REFLECTANCE EXPERIMENT LABORATORY (RELAB) DESCRIPTION AND USER'S MANUAL

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1 Overview

Spectroscopic data acquired in the laboratory provide the interpretive foundation upon which compositional information about unexplored or unsampled planetary surfaces is derived from remotely obtained reflectance spectra. The Brown University Reflectance Experiment Laboratory (RELAB) is supported by NASA as a multi-user spectroscopy facility, and laboratory time can be made available at no charge to investigators who are funded through NASA programs.

RELAB has two operational spectrometers available to users:

- A near-ultraviolet, visible, and near-infrared bidirectional spectrometer
- A Thermo-Nexus 870 near- and mid- infrared FT-IR spectrometer.

The overall purpose of the design and operation of the bidirectional spectrometer is to obtain high precision, high spectral resolution, bidirectional reflectance spectra of earth and planetary materials. One of the key elements of its design is the ability to measure samples (hereafter referred to as **specimens**) using viewing geometries specified by the user. This allows investigators to simulate, under laboratory conditions, reflectance spectra obtained remotely (i.e., with spaceborne, telescopic, and airborne systems) as well as to investigate geometry dependent reflectance properties of geologic materials.

The Thermo Nexus 870 FT-IR spectrometer is commonly operated in reflectance mode from 0.9 to 100 μ m but can also be used for transmission measurements. An FTIR microscope (Thermo Contin μ um) is also attached to the bench FTIR and can be used in reflectance or transmission mode to measure spots as small as 50 μ m on appropriate specimens.

Use and scheduling of the RELAB is monitored by an advisory committee. NASA investigators should direct inquiries to the Science Manager or RELAB Operator.

2 Contact Information

RELAB Web Site:

http://www.planetary.brown.edu/relab/

Relab Address:

MacMillan Hall

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Providence, Rhode Island 02912

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3 Instrument Specifications

3.1 UV-VIS-NIR BIDIRECTIONAL SPECTROMETER

Operating Spectral Range: Nominal (0.32 to 2.55 μ m); Possible (0.3 to 2.6 μ m)

| Mode | Range (μm) | Resolution (nm) | Grating | Detector | Light source |
|------|------------|-----------------|---------|-----------------|--------------|
| Α | 0.30-0.42 | < 1.7 | 1200 | Photomultiplier | Xenon |
| В | 0.40-0.85 | < 1.7 | 1200 | Photomultiplier | Halogen |
| С | 0.60-1.80 | < 3.4 | 600 | InSb | Halogen |
| D | 1.70-2.60 | < 6.8 | 300 | InSb | Halogen |

Sampling Interval: 5 or 10 nm standard, 1 nm minimum.

Precision: Instrumental error is less than 1/4 % in reflectance.

Geometry: Bidirectional reflectance; Spectral goniometry.

Incident and reflected beam can each be varied from normal to 70°.

(-10 < i < 70; -70 < e < 70).

Phase angle minimum 12°, maximum 140°.

Specimen: Particulate specimen or soil (reflectance):

Measured horizontal and uncovered (normally rotated slowly).

Optimal sample amount is 500 mg.

Specimen should be no smaller than 20 mg.

Specimen should be no larger than 10 g.

Chip or rock (reflectance):

Measured horizontal and uncovered on a height-adjustable stage.

Smallest reliable spot size is ~1.5 mm.

Maximum Specimen diameter is 10 cm (2.5 cm if it is to be spun).

Thin section (reflectance or transmittance):

Measured horizontal on halon (reflectance) or on an aperture (transmittance).

Regions to be measured should be no smaller than 1.5 mm.

Surface should be polished and clean (no carbon coating).

Reference Standard: Halon (pressed) or Spectralon (by Labsphere).

Corrections based on the NBS calibration and relative measurement to diffuse gold (at

longer than 2 µm in wavelength) are applied automatically.

Light Source: Quartz halogen or Xenon lamp. Oriel monochromator.

Optics: Order sorting filters, front surface mirrors, depolarizer, apertures.

Typical Run Time: Measurements over a spectral range of 0.32 to 2.55 μm at 5 nm sampling interval take

~2 hours per specimen.

3.2 Thermo Nexus 870 FT-IR SPECTROMETER

Operating Spectral Range: Nominal (1.0 to 50 μm) Possible (0.8 to 200 μm)

| Mode | Range (μ m) | Light Source | Beam Splitter | Detector |
|-----------|------------------|--------------|-----------------|-----------------|
| Α | 1.0-4.7 | Quartz | Si-on-CaF2 | TE cooled DTGS |
| A* | 0.9–4.5 | Quartz | Si-on-CaF2 | LN2 cooled InSb |
| В | 1.3 - 28 | Glowbar | Ge-on-KBr | TE cooled DTGS |
| С | 14.3-200 | Glowbar | Solid substrate | DTGS |

Resolution: 16, 8, 4, 2, 1 or 0.5 cm⁻¹

Default: 4 cm⁻¹

Geometry: Diffuse reflectance: Biconical, off-axis for Pike specimen holder

Transmission: normal incidence (collimated)

Sample: Particulate specimen or soil (reflectance):

Measured horizontal and uncovered in purged (H₂O, CO₂ free) environment.

Desired specimens amount is 50 - 500 mg.

Specimen should be no smaller than 20 mg.

More than 1 g is unnecessary.

Multiple specimens can be measured in sequence (same environment)

Chip (reflectance):

Measured horizontal and uncovered.

Regions to be measured should be no smaller than 1 mm.

Maximum size is 1 cm in height and 3 cm in diameter.

Thin section and single crystal (transmission):

Measured vertical, attached to an appropriate aperture board.

Regions to be measured should be no smaller than 1.5 mm.

Surface should be polished and clean (no carbon coating).

Reference Standard: Brushed diffuse gold (reflectance)

Blank (transmittance)

Additional Attachments: Pike AutoDiff Diffuse Reflectance Autosampler

Continuum Microscope system

Transmission mode currently operational

Reflectance mode (with 2-D capabilities) being tested.

Software: OMNIC, Atlµs [new]

4 General Operations

Use of the RELAB should be initially arranged through the Science Manager. New Investigators must fill out the attached *User Registration Form*. All investigators should provide information for each specimen to be measured using the attached *Specimen Information Form* and *Compositional Analysis Form* if chemical or mineral composition is available. A completed *Measurement Request From* must be provided for each set of specimens to be measured under a common measurement condition. This information is very important in order to maintain a useful and up-to-date data base of spectroscopic data.

4.1 Bidirectional Spectrometer:

Powders, chips, or slabs can be measured using the RELAB bidirectional spectrometer. Although specimen dishes come in various sizes, the smallest specimen that can be accurately handled is about 20 mg, while the optimum specimen size is about 500 mg. In all cases it is desirable for the specimens to be optically thick over the wavelength region of interest for reflectance measurements.

The standard specimen dish for the bidirectional spectrometer is aluminum coated with black teflon. Its reflectance is less than 3% throughout the entire spectral range of the bidirectional spectrometer.

For analysis of heterogeneous specimens, viewing optics include precision apertures for measurements from broad specimen areas up to 1 cm in diameter down to areas as small as 1 mm in diameter.

To initiate a data run the USER must supply and specify the following run parameters: (a) specimen name and properties; (b) angle of incidence (light source) and angle of emission (reflectance); (c) wavelength range (start and stop); and (d) sampling interval. Nominal settings are provided.

Based on these run parameters specified by the user, the RELAB Operator configures the system and performs all the data acquisition. A complete spectrum from 350 to 2550 nm at 5 nm sampling interval requires about 2 hours of laboratory run time per specimen, depending on specimen characteristics.

At the end of a run, values for the specimen signal, the standard signal, the offset, the ratio of specimen/halon (after offset subtraction), and the standard deviation of signal variance during integration on the specimen are recorded on disk in a file with all run parameters and text. These data files, each identified by a unique measurement ID, become part of the database collection. NBS calibration of halon is a multiplicative correction to the ratio data, producing absolute reflectance values for the specimen.

4.2 FT-IR Spectrometer:

A Nicolet Nexus 870 FTIR spectrometer is operational for particulate specimens using a PIKE AutoDiff multi-sample attachment. Infrared [off-axis] biconical reflectance spectra are normally produced relative to a gold standard. Infrared spectra may be scaled to and merged with bidirectional reflectance spectra to produce continuous spectra from 0.3 to 26 μ m. The PIKE multi-sample biconical reflectance attachment is normally requested by outside users as the standard mode for mid-IR data. Use of the Nicolet Continuµm microscope is available as well, but use of this instrument requires training and/or piror experience. Contact the RELAB science manager or operator for information on the use of the Continuµm FTIR microscope.

5 RELAB Data in the NASA Planetary Data System

Spectra acquired at RELAB are archived in the NASA Planetary Data System (PDS, <u>pds.nasa.gov</u>). The data are incorporated into the PDS Geosciences Node Spectral Library (<u>pds-geosciences.wustl.edu/spectrallibrary</u>). They are registered with the PDS using the PDS Bundle Logical Identifier **urn:nasa:pds:relab**, and they may be searched, displayed, and downloaded using the PDS Geosciences Node Spectral Library web interface (<u>pds-speclib.rsl.wustl.edu/</u>).

In the PDS archive each RELAB measurement has a unique Logical Identifier and a PDS label that records the metadata about the measurement, the instrumentation, and the sample measured. The label is expressed in XML (eXtended Markup Language) so that it is both human- and software-readable. The metadata parameters in the label are governed by the PDS Core Data Dictionary and the PDS Spectral Library Data Dictionary. The definitions and structure of the Spectral Library dictionary are summarized in Appendix A, with notes about their specific application to RELAB data. This appendix includes an example of the XML metadata.

More information about PDS archives may be found at pds.nasa.gov/datastandards/documents/.

6 User Instructions

- 1) After the initial contact with the RELAB Science Manager to arrange use of the facility, users should contact the RELAB Operator directly to schedule specimens to be measured. Investigators should carefully select the most appropriate specimen preparation and RELAB configuration for their specific science requirements. If a user is uncertain of measurement strategy, he or she should contact the RELAB Operator or Science Manager for advice or suggestions. [During periods of heavy use of the facility, requests for extensive numbers of spectra may be given lower priority in the measurement queue, therefore it is important to prioritize measurements in any large request.]
- 2) Investigators (and/or their students) should fill out the attached User Registration Form with up-to-date information. Specimen IDs assigned at the RELAB use the investigators' three initials. If you have published work using RELAB spectra, please also include a publication list. These will be included in a public spectroscopy bibliography on the RELAB website. (It is unnecessary to send references already included.)
- 3) For each set of specimens to be measured under common conditions (same geometry, wavelength range, sample interval, etc), the investigator is requested to fill out the attached Measurement Request Form. It includes information to specify the type of measurement to be made in the RELAB.
 - a) Applicable Specimens: Identify all the submitted specimen names which are to be measured under a common measuring condition described in the form, or write "All".
 - b) Research Type: For accounting purposes, circle at least one category that accounts for support of this research, and <u>please include NASA award number when applicable</u>. The research type should reflect the NASA involvement of the PI/CoI or Sponsor.
 - c) Wavelength Range and Sampling Interval or Resolution: Choose one of standard values or specify.
 - d) Geometry: Incidence and emergence angles are measured from the vertical direction in positive and negative values of degrees (negative values are on the opposite site). For example, a geometry with source light at 30° inclination and detector at 20° inclination from the vertical direction would be (30, -

- 20) which makes 50° phase angle. Phase angle must be 12° or larger for the Bidirectional Spectrometer and all measurements are currently made in the plane of scattering. Geometry for the FTIR Spectrometer is fixed, with broad conical incidence and reflectance at (30, -30), but out of the plane of scattering.
- e) Date Desired: Indicate the date spectral data need to be completed.
- f) Public Release Date: Specify when spectroscopic data on this specimen can be included in a public data base available to other investigators in digital form. Maximum period is three years. Default is immediate release.
- g) Data Transfer Preference: All files and data will be sent to the user electronically (e.g., e-mail).
- 4) For *each specimen* the investigator must fill out the attached **Specimen Information Form**. The information requested includes:
 - a) Specimen Name & Description: Formal name or the investigator's name for the specimen (can be used in a database search) as well as a brief description of the sample
 - b) Specimen Collection Location: The geographical site from which the specimen was obtained or 'synthetic' if it is not a natural material. If it is extraterrestrial, provide appropriate information Meteorite fall/find location, Apollo lunar site, etc.
 - c) Owner Name & Location: Owner and location where the specimen is likely to be (semi)permanently stored.
 - d) Organic Type: Primarily inorganic, organic, or mixture (e.g., tar sands would be a mixture)
 - e) Origin: Is the specimen natural, synthetic, both, or is it a synthetic sample derived or constructed from naturally occurring materials (e.g., a human made mixture of different natural minerals)?
 - f) Texture: Powder, slab, coarse-grained sand, fine-grained soil, thin section, etc.
 - g) Minimum and Maximum Particle Size: For particulate specimens, the maximum and minimum (if known) particle sizes in micrometers.
 - h) Material Type and Names of Minerals, Rocks if applicable: Please mark the appropriate category and include names of minerals or rock types (sedimentary, igneous, metamorphic) when applicable.
- 5) Whenever available, modal mineralogy for the specimen and/or chemical analysis for either the bulk specimen or for individual mineral constituents should be provided on the **Compositional Analysis Form**. This important information will be stored in a separate file linked to the specimen. If such data are not currently available but are expected to be available in the future then please indicate this.
- 6) Specimens should be sent to the RELAB Operator with completed forms and any other necessary instructions. Although not necessary, any NASA investigator is welcome to visit the RELAB at Brown University to prepare their specimens for measurement in person and to use available data analysis tools. This should be prearranged to prevent schedule conflicts. A small office is available for visitors.
- 7) Data products are sent to the investigator (digital copy). Special requirements should be discussed with the RELAB Operator.

8) RELAB forms are downloadable in PDF form from our web site along with Microsoft Word files. Contact the

7 User Registration Form

NASA-funded projects have access to RELAB at no charge to User.

Each group of measurements must be accompanied by Measurement Request Forms.

| Principal Contact: | | Date _ | | | |
|--------------------|----------------|----------------|------|--|--|
| Full Name: | | | | | |
| | First | Middle Initial | Last | | |
| Affiliation: | | | | | |
| Mailing Address: | | | | | |
| | | | | | |
| E-Mail Address: | | | | | |
| Phone: | | Fax: | | | |
| Secondary (or Stud | lent) Contact: | | | | |
| Full Name: | | | | | |
| | First | Middle Initial | Last | | |
| Affiliation: | | | | | |
| Mailing Address: | | | | | |

| E-Mail Address: | |
|------------------|----------|
| | |
| Phone: | Fax: |
| | |
| | |
| | |
| | |
| * For RELAB use: | |
| | |
| PI Code: | SI Code: |

7.1 Specimen Information Form (One for each specimen) Investigator: _____ Specimen Name & Description: _____ Specimen Collection Location: Owner Name & Location: Organic Type (mark one): Inorganic ____ Organic ____ Mixture ____ Origin (mark one): Natural Natural & Synthetic Entirely Synthetic Synthetic From Natural (e.g., mixture of natural mineral powders) Flight Hardware Texture (e.g. particulate, non-particulate, pressed powder, etc.): Particle Size: _____ μm (Minimum) (Maximum) Material Type (mark one): Mineral____ Rock___ Element___ Organic___ Amorphous___ Ice____ Unconsolidated Mixture___ Consolidated Mixture___ Single Particle____ Mineral Name(s) (if applicable): Rock Type(s) (if applicable):

Is compositional information available? () Yes () No () Not currently, but will be acquired

| (If yes, please also submit Compositional Analysis Form.) | | | | | | |
|---|-----------------------------|---------------|--|--|--|--|
| Priority Level: | (used in Measurement | Request Form) | | | | |
| * For RELAB use: | | | | | | |
| MM Analysis #: | | Bulk Chem. #: | | | | |
| ID: | | | | | | |
| PI: | SI: | PO: | | | | |

| Investigator: | | | | | | | |
|---------------------------------|-------------------|----------------------------------|--------------|----------------------------------|-----------|---------------------------------|------------|
| Specimen Name | :: | | | | | | |
| Text (identify fa | cility, method, a | and investigator p | erforming | analysis): | | | |
| | | | | | | | |
| Chemical Analys | sis (wt%): | | | | | | |
| SiO ₂ : | % | TiO ₂ : | % | Al ₂ O ₃ : | % | Cr₂O₃: | % |
| V ₂ O ₃ : | % | Fe ₂ O ₃ : | % | FeO: | % | CoO: | % |
| NiO: _ | % | MnO: | % | MgO: | % | ZnO: | % |
| CaO: | % | Na ₂ O: | % | K₂O: | % | P ₂ O ₅ : | % |
| : _ | % | : | % | : | % | : | % |
| Include minor o | r trace element | s information on | a separate : | sheet. | | | |
| Modal Minerald | ogy: | | | | | | |
| Mineral / Co | omponent | (wt/vol) % |) | Mineral / 0 | Component | | (wt/vol) % |

7.2 Compositional Analysis Form (One for each specimen if available)

| | _ | _ | | |
|----------------------------------|-------------------------|---------------|-----------------|---|
| | | | | |
| | | | | |
| | <u> </u> | | | - |
| | | | | |
| | | | | |
| | _ | | | |
| | | | | |
| If available, provide chemical a | analysis for individual | minerals on s | eparate sheets. | |
| | | | | |
| | | | | |
| | | | | |
| * For RELAB use: | | | | |
| | | | | |
| Specimen ID: | | | | |
| | | | | |
| | | _ | 5 A 1 ' ' '' | |
| M Mineral #: | <u> </u> | (| C Analysis #: | |

| specimens) | | | | | | | | |
|---|------------------------------|--|-------------|--|--|--|--|--|
| Investigator Name: | | | | | | | | |
| Applicable Specimens: | Applicable Specimens: | | | | | | | |
| | | | | | | | | |
| Research Type (circle at lea | | | | | | | | |
| | 1DAP PSTAR DDAP | - | proparation | | | | | |
| LARS CDAP NFDAP Active missions Mission planning Proposal preparation Other: | | | | | | | | |
| NASA PI/Col or Sponsor (if | different from Investigate | or) : | | | | | | |
| Bidirectional Spectrometer | r (* Standard parameters) | | | | | | | |
| Wavelength Range: | ()* 0.32-2.55 μm | () 0.3-2.6 μm | () Other | | | | | |
| Sampling Interval: | ()* 10 nm | () 5 nm | () Other | | | | | |
| Geometry (incidence, e | mergence angles): | ()* (30, 0) | () Other | | | | | |
| | | | | | | | | |
| FT-IR Spectrometer (* Stan | dard parameters) | | | | | | | |
| Wavelength Range: | () 1-4 μm ()* 2-2 | 25 μm () 17-50 μm | () Other | | | | | |
| Wavenumber Resolution | on: () 1 cm ⁻¹ (|) 2 cm ⁻¹ ()* 4 cm ⁻¹ | () Other | | | | | |
| | | | | | | | | |

7.3 Measurement Request Form (One for each group or subgroup of

Schedule (* Maximum and default)

| Date desired for the priority levels specified in the Specimen Information Forms | | | | | | |
|--|---------------|----------|------------|--------------|--|---|
| Priority Level: | | | | | | |
| Date Desired: | | | | | | _ |
| Public Release Date: | () Immediate | ()1 Year | () 2 Years | ()* 3 Years | | |

Appendix A—The PDS Spectral Library Data Dictionary User's Guide Definitions Annotated for RELAB

PDS Spectral Library Data Dictionary User's Guide

November 22, 2019

Susan Slavney, PDS Geosciences Node

1 Introduction

1.1 Purpose of this User's Guide

This guide describes the organization and contents of the Spectral Library Data Dictionary, one of several Discipline Dictionaries maintained by the Planetary Data System (PDS). This dictionary is used when creating PDS labels for laboratory spectral data. It contains terms that describe laboratory spectral measurements and the specimens measured.

1.2 Audience

This guide is intended for users and data providers of Spectral Library data products. In particular, users may wish to refer to Section 5, Definitions, to better understand the terms in the PDS labels of data products. Data providers may want to read the entire guide to understand how to create PDS labels for their spectral data.

1.3 Applicable Documents

PDS4 Concepts, https://pds.nasa.gov/datastandards/documents/concepts/, a high-level view of the PDS4 archiving standard

The Planetary Data System Standards Reference, https://pds.nasa.gov/datastandards/documents/sr/current/, the complete reference for the PDS4 Information Model

The PDS4 Data Dictionary, https://pds.nasa.gov/datastandards/documents/dd/current/, the PDS4 core (or "common") dictionary in an easily searchable HTML format

Data Providers' Handbook: Guide to Archiving Planetary Data Using the PDS4 Standard, https://pds.nasa.gov/datastandards/documents/dph/current/, a step-by-step guide for creating a PDS archive

The PDS4 Information Model Specification, https://pds.nasa.gov/datastandards/documents/im/current/, the same information as in the PDS4 core dictionary, in a formal specification for use by programmers and data engineers

2 Overview of the Spectral Library Data Dictionary

A spectral library is a collection of spectral measurements of laboratory samples, also known as specimens. Specimens may be rocks, minerals, ice, meteorites, etc. They may be in various physical forms. They may be naturally-occurring or synthetic. A given specimen may have many measurements. The measurements may

consist of reflectance spectra, Raman spectra, XRD, XRF, LIBS, and other types. In the PDS Spectral Library, each measurement's data is contained in a single file and is accompanied by a PDS4 label that describes the measurement and the specimen that was measured. Together the data file and PDS4 label are considered one data product.

The Spectral Library Data Dictionary is maintained by Susan Slavney at the PDS Geosciences Node. It may be revised when new spectra are submitted to the library. Questions about it may be addressed to geosci@wunder.wustl.edu.

3 How to Include the Spectral Library Dictionary in a PDS4 Label

PDS4 labels are written in XML (https://www.w3.org/XML/) and are governed by the PDS4 XML schema that defines the label structure and contents. The XML schema not only defines the individual attributes in the label, but also defines the order in which they appear in the label. The main PDS4 XML schema may be supplemented with additional, specialized schemas as needed for particular applications. The Spectral Library Data Dictionary is one such specialized schema.

The schema that defines the main, or "core", PDS4 Dictionary is available at https://pds.nasa.gov/datastandards/schema/released/#pds. The schema that defines the Spectral Library Data Dictionary is at https://pds.nasa.gov/datastandards/schema/released/#speclib. Here you will see that a dictionary is made up of several files, but only these two are needed for reference in a Spectral Library product label:

| PDS4_SPECLIB_xxxx_yyyy.xsd | The schema file itself, containing dictionary definitions. Like PDS |
|----------------------------|--|
| | labels, the schema file is written in XML. xxxx is the version number of |
| | the PDS Core Dictionary and yyyy is the version number of the |
| | Spectral Library Data Dictionary. |
| PDS4_SPECLIB_xxxx_yyyy.sch | The Schematron file, containing rules about the use of dictionary |
| | terms, also in XML |

The Spectral Library dictionary files are referenced at the beginning of a data product label, as shown in red in this example:

```
<?xml version="1.0" encoding="UTF-8"?>
<?xml-model
   href="https://pds.nasa.gov/pds4/pds/v1/PDS4_PDS_1B00.sch"
   schematypens="http://purl.oclc.org/dsdl/schematron"?>
<?xml-model
   href="https://pds.nasa.gov/pds4/speclib/v1/PDS4_SPECLIB_1B00_1000.sch"
   schematypens="http://purl.oclc.org/dsdl/schematron"?>
<Product_Observational xmlns="http://pds.nasa.gov/pds4/pds/v1"
   xmlns:speclib="http://pds.nasa.gov/pds4/speclib/v1"
   xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
   xsi:schemaLocation="http://pds.nasa.gov/pds4/pds/v1
   https://pds.nasa.gov/pds4/pds/v1/PDS4_PDS_1B00.xsd
   http://pds.nasa.gov/pds4/speclib/v1
   https://pds.nasa.gov/pds4/speclib/v1
   https://pds.nasa.gov/pds4/speclib/v1/PDS4_SPECLIB_1B00_1000.xsd">
```

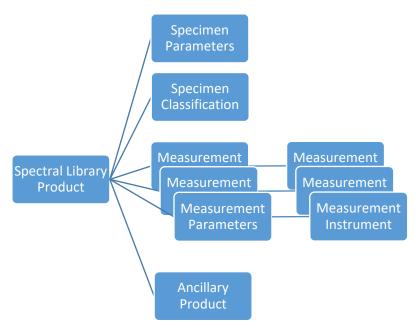
The Spectral Library Data Dictionary defines the metadata terms that describe the data products in the Spectral Library. In a PDS4 data dictionary individual elements are called attributes, and groups of associated attributes are called classes. A class may contain other classes, known as subclasses. The Spectral Library Data Dictionary, referred to in PDS4 labels as "speclib", consists of the top-level **Spectral_Library_Product** class and four subclasses: **Specimen_Parameters**, **Specimen_Classification**, **Measurement_Parameters**, and **Ancillary_Product**. The Measurement_Parameters subclass itself has a subclass, **Measurement_Instrument**. This top level class and its subclasses belong in the **Discipline_Area** section of a PDS4 label. For examples of labels of actual products, see section 6.

4 Organization of Classes and Attributes

This section shows the organization of Spectral Library classes and attributes in the order in which they are required to appear in the label. Section 5 lists the attributes and their complete definitions in alphabetical order.

4.1 Class < speclib: Spectral Library Product>

Spectral_Library_Product is the superclass that encompasses all other Spectral Library classes and attributes. It has the following structure.



Hierarchy of classes in the Spectral Library Product superclass

This structure is expressed in the label as shown below. Note that the **Spectral_Library_Product** class includes two attributes that are not in a subclass: **processing_description** and **measurement_segments**. It is possible for a spectral measurement to be made up of multiple segments measured by different instruments. The attribute **processing_description** explains this set of measurements for a given spectrum. The attribute **measurement_segments** gives the number of segments that make up the spectrum. For each segment, a separate instance of the **Measurement_Parameters** class is provided.

```
</speclib:processing description>
   <speclib:Specimen Parameters>
      [Specimen Parameters attributes]
   </speclib:Specimen_Parameters>
   <speclib:Specimen Classification>
      [Specimen Classification attributes]
   </speclib:Specimen Classification>
   <speclib:measurement_segments>2</speclib:measurement_segments>
   <speclib:Measurement_Parameters>
      [Measurement Parameters attributes for the first segment]
   </speclib:Measurement Parameters>
   <speclib:Measurement Parameters>
      [Measurement Parameters attributes for the second segment]
   </speclib:Measurement_Parameters>
   <speclib:Ancillary Product>
      [Ancillary Product attributes]
   </speclib:Ancillary Product>
</speclib:Spectral Library Product>
```

The four classes **Specimen_Parameters**, **Specimen_Classification**, **Measurement_Parameters**, and **Ancillary_Product** are described in the sections that follow. The **Ancillary_Product** section is optional; all others are required, and they must appear in the order shown.

The table below describes each component of the **Spectral_Library_Product** class. Asterisks (*) indicate required components. More complete definitions are in Section 5. Throughout this document class names are given with each word capitalized and attribute names are given in all lowercase, following PDS custom.

| Spectral_Library_Product Class | |
|--------------------------------|--|
| Component | Description |
| processing_description | The processing_description attribute provides information about |
| | how measurement(s) for a particular data product were made, in |
| | addition to the information given in the Measurement_ |
| | Parameters class. In the case of a product created by merging |
| | multiple measurements, this attribute describes how the merge |
| | was done. The description can be as long as necessary. |
| *Specimen_Parameters Class | The Specimen_Parameters class provides information that |
| | describes the specimen (sample) that was analyzed, such as |
| | particle size, collection location, and specimen owner. The class |
| | can appear only once in the label. |
| *Specimen_Classification Class | The Specimen_Classification class classifies the specimen as to its |
| | composition and physical state. The class can appear only once in |
| | the label. |
| *measurement_segments | The measurement_segments attribute gives the number of |
| | measurement segments that were merged to create the |
| | spectrum. If the spectrum is not merged from multiple segments, |
| | then the value of measurement_segments is 1. There will be one |
| | instance of the Measurement_Parameters class for each |
| | segment. |
| *Measurement_Parameters Class | The Measurement_Parameters class contains attributes that |
| | describe the conditions under which a spectral measurement was |
| | made. There will be one instance of the |

| | Measurement_Parameters class for each segment of the |
|-------------------------|---|
| | spectrum. |
| Ancillary_Product Class | The Ancillary_Product class points to an ancillary data product |
| | that contains additional data about the specimen (for example, |
| | an XRD measurement or an image of the specimen). This class can |
| | appear more than once, or may not appear at all. |

4.2 Class < speclib: Specimen Parameters >

The **Specimen_Parameters** class identifies and describes the laboratory specimen that is the target of the spectral measurement.

The class is expressed in the label as shown below. This class has no subclasses.

```
<speclib:Spectral Library Product>
   <speclib:Specimen Parameters>
     <speclib:specimen id>
          [identifier unique within the Spectral Library]
      </speclib:specimen id>
     <speclib:specimen name>[common name]</speclib:specimen name>
      <speclib:specimen description>
          [specimen description]
      </speclib:specimen description>
      <speclib:source specimen id>
          [identifier of source specimen from which this one was derived]
      </speclib:source specimen id>
      <speclib:specimen min size unit="micrometer">
          [minimum size]
      </speclib:specimen min size>
      <speclib:specimen max size unit="micrometer">
          [maximum size]
      </speclib:specimen max size>
      <speclib:specimen collection location>
          [location where specimen was collected]
      </speclib:specimen collection location>
      <speclib:specimen owner location>
          [facility that owns the specimen]
      </speclib:specimen owner location>
      <speclib:specimen owner name>
          [name of specimen owner]
      </speclib:specimen owner name>
   </speclib:Specimen Parameters>
</speclib:Spectral Library Product>
```

The table below describes the components of the **Specimen_Parameters** class. Asterisks (*) indicate required components. More complete definitions are in Section 5.

| Specimen_Parameters Class | |
|---------------------------|--|
| Component | Description |
| *specimen_id | The specimen_id attribute uniquely identifies the specimen within the Spectral Library. |

| specimen_name | The specimen_name attribute provides a name or identifier for |
|-------------------------------|--|
| | the specimen. The value is typically assigned by the person who |
| | owns the specimen or the person who made the measurement, |
| | and is not guaranteed to be unique. There are no formation |
| | rules or constraints on the value, only that the name has to be |
| | less than 255 characters long. |
| specimen_description | The specimen_description attribute provides a short description |
| | of the specimen up to 300 characters long. |
| source_specimen_id | The source_specimen_id attribute identifies the source |
| | specimen from which the observed specimen is derived. |
| *specimen_min_size | The specimen_min_size attribute identifies the minimum |
| | particle size of the observed specimen. Units are specified with |
| | the 'unit' XML attribute. Allowable units are 'AU', 'Angstrom', |
| | 'cm', 'km', 'm', 'micrometer', 'mm', and 'nm'. The attribute may |
| | be present but with a null value. |
| *specimen_max_size | The specimen_max_size attribute identifies the maximum |
| | particle size of the observed specimen. Units are specified with |
| | the 'unit' XML attribute. Allowable units are 'AU', 'Angstrom', |
| | 'cm', 'km', 'm', 'micrometer', 'mm', and 'nm'. The attribute may |
| | be present but with a null value. |
| *specimen_collection_location | The specimen_collection_location attribute provides the place |
| | where the specimen was collected. The attribute may be present |
| | but with a null value. |
| *specimen_owner_location | The specimen_owner_location attribute provides the institution |
| | or facility that owns the specimen at the time the measurement |
| | |
| | is taken. Use the value 'Unknown' if the location is not known. |
| *specimen_owner_name | is taken. Use the value 'Unknown' if the location is not known. The specimen_owner_name attribute identifies the individual or |
| *specimen_owner_name | |
| *specimen_owner_name | The specimen_owner_name attribute identifies the individual or |

4.3 Class <speclib:Specimen_Classification>

The Specimen_Classification class provides information about the type of the specimen that is the target of the spectral measurement.

The class is expressed in the label as shown below. This class has no subclasses.

```
</speclib:synthetic type>
     <speclib:material state>[Solid, Liquid, or Gas]/speclib:material state>
     <speclib:organic type>
          [Inorganic, Organic, or Mixture]
     </speclib:organic type>
     <speclib:material_type>[general type of specimen]</speclib:material_type>
     <speclib:material_subtype>
          [more specific material subtype]
     </speclib:material subtype>
     <speclib:mineral_type>
         [required if material type is Mineral]
     </speclib:mineral type>
     <speclib:mineral subtype>
         [more specific mineral subtype]
     </speclib:mineral subtype>
     <speclib:rock type>
         [required if material type is Rock]
     </speclib:rock_type>
     <speclib:rock subtype>
         [more specific rock subtype]
     </speclib:rock subtype>
     <speclib:volatile type>[Poor, Rich, or Unknown]
     <speclib:synthetic processing description>
         [descriptive text]
     </speclib:synthetic_processing_description>
  </speclib:Specimen_Classification>
</speclib:Spectral Library Product>
```

The table below describes the components of the **Specimen_Classification** class. Asterisks (*) indicate required components. More complete definitions are in Section 5.

| Specimen_Classification Class | |
|--------------------------------|--|
| Component | Description |
| *specimen_type | The specimen_type attribute gives one or more terms that |
| | classify the origin of the specimen. Allowable values are |
| | 'Terrestrial Sample', 'Lunar Meteorite', 'Mars Meteorite', |
| | 'Other Meteorite', 'Returned Lunar Sample', 'Returned |
| | Asteroid Sample', and 'Synthetic Sample'. |
| | Other values may be added to the dictionary as needed. |
| material_common_name | The material_common_name attribute gives a specific name |
| | of the specimen material that would be useful for searching in |
| | a database. |
| *material_origin | The material_origin attribute specifies whether the specimen |
| | is a natural or synthetic material. The allowable values are |
| | 'Natural' and 'Synthetic'. |
| synthetic_type | The synthetic_type attribute identifies the nature of a |
| (required if material_origin = | synthetic specimen. Possible values are 'Entirely Synthetic', |
| Synthetic) | 'Natural and Synthetic', 'From Natural', and 'Hardware'. |
| *material_state | The material_state attribute identifies the physical state of |
| | the specimen. Allowable values are 'Solid', 'Liquid', