Interlaboratory Comparison Study of Visible and Near-Infrared Reflectance Spectra Using a Set of Common Standard Materials

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Introduction: Visible and near-infrared (VNIR) reflectance spectroscopy has been a useful technique in obtaining compositional information of rocky surfaces of airless planetary bodies. Therefore, many laboratory studies employed VNIR spectrometers to accumulate spectral data of common geologic minerals and the like. However, consistency or accuracies of their wavelength and reflectance values have not been often checked among different laboratories. This study is one of such efforts [1] employing four different instruments located in three different laboratories.

Experimental: The standard materials used for this study were Spectralon (SRS-99-010) and a wavelength calibration standard (CSTM-WCS-MC) purchased from Labsphere. Bidirectional diffuse reflectance (BDR) spectra of the latter relative to the former were measured by four different spectrometers: Reflectance Experiment Laboratory (RELAB) [2, 3] BDR spectrometer, Bunko-Keiki spectrometer at Osaka University, Bruker Vertex 70v at Tohoku University, and ASD Fieldspec 3 at RELAB.

The average incidence and emergence angles were set to 30 and 0 degrees, and the incidence beam footprint sizes were 3±1 mm. The incidence and emergence cone angles are estimated as: 8 and 4 degrees for RELAB BDR, 13 degrees each for Bunko-Keiki, 12.5 and 25 degrees for Bruker, and 25 degrees each for ASD. The sample was spun for RELAB BDR and ASD measurements to average out possible heterogeneity around the azimuth axis.

The wavelength range was 350-2050 nm, and the sampling interval was 1 nm except for Bruker which sampled data at an interval that is half the wavelength resolution. The nominal wavelength resolutions were 2-8 nm for RELAB BDR, 5 nm for Bunko-Keiki, 0.25-3.2 nm (16-8 cm^{-1}) for Bruker, and 3-10 nm for ASD. When neighboring segments of each spectrum differ in reflectance, the side that is known to be more trustable was adopted and the other side was scaled and spliced to the former. In general, there were discrepancies of up to 5 % in reflectance.

Wavelength Resolutions and Positions: Before comparing wavelength positions, resolution differences have to be examined and taken into account. As shown in Fig. 3, Bunko-Keiki and ASD spectra are best matched with RELAB BDR spectrum that is moving-averaged over 7 data points. Assuming that RELAB BDR spectrometer truly has a 2 nm resolution, this result suggests Bunko-Keiki and ASD spectrometers have a resolution of about 8 nm.

However, the ASD resolution decreased toward the shorter wavelengths and increased toward the longer wavelengths. An alternative explanation is that RELAB BDR and Bunko-Keiki spectrometers have variable wavelength resolutions over the visible range, that increase toward shorter wavelengths and decrease toward longer wavelengths.

Lastly, RELAB BDR spectrum is best matched with Bruker spectrum that is moving-averaged over 9 data points. Because Bruker sampled at double the frequency of the wavelength resolution, this result suggests that at 500 nm (20,000 cm^{-1}), the RELAB BDR wavelength resolution is estimated to be

$$(16\ cm^{-1} \times 5) / 20000\ cm^{-1} \times 500\ nm = 2\ nm$$

which is consistent with the wavelength resolution of RELAB BDR spectrometer.

Because the wavelength resolution of Bruker is constant at 16 cm^{-1} over this visible range in the wavenumber scale but is variable in the wavelength scale, the excellent match in Fig. 3 suggests that RELAB BDR also has a variable wavelength resolution centering on 2 nm around 500 nm in wavelength, increasing toward shorter wavelengths and decreasing toward longer wavelengths. This is consistent with the above results.

After taking care of these wavelength resolution differences, wavelength positions appear to be very consistent among the spectrometers, except RELAB ASD spectrometer showing up to 1 nm deviation from RELAB BDR spectrometer (Fig. 4) which is naturally expected as a portable spectrometer.

