

**INTRODUCTION TO THE PDS GEOSCIENCES NODE SPECTRAL LIBRARY WEBSITE.** D. Scholes<sup>1</sup>, E. A. Guinness<sup>2</sup>, S. Slavney<sup>3</sup>, and R. E. Arvidson<sup>4</sup>, McDonnell Center for the Space Sciences, Department of Earth and Planetary Sciences, Washington University in St. Louis, 1 Brookings Drive, Campus Box 1169, St. Louis, Missouri, 63130, <sup>1</sup>[scholes@wunder.wustl.edu](mailto:scholes@wunder.wustl.edu); <sup>2</sup>[guinness@wunder.wustl.edu](mailto:guinness@wunder.wustl.edu); <sup>3</sup>[slavney@wunder.wustl.edu](mailto:slavney@wunder.wustl.edu); <sup>4</sup>[arvidson@wunder.wustl.edu](mailto:arvidson@wunder.wustl.edu).

**Introduction:** The PDS Geosciences Node Spectral Library website (Spectral Library, <https://pds-speclib.rsl.wustl.edu>) is a web-based interface that provides search, review, and download options for spectral data that has been archived by the PDS. The website's catalog (database) currently contains the Reflectance Experiment LABORatory (RELAB) [1] data set that was released as a PDS4 data collection in April 2020. The website currently contains 17,896 spectral measurements of 10,272 geologic samples (specimens).

**Planning and Development:** The design and planning of the website were developed with close collaboration between RELAB and the PDS Geosciences Node. Funding was provided through the NASA PDART program. The PDART PI was Ralph Milliken, the Manager of RELAB, Brown University.

*RELAB data set.* The first step of the project was to design the organization, format, and necessary metadata for archiving the RELAB data set in the PDS using the PDS4 data standard [2]. PDS4 uses a standardized XML format for observation metadata (PDS label), stricter data format standards, and data dictionaries for uniform lookup values. The PDS4 format provides consistent structure and values for data users and better supports software development and machine learning.

*Website design.* Several iterations of review and discussion between RELAB and the PDS Geosciences Node shaped the Spectral Library interface design. An emphasis was placed on usability and providing useful context for the measurements to help users efficiently locate and download relevant measurements (PDS products). A framework that could expand to catalog other data collections was an additional priority.

*External review.* As part of a PDS data release, a peer review was conducted on the RELAB PDS4 data collection and the Spectral Library, prior to public release. The peer review provided helpful recommendations for website enhancements, as well as additional clarification in the RELAB PDS4 archive.

*Public release and first update.* The RELAB PDS4 data collection [3] (<https://pds-geosciences.wustl.edu/speclib/urn-nasa-pds-relab/>) and the Spectral Library were released to the public in April 2020. Both are hosted by the PDS Geosciences Node. An update was made to the PDS archive in

October 2020 as additional specimen measurements, specimen chemical analyses, and specimen images became available. The Spectral library was updated to reflect the additional measurement data and ancillary files. The Spectral Library was also enhanced with additional search filters, including a chemistry element search.

**Website Features:** The Spectral Library has been designed to provide a highly interactive interface for filtering results, viewing measurement metadata and supporting ancillary files, plotting measurement data, and downloading selected measurement files. The system is designed around the concept that each specimen may have one or more measurements. A measurement typically corresponds with one PDS product, although multiple measurements may be included in one PDS product based on the archived data. Key interface features are listed, as follows.

*Faceted Search.* From the search page, the faceted search filters allow users to rapidly narrow the search criteria with immediate feedback from updated filter counts and an updated results list. Highlights include a keyword search, chemistry element search, and specimen type, in addition to measurement type, measurement range, and other typical geology filters. Figure 1 shows an example of the faceted search set for terrestrial samples containing Olivine.

*Search Results List.* The faceted search interactively updates the search result list, which is displayed on the same screen. The search result list is organized by displaying matching specimens, with each having an expandable list of corresponding measurements. Measurements have links that can be clicked to open a new browser tab for viewing measurement details. The results list page displays a summary of the currently filtered count of matching specimens and measurements, along with the applied filters. All search results can be added to the user cart or individual measurements can be added. Icons indicate measurements that have associated chemical analysis files and photographs available through the website.

*Quick View.* The right side of the Spectral Library search interface contains a quick view window for comparing multiple plots from the search results list. The measurements must be of the same type, such as reflectance or absorption. The plotting options allow a

user to filter the x and y ranges, as well as download an image of the plot.

**Detail page.** The measurement detail pages correspond with PDS products. The top section of the detail page contains metadata about the specimen, such as its description, owner, material classification, and links to any chemical analyses that are available. Specimen images are displayed when they are available. Measurement details are provided, along with direct links to the measurement label and data file. Any ancillary files may be downloaded directly, or the entire set of measurement and supporting files can be added to the user cart. The measurement is plotted for display, with options for cropping the plot's x and y axis. Any tagged references and DOIs are also displayed on the page. Figure 2 shows an example Spectral Library measurement detail page.

**Cart download option.** All data that is archived in the PDS is freely available to the public. The Spectral Library has a user cart feature to support convenient bulk downloads of selected data. Measurements can be added to the cart from the search results list or the measurement detail pages. The cart checkout page allows the user to review the cart selections, and select the desired packaging format of zip, tar, or tar.gz for the requested files. After submitting the cart request, a service at the PDS Geosciences Node will package the files of the user request into the desired packaging format and email the user an HTTPS link for direct file download.

**Future work:** The PDS Geosciences Node plans to continue to expand and improve the Spectral Library.

**Additional data sets.** We are in the process of developing website updates to integrate two additional PDART data sets into the website. They will require additional search parameters and additional metadata displays, which will further expand the functionality of the Spectral Library. One data collection includes x-ray absorption spectroscopy measurements, while the other includes RAMAN spectra of brines. We anticipate the addition of future data collections along with periodic additions from RELAB.

**Web API.** The PDS is currently developing a standard REST API format. Once the format is in a mature state, a REST API will be created for the Spectral Library. This functionality will improve the ability for data discovery and the use of scripts and other software to access the cataloged data collections.

**Contact Information:** As always, the PDS Geosciences Node appreciates user feedback and suggestions, which may drive additional interface updates. To share feedback or ask questions, please send email to [speclib@wunder.wustl.edu](mailto:speclib@wunder.wustl.edu).

**Acknowledgments:** The Spectral Library was developed in collaboration with RELAB, and funding was provided from the NASA PDRART program. Continued support has been provided through funding provided to the PDS Geosciences Node from NASA. We would like to thank the peer reviewers who provided valuable feedback that helped drive some of the features of the website.

**References:** [1] R.E. Milliken et al (2016), LPS 47th, Abstract #2058. [2] PDS4 Information, <https://pds.nasa.gov/pds4/about/>. [3] Milliken, R. (2020) Spectral Library Bundle of reflectance spectra and ancillary data acquired by RELAB at Brown University [Data set]. PDS Geosciences Node. <https://doi.org/10.17189/1519032>

**Search Filters** [?] [Reset All](#)

▼ **Spectral Database**

RELAB [\[i\]](#) 852

**Note:** Purity or composition of samples sent by users to the NASA RELAB facility are not independently verified by the RELAB spectroscopy facility.

▼ **Keyword Search**

[x]

Case sensitive  Include Specimen ID in search  
Searches specimen name, measurement id, description, and material common name

**Optional Secondary Keyword**

And  Or

Case sensitive  Include Specimen ID  
Searches specimen name, measurement id, description, and material common name

► **Chemical Composition**

▼ **Specimen Type**

Lunar Meteorite 0

Mars Meteorite 15

Other Meteorite 70

Returned Lunar Sample 13

Synthetic Sample 152

Terrestrial Sample 469

Figure 1: The faceted search form filtering RELAB terrestrial samples that contain olivine.

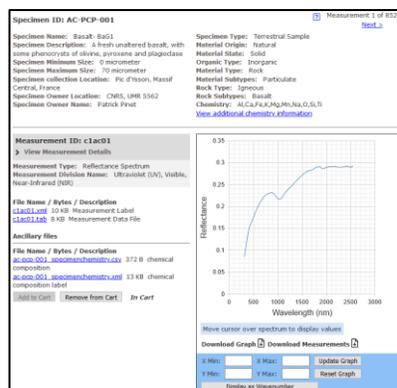


Figure 2: An example measurement detail page displaying specimen and measurement data, along with direct file download links and measurement plot.