMSE or slope values below these thresholds are considered to lack influence from the black disk, indicating that the spot size is smaller than the aperture for that disk.

Spot sizes at a range of geometries are shown in Table 2 in the main text. The low end of the reported spot size range is the smallest diameter based on RMSE and slope where the black paper does not influence the spectrum based on the low confidence threshold. The high end of the reported spot size range is the same based on the high confidence threshold. Spot sizes range from <1.6 cm at e = 0° to <3.5 cm at e = 70°.

Text S4. Vibration Characterization

Vibration caused by TANAGER could cause samples to shift, resulting in changes in the field of view over the duration of a run, either from particulate material settling over time or from variations in light source or detector pointing due to vibration. To assess the baseline vibration from TANAGER, we used the *Vibration Analysis* mobile phone application (Kharutskiy, 2014). All measurements were taken with a phone placed on

TANAGER's sample tray, except "Lab bench" (Figure S4), which was collected with the phone on the lab bench as a baseline for the lab's vibration. We assessed the following possible sources of vibration: TANAGER itself while still; TANAGER incidence, azimuth, and sample tray movement; and the slamming of self-closing fire doors adjacent to the lab. We measured vibration at a sampling rate of 100 Hz in the units of g. The intensity of vibration is reported as the minimum value for a measurement subtracted from the maximum value.

All measurements except azimuth movement and tray movement yielded vibration intensity less than the resolution of the measurements (0.018g based on the software and hardware limitations; Allan, 2011), which we consider to be negligible. Tray movement vibration intensity is up to 3x the data resolution (0.057g in the x-axis), and azimuth movement intensity is up to 12x the data resolution (0.221g in the y-axis) (Figure S4). These values are still considered low and since neither movement happens during data collection, the likelihood of impact is low.

Repeat imagery of mixed particulate material in a TANAGER sample cup further confirms that TANAGER movements are unlikely to shift materials and negatively impact the quality and consistency of spectra (Figure S6). Spectral repeatability of variable surfaces in Section 4.2 also suggests that pointing and illumination are consistent and not affected by instrument vibration.

Text S5: Polarization Artifact Characterization

TANAGER design parameters require that polarization artifact peaks at ~1100 and 1300 nm (Section 2.7) are less than 0.1 reflectance for dark basalt samples. Since delivery, TANAGER data has rarely shown these artifacts and, qualitatively, peaks are diffuse and muted compared to data collected with the contact probe or with spectrometers comparable to the FieldSpec.

We evaluated these polarization artifacts (Section 2.7, Figure 18) for TANAGER spectra using a full hemispheric dataset of coated basalts from Hawai'i. The artifacts were not visible in most spectra, but some of those at larger phase angles displayed clear artifacts with peaks at ~1100 and 1300 nm (Figure S7). We quantified the difference between polarization artifacts and the continuum by dividing the maximum difference between measured values and a continuum by the continuum value at that wavelength. Percent differences are between 0.76% and 2.15%, with slightly lower differences for the 1100 nm peaks than the 1300 nm peaks. All measured percent differences, therefore, are well below the 10% threshold required by TANAGER parameters and are qualitatively rare and small in TANAGER data. Therefore, we do not consider polarization artifacts to be an ongoing concern in our datasets.

Text S6: Recommendations for Long-Term TANAGER Operations

After two years and more than 300 hours of use, we reevaluated a selection of TANAGER's requirements (Table 1) for data quality, alignment of key parts, and consistency of movement. We compared results to the initial assessments performed by First Mode, LLC on delivery of TANAGER in the spring of 2021, and found that most requirements are still met (Table S1). The only hardware aspect with measurable degradation was the consistency in sample tray positioning, which varied an average of 0.8 mm with a maximum variability of 1.8 mm (a considerable increase from values on delivery). Higher errors resulted from "jerky" movements of the sample tray, which we attribute to degradation of its motor.

We also found that the accuracy of the intersecting lasers on the incidence arm (that indicate the plane of measurement) can shift over time. These lasers had no quantitative design requirements, but we evaluated them after ~250 hours of TANAGER run time when one of the lasers needed replacement. It is unclear how significant laser shift is over time, but due to their importance for sample positioning, we recommend recalibrating the lasers periodically to ensure they intersect in the center of the incidence light footprint and 11" above the baseplate, and before long (> 1 day) runs or before datasets intended for publication.

In summary, we recommend reevaluating most performance requirements every 300-500 hours, and more frequently for the lasers, sample tray repeatability, and other items as concerns arise. When any components are replaced (e.g., light source, motors), the relevant performance requirements should be evaluated promptly.

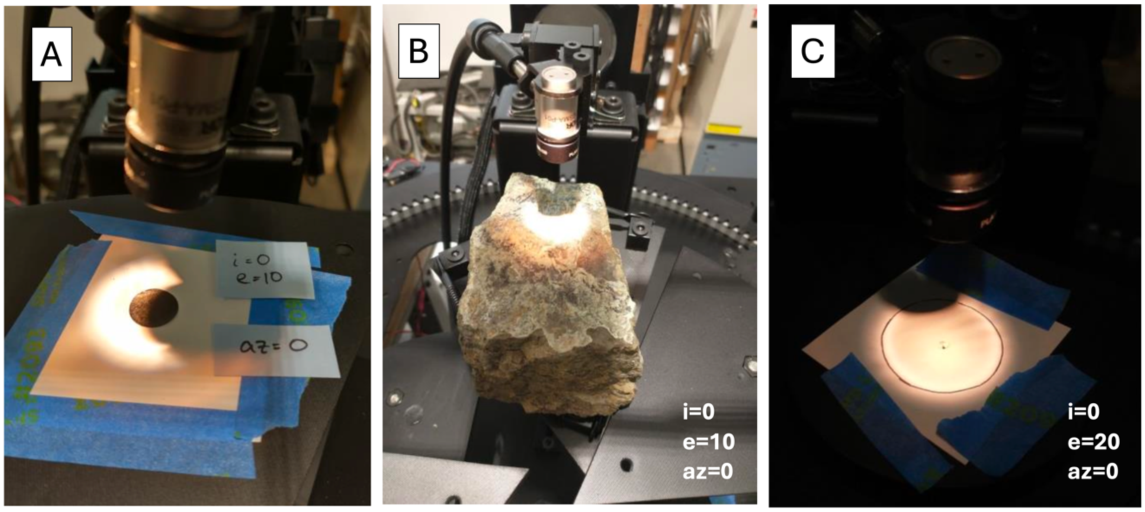

Figure S1. Examples of shadows cast by TANAGER's detector for phase angles g=10° (a-b) and g=20° (c). The requirement that the detector head not fall inside the incident light beam for g >= 20° (sub-requirement 1.1, Table 1) is not met, as shown in (c), but we find this to be acceptable because the shadowed region is outside the detector pointing.