Results: Shown in Fig. 1 are the entire spectra of WCS relative to Spectralon by four different instruments. In general, all the four instruments produced highly consistent reflectance spectra of the common standard pair of materials. There are up to 6 % reflectance scatters, and the RELAB BDR spectrum seems to represent the central value of all. Bunko-Keiki spectrum is very close to RELAB BDR one over the entire wavelength range, and Bruker and ASD spectra seem to have slightly bluer continua than RELAB BDR and Bunko-Keiki continua. Another notable difference is their wavelength resolution variation as depicted in Fig. 2 over the visible range. This issue will be investigated using simple moving average operations below.

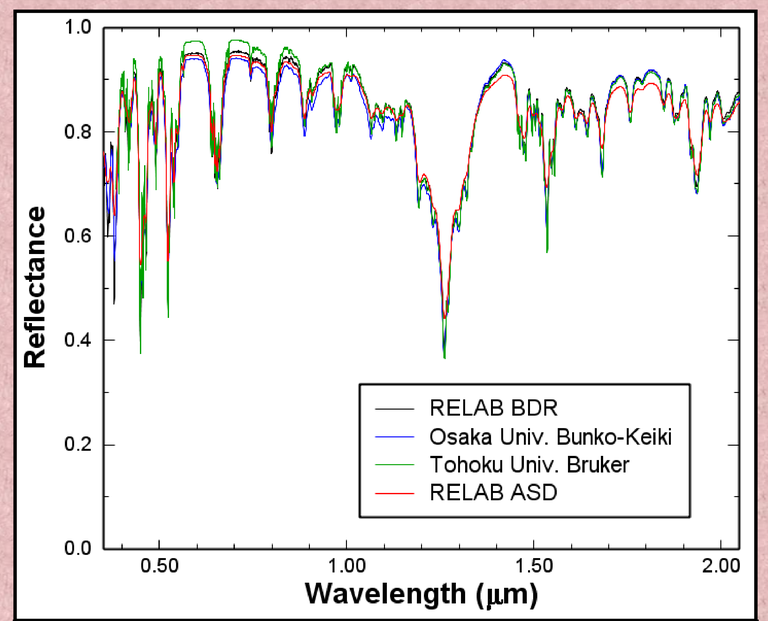

Fig. 1. Reflectance spectra of CSTM-WCS-MC relative to Spectralon measured by four different instruments.

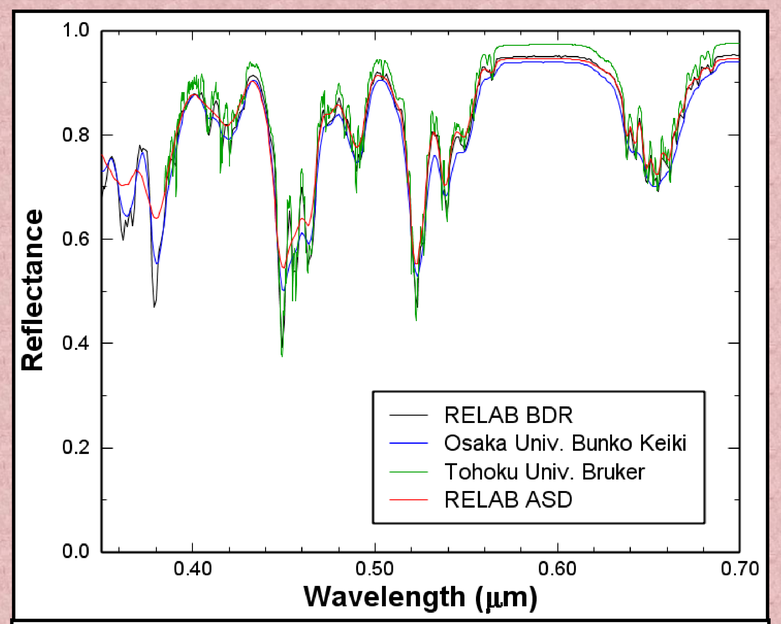

Fig. 2. An enlarged view of the visible range of the spectra in Fig. 1, depicting the wavelength resolution variation.

