AN INTERLABORATORY UV/VIS/NIR WAVELENGTH CALIBRATION STUDY.

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Introduction: Analytical Spectral Devices (ASD) spectrometers are becoming increasingly common and used within the Earth and planetary sciences community both in the laboratory as well as in the field. They generally cover the wavelength range of 350 to 2500 nm by utilizing a silicon array detector (350-1000 nm) and two Peltier cooled graded index InGaAs photodiodes (SWIR1: 1000-1830 nm, SWIR2: 1830-2500 nm). The spectral resolutions of the instruments have varied over the years and between different models from 2-3 nm at 700 nm and 7-12 nm at 2100 nm [1]. One advantage of the ASD spectrometer is that even with the resolutions ranging from 2-12 nm, the spectral sampling interval, defined as the spectral distance between the centers of adjacent spectral channels sampled along a spectrum [2] is independent of resolution and ranges between 2 and 5 samples per full-width-half-maximum. This has remained the same across the different models, being 1.4 nm in the 350-1000 nm range and 2.0 nm in the 1000-2500 nm range. Spectra are ultimately output at 1 nm spacing via internal interpolation by the instrument. [1] The goal of this project is to assess the performance of different ASD spectrometers in terms of wavelength calibration, and effects of varying spectral resolution, and band passes, using a common set of calibration standards. We currently have a set of wavelength calibration diffuse reflectance standards circulating among seven facilities being investigated with nine ASD Fieldspec spectrometers of various ages and models (Fig.1).

Spectrometer	Unit #	Resolution (nm)		
Fieldspec Pro HR	6462	2 @ 700	7 @ 1400	7 @ 2100
Fieldspec 3	16452	3 @ 700	10 @ 1400	10 @ 2100
Fieldspec 3	16426	3 @ 700	10 @ 1400	10 @ 2100
Fieldspec Pro	6516	3 @ 700	10 @ 1400	10 @ 2100
Fieldspec Pro	6398	3 @ 700	10 @ 1400	10 @ 2100

Fig 1: List of spectrometers utilized to date with spectral resolutions of each spectrometer separated by each detector. Measurements will be made with an additional four spectrometers.

The wavelength calibration standards are from Labsphere and consist of three rare earth oxide doped Spectralon® pucks (99.99% pure) covering the UV/VIS/NIR region of the spectrum. Each standard exhibits well-defined absorption bands at specific wavelengths. The calibration is traceable to National Institute of Standards and Technology (NIST) where the data were collected with an integrating sphere setup up as an 8° hemispherical reflectance accessory. Holmium oxide (WCS-HO-010) is used for the UV/VIS/NIR regions, erbium oxide (WCS-EO-010) for the VIS/NIR regions and dysprosium oxide (WCS DO-010) covers the NIR region. Here we discuss only the results for the holmium oxide as it has bands in all three detector ranges

Methodology: The diffuse reflectance spectra were collected by each participant using the light source, setup and procedures they most commonly employ. The only request was that the viewing geometry of the setup had i=30° and e=0° and the spectra were acquired relative to the same Spectralon® 99% reflectance standard (SRS-99-010).

Results: To date, we have received data from five ASD spectrometers, and the results are as follows:

VNIR (350 - 1000 nm) Band centers for this region have a ± 1 nm variance [3]. The largest observed variation in band position is a 5 nm difference at wavelengths less than 500 nm. These differences decrease to 3 nm between 500-600 nm to 2 nm within the 600-1000 nm range.

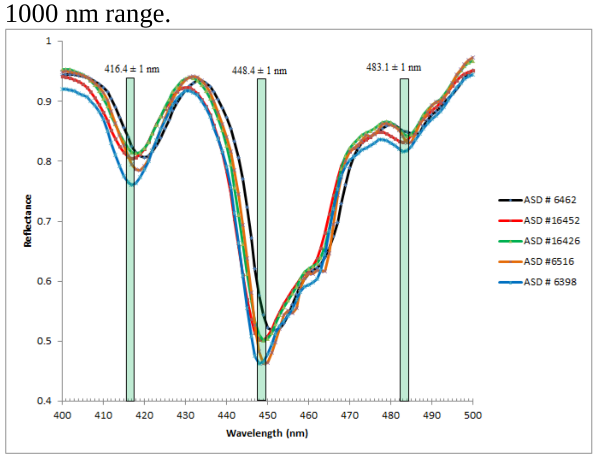

Fig 2: Reflectance spectra of holmium oxide between 400 and 500 nm. Shaded bars represent expected band minima with allotted variance of ±1 nm.

SWIR1 (1000 - 1830 nm) The SWIR1 detector was found to have less scatter than the VNIR, as the band centers fell within the allotted ± 2 nm zones [3]. For the lower resolution instruments, the band positions tend to be accurate but the overall band shapes are less well defined.

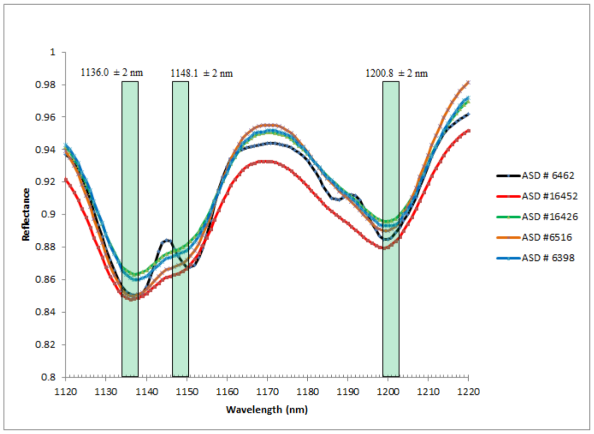

Fig 3: Reflectance spectra of holmium oxide between 1120 and 1220 nm. Shaded bars represent expected band minima with allotted variance of ± 2 nm.

SWIR2 (1830 - 2500 nm) The SWIR2 detector was accurate for the higher resolution instrument as the absorption band centers fell within the given range of ± 2 nm. The lower resolution spectrometers however, did not resolve the multiple absorption features present in this wavelength region. Many of the narrow bands became amalgamated into one larger feature that was offset slightly (Fig. 4).

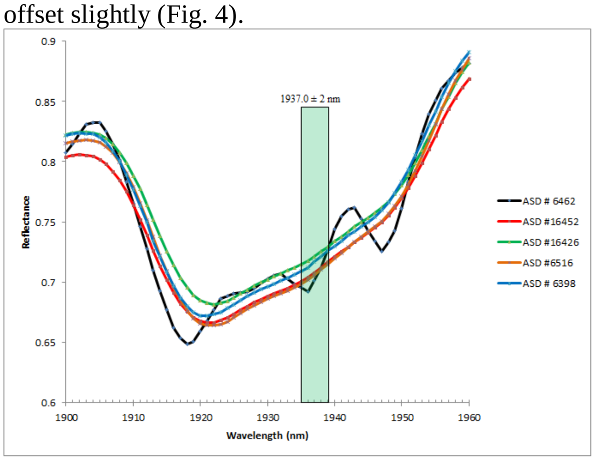

Fig 4: Reflectance spectra of holmium oxide between 1900 and 1960 nm. Shaded bar represents expected band minima with allotted variance of ± 2 nm.

Discussion: Variations exhibited by the VNIR detectors can be attributed mostly to unit #6462 falling outside the high end of the acceptable range. All band centers below 600 nm for this instrument are higher than expected values.

The two thermoelectrically cooled InGaAs detectors appear to be the most accurate with the least variation between the different ASD instruments. This however could just be a result of them having a broader spectral resolution so that if there were any offsets of a few nm between different spectrometers, the differences get averaged across the 7-10 nm bandpass. One consequence of having lower spectral resolution is that many of the absorption bands change their apparent shape or position or are diminished altogether for the four spectrometers that have a broader 10 nm resolution (Fig. 4).

Temperature of the wavelength standards can also play a role in band position but [4] examined these effects and found there to be only 0.3 nm difference between 20°C and 30°C, which is well within the 2 nm allotted variance. [4] also looked at the influence of instrument sensitivity. They compared a Varian-Cary 2390 spectrophotometer against the reference spectrometer [4] at the National Bureau of Standards (now NIST) using a spectral band width of 5 nm and found there to be an uncertainty of approximately 1 nm.

Future Work: Measurements with four other ASD spectrophotometers are ongoing as well as at Reflectance Experiment Laboratory (RELAB). These results will be grouped and analyzed in the same manner as the others. Another aspect that needs to be assessed is the variability across the surface of a single standard. We will collect multiple spectra at different points on the standard to see if there are any uncertainties. Assessing multiple Labsphere wavelength standards of the same type will also be worthwhile.

Conclusion: This study was initiated after noticing a possible small drift in the visible region of unit #6462. This work has proven useful to understand the effects of variations in spectral resolution, sampling intervals, and accuracy and reliability of reflectance standards.

References: [1] Hatchel D. C. (1999) *Analytical Spectral Devices, Inc. (ASD) Technical Guide*. [2] Swayze G. A. et al. (2003) *JGR*, 108, NO. E9, 5105. [3] *Spectralon® wavelength calibration standards data sheet*, Labsphere.com. [4] Weidner V. R. et al. (1986) *J. Res. Nat. Bur. Stand.* , 91, 243-253. [5] Venable W. H. et al. (1976) *Nat. Bur. Stand. Tech. Note* 594-11, 1-41.

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