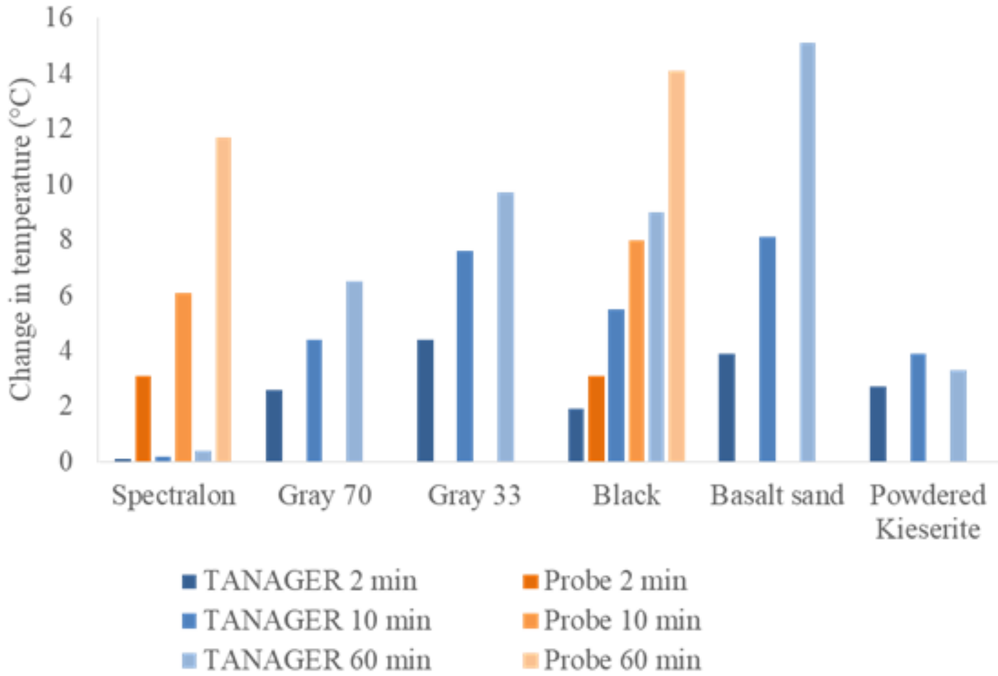

Figure S2. Changes in temperature under TANAGER's incident light source for a range of solid and particulate targets. Changes in temperature under a Malvern Panalytical Contact Probe for the Spectralon® and Black color standard are shown for comparison.

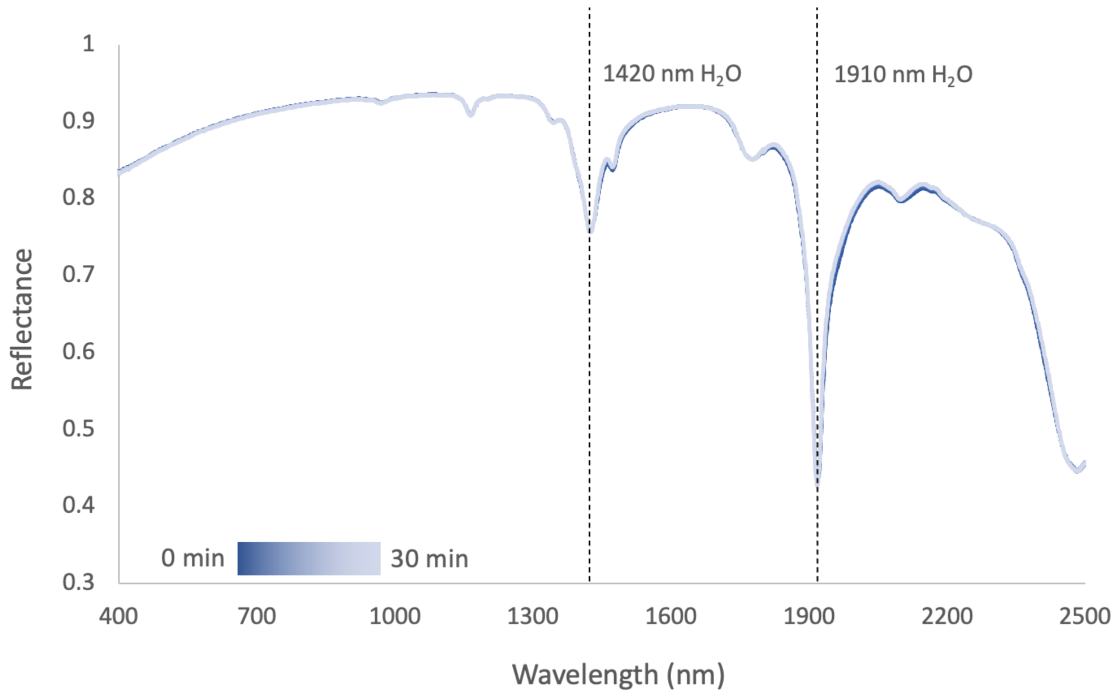

Figure S3: Fifteen spectra of anhydrite ($CaSO_4$) acquired over 30 minutes of continuous exposure to TANAGER's incident light source. Prominent absorption bands due to hydration are labeled. No meaningful changes to these absorptions (or any other spectral features) were observed during heating experiments, implying that TANAGER's light source is unlikely to drive off adsorbed water from mineral grains (or otherwise dehydrate samples).

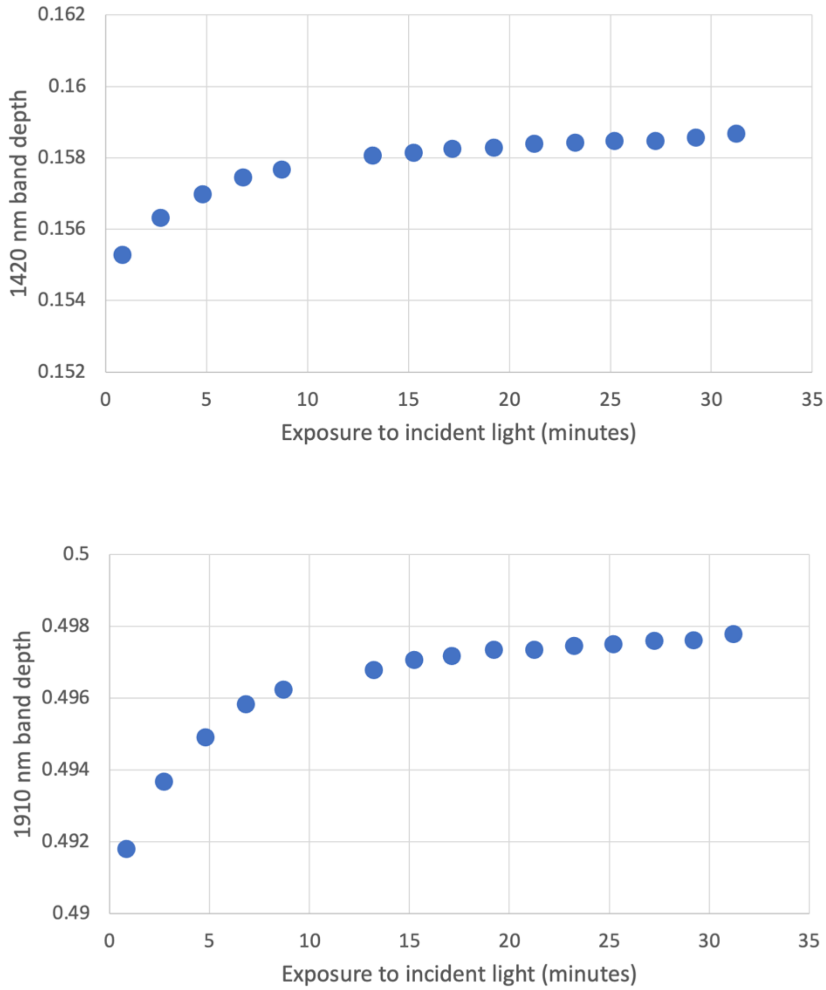

Figure S4: Changes to hydration band depths due to adsorbed water on anhydrite grains during continuous exposure to TANAGER's light source. Above: 1420 nm band depth beneath a continuum with shoulders at 1330 nm and 1500 nm; Below: 1910 nm band depth beneath a continuum with shoulders at 1820 nm and 2050 nm.

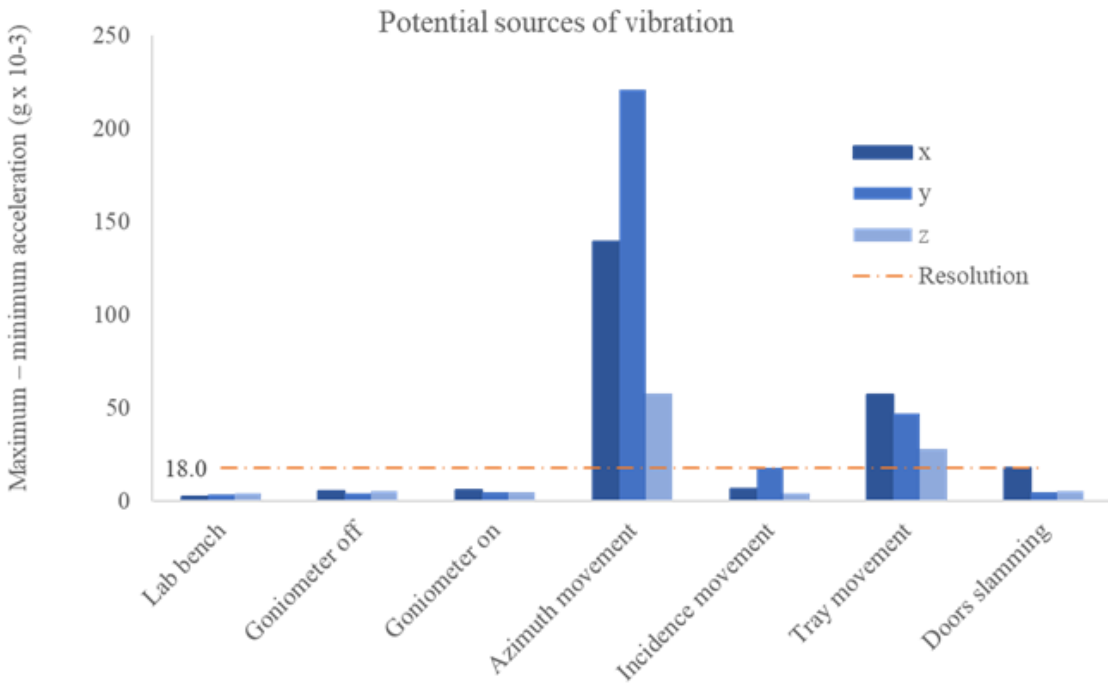

Figure S5: Total variation (maximum – minimum acceleration values) for x, y and z axes yielded from possible TANAGER vibration sources. The dashed horizontal line represents the resolution of the hardware and software.

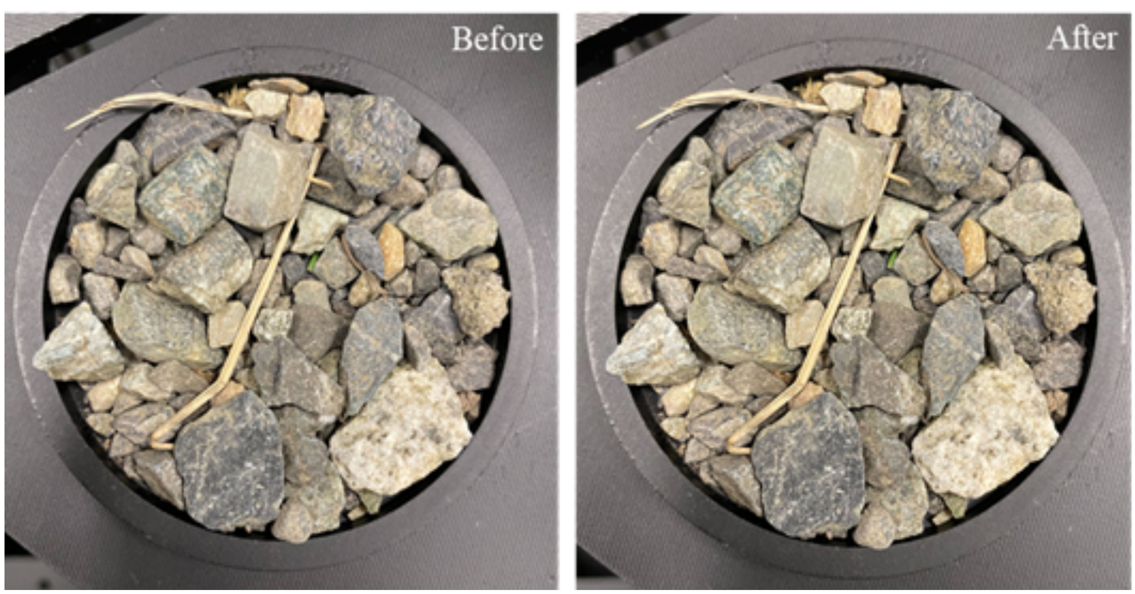

Figure S6: A mixture of loose gravel and grass in a TANAGER sample cup before and after being subjected to a full 360° rotation of the sample tray in 60° increments; and 360° of azimuth rotation (0° to 180° and 180° back to 0°).

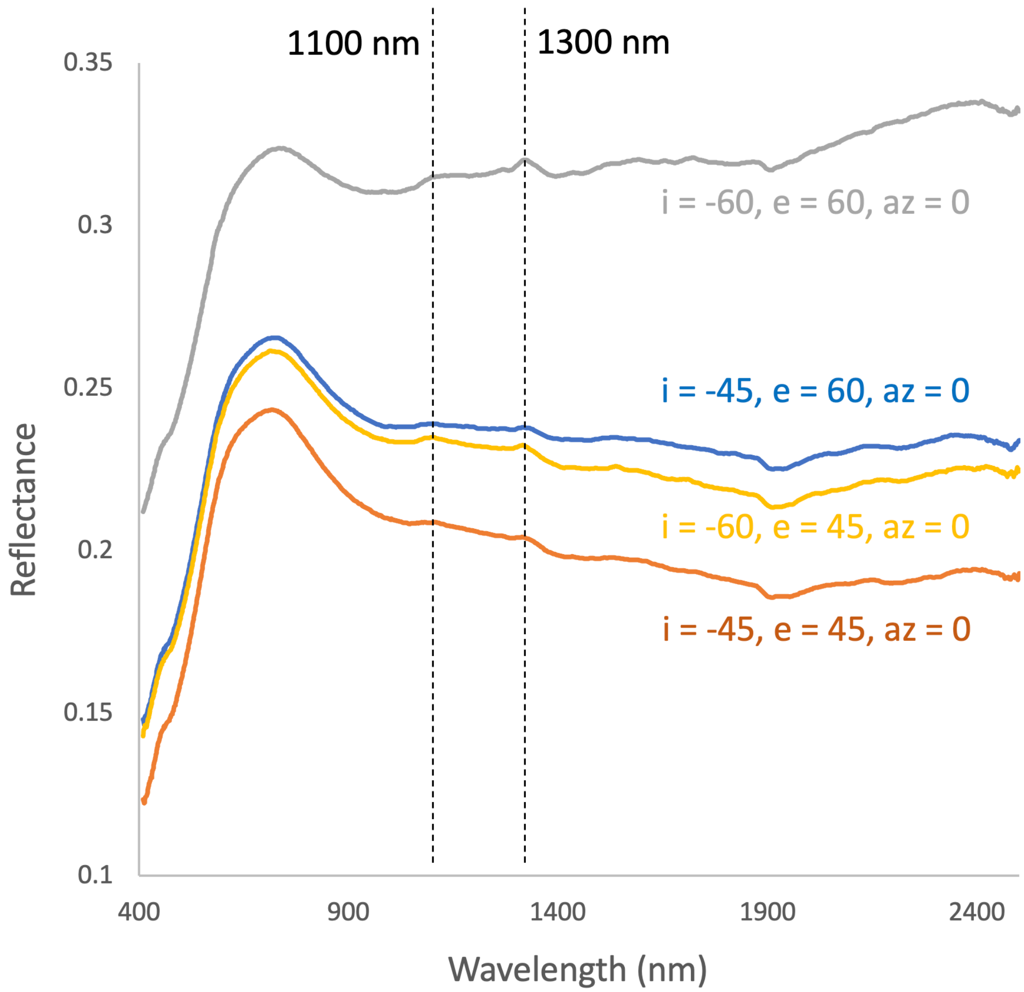

Figure S7: Spectra of a coated basalt from Hawaii with minor polarization artifacts at 1100 nm and 1300 nm.

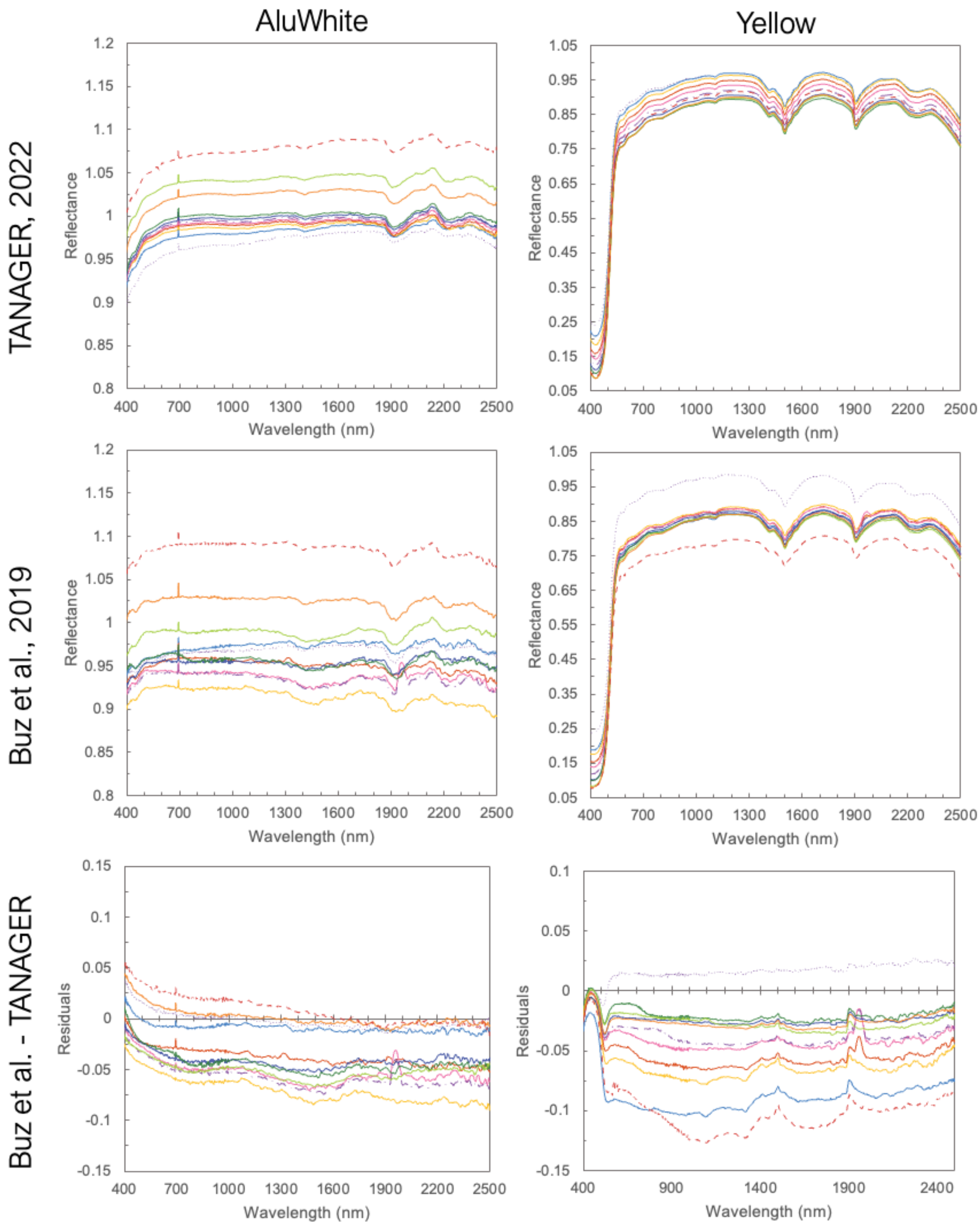

Figure S8: Spectra of the AluWhite and yellow Mastcam-Z caltarget witness samples at multiple viewing geometries from TANAGER (top) compared to Buz et al. (2019) (middle), with residuals (bottom). All measurements were acquired at i = 30° and az = 0°.

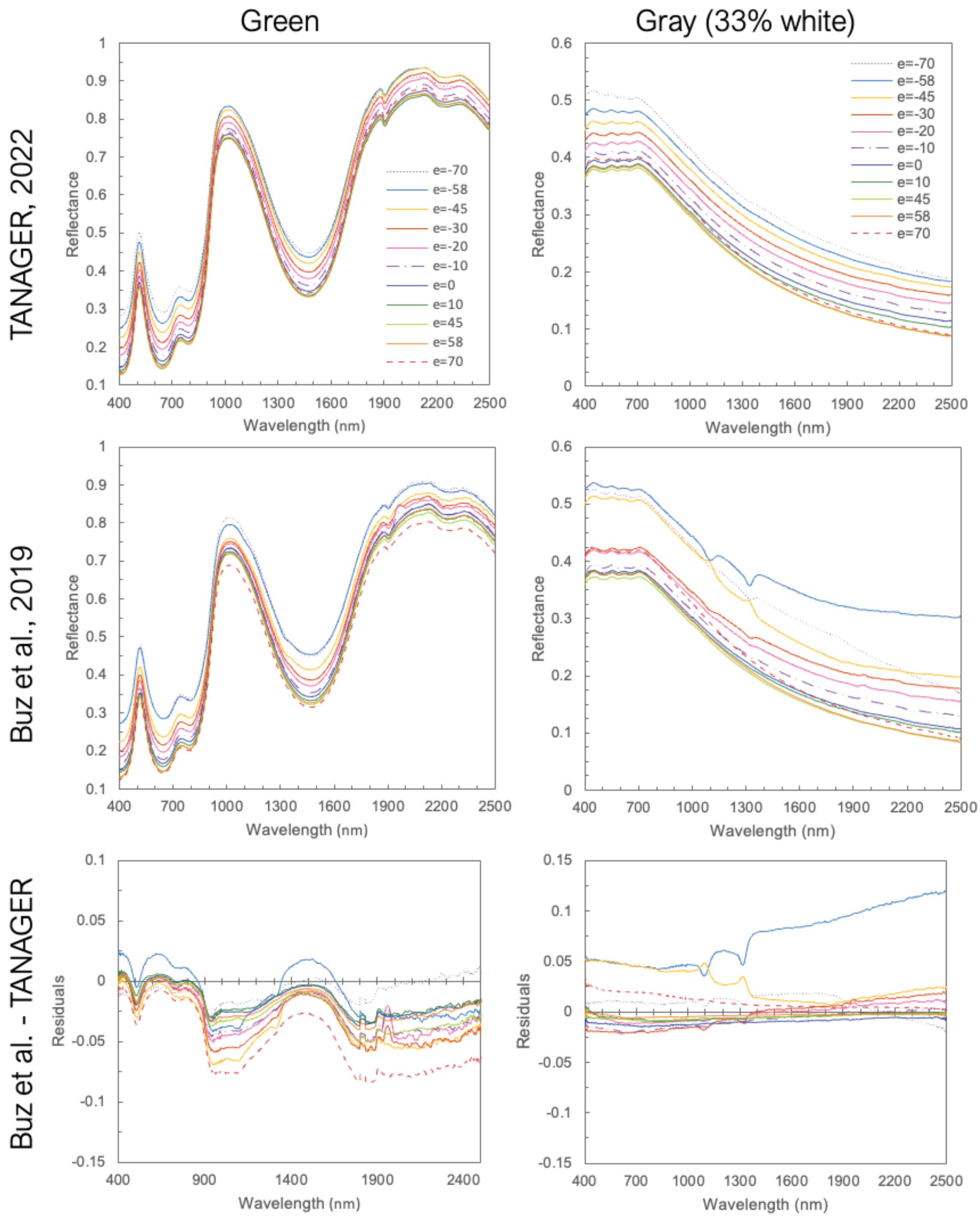

Figure S9: Spectra of the green and dark gray (33% white) Mastcam-Z caltarget witness samples at multiple viewing geometries from TANAGER (top) compared to Buz et al. (2019) (middle), with residuals (bottom). All measurements were acquired at i = 30° and az = 0°.

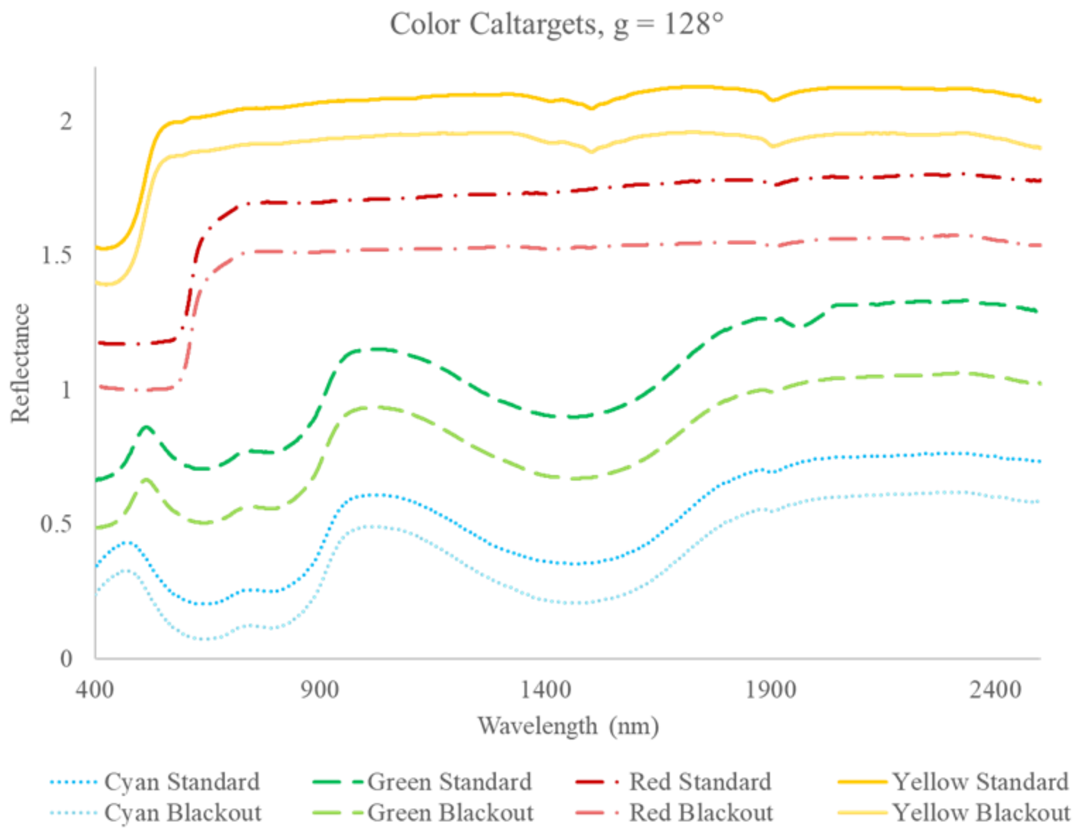

Figure S10: Spectra of color caltargets collected with TANAGER in a very forward-scattering geometry (g = 128º) with and without blackout curtains on the lab cabinetry ("Blackout" vs. "Standard"). The curtains reduce stray light reflected from lab surfaces and reduce overall reflectance (but do not otherwise change spectral shape). Spectra are offset for clarity (Cyan by -0.55; Green by -0.15; Red by +0.40; Yellow by +0.80).

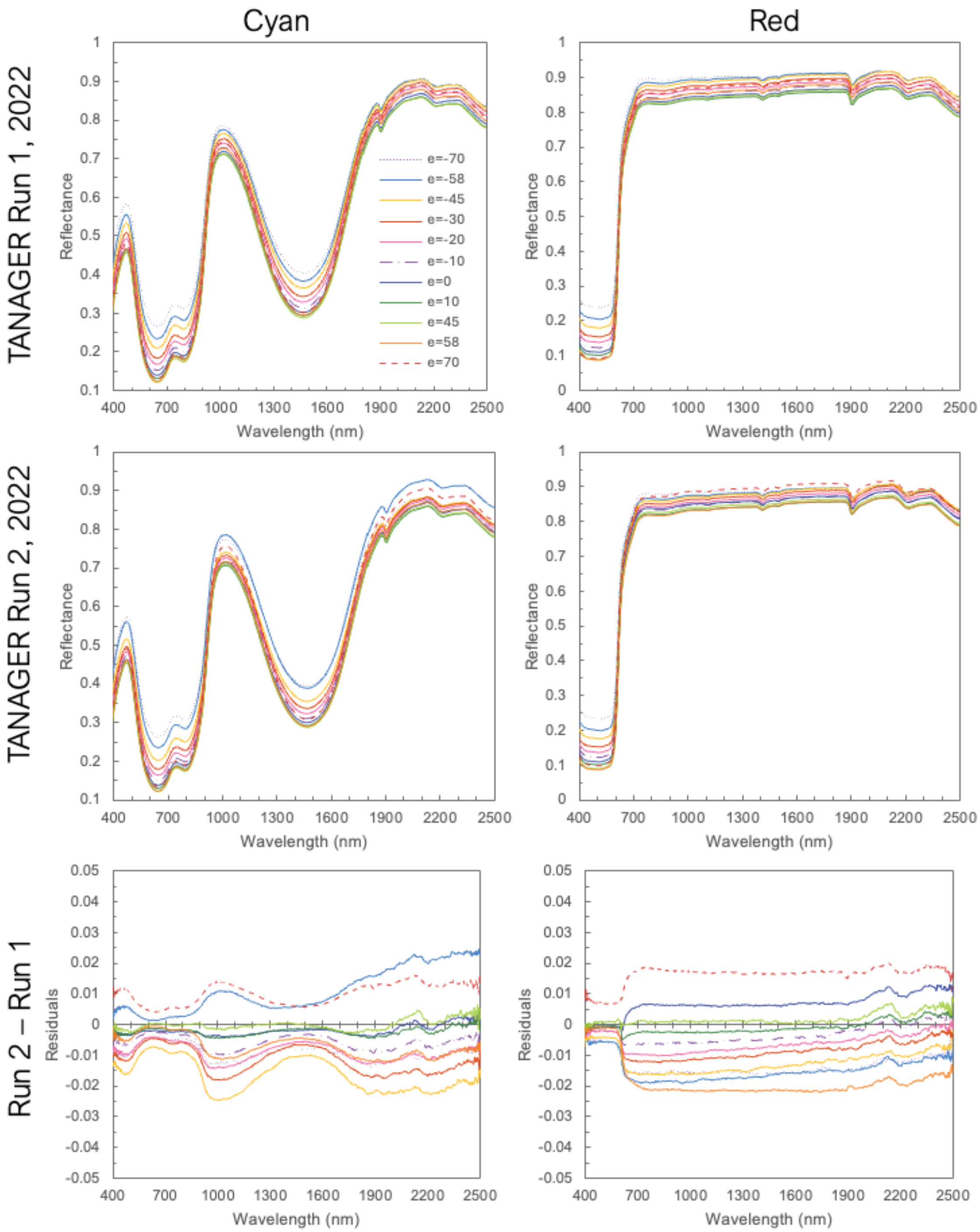

Figure S11: Spectra of the cyan and red Mastcam-Z caltarget witness samples from two TANAGER data collection runs (top and middle) with residuals (bottom). All measurements were acquired at i = 30° and az = 0°.

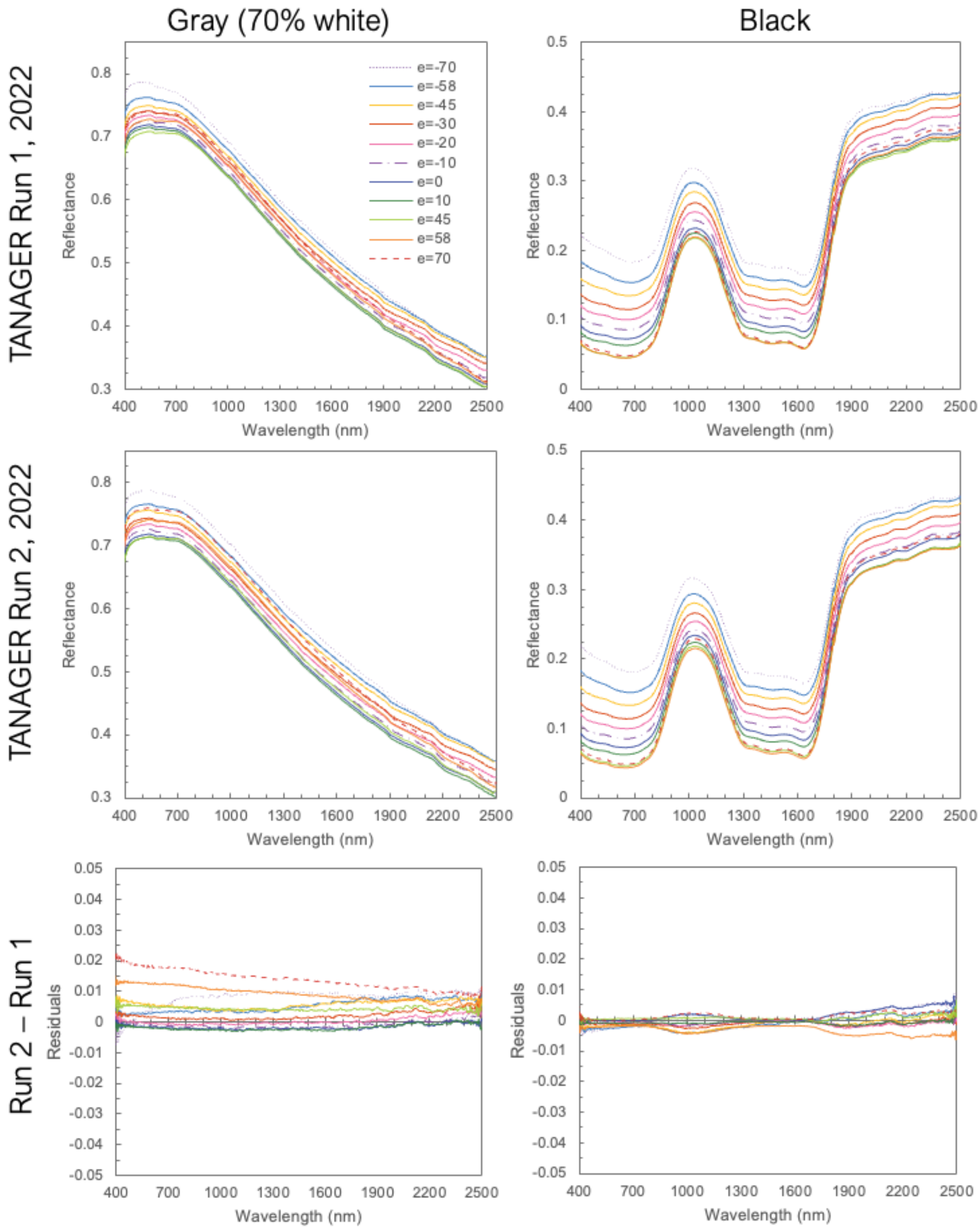

Figure S12: Spectra of the light gray (70% white) and black Mastcam-Z caltarget witness samples from two TANAGER data collection runs (top and middle) with residuals (bottom). All measurements were acquired at i = 30º and az = 0º.

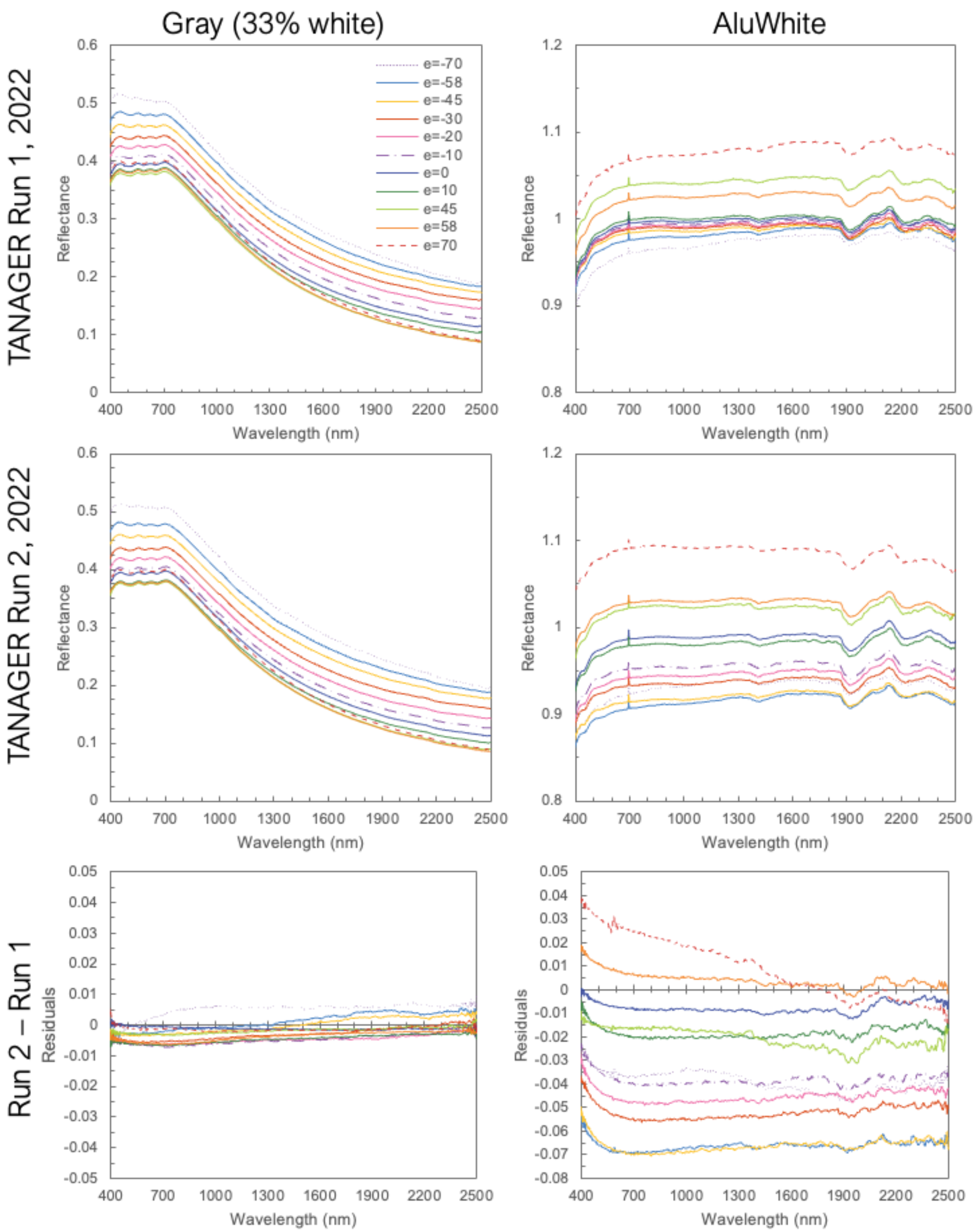

Figure S13: Spectra of the dark gray (33% white) and AluWhite Mastcam-Z caltarget witness samples from two TANAGER data collection runs (top and middle) with residuals (bottom). All measurements were acquired at i = 30° and az = 0°.

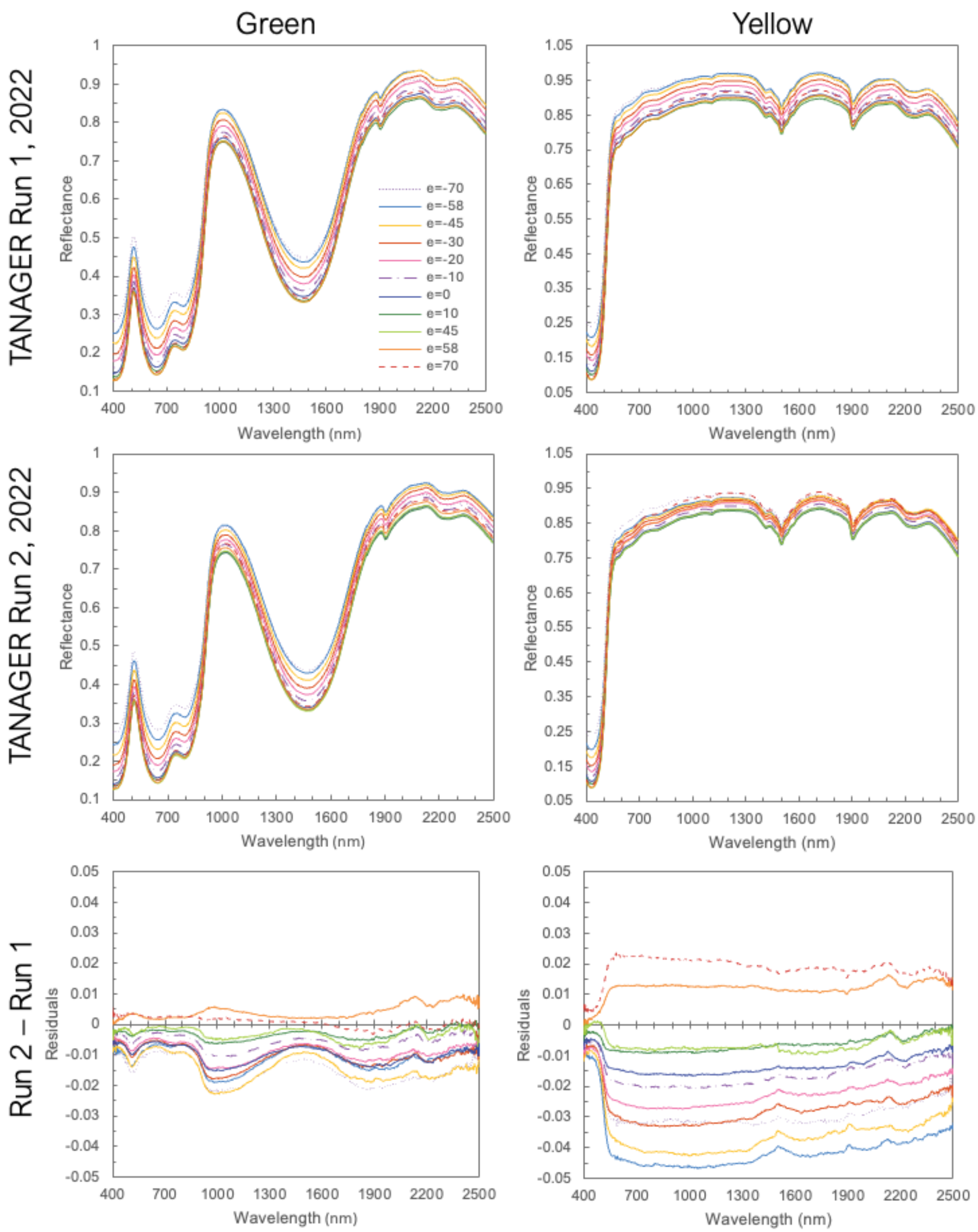

Figure S14: Spectra of the green and yellow Mastcam-Z caltarget witness samples from two TANAGER data collection runs (top and middle) with residuals (bottom). All measurements were acquired at i = 30° and az = 0°.

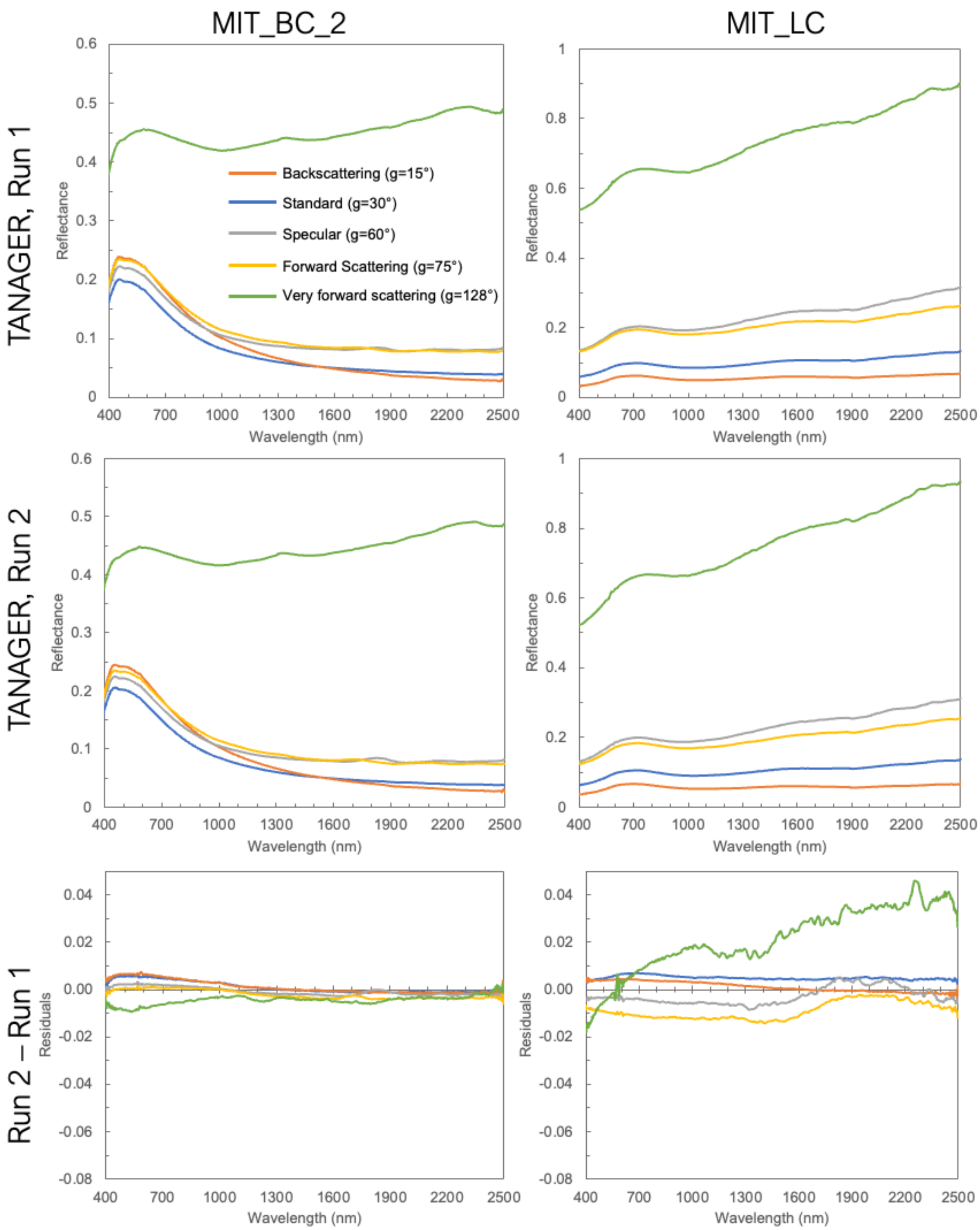

Figure S15: Spectra of heterogenous, naturally-coated basalt samples (MIT_LC and MIT_BC, see Figure 25) from two TANAGER data collection runs (top and middle) with residuals (bottom). All measurements were acquired at i = 30° and az = 0°.

Requirement	Reevaluation	Recommendation
1.11 Signal drift from heating at small phase angles	Standard deviation is less than 0.005 over 15 minutes of exposure to incident light	Reevaluate every 300-500 hours of use, and when a new bulb is installed
1.12 Noise	Noise values < 0.001 at all wavelengths (quantified by subtracting an original spectrum from its Savitzky-Golay smoothed spectrum; window size = 19, order = 2)	Reevaluate every 300-500 hours of use
1.13 Polarization artifacts	Measured < 0.01 difference in reflectance from artifact to continuum (or as high as 2.2% of the continuum)	Reevaluate every 300-500 hours of use
1.3 Angular control	All angular controls have an accuracy <1°: • Incidence: 0.3° average, 0.8° max variability • Emission: 0.3°average, 0.9° max variability • Azimuth: <0.1° average, 0.1° max variability	Reevaluate every 300-500 hours of use
1.5 Pointing accuracy - light source	illumination pointing to varies with azimuth motion by 1.0 mm - 1.6 mm (4% - 6% of incidence spot size)	Reevaluate every 300-500 hours of use
1.6 Pointing accuracy - detector	Detector spot deviates from the target point by 4.5% of the detector spot size diameter	Reevaluate every 300-500 hours of use
2.3 Sample tray repeatability	Average repeatability of 0.8 mm and a maximum variability of 1.8 mm	Reevaluate every ~100 hours to assess for further motor degradation

Table S1. Summary of TANAGER requirements that were reevaluated after ~300 hours of instrument use, with recommendations for how often they should be revisited in long-term operations. Details of requirements are given in Table 1.