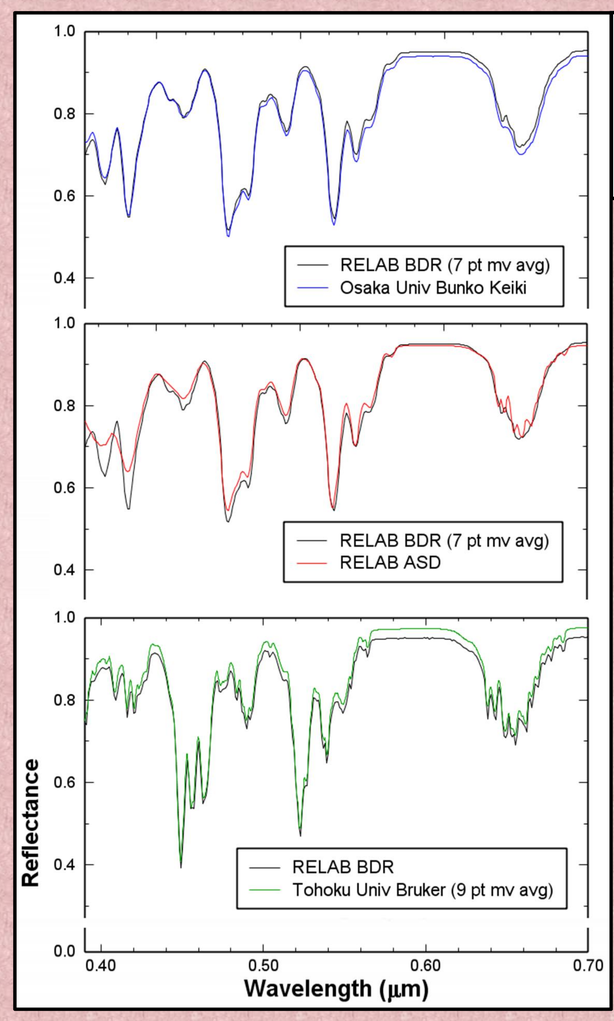

Fig. 3. Comparison of RELAB BDR, Osaka Univ. Bunko-Keiki, and Tohoku Univ. Bruker visible spectra after adjusting their wavelength resolutions.

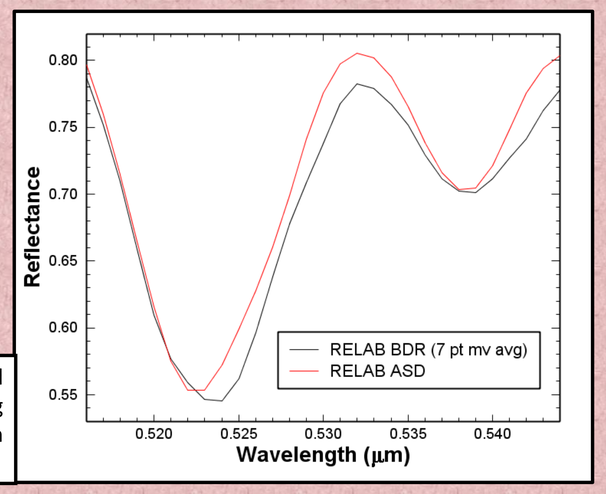

Fig. 4. RELAB BDR and ASD spectra, showing up to 1 nm deviation in wavelength.

Summary: As a result of measuring the relative VNIR spectra of a pair of standard materials by four different spectrometers, a high level consistency in both reflectance and wavelength position has been obtained. With careful handling and configuration of the samples and optics, these instruments should be able to reproduce mutually consistent VNIR reflectance spectra, except for their wavelength resolution differences and small wavelength shifts with ASD spectrometer.

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References: [1] Mann P. (2014) *LPS XLV*, Abstract #2392. [2] Pieters C. M. and Hiroi T. (2004) *LPS XXXV*, Abstract #1720. [3] RELAB home page: http://www.planetary.brown.edu/relab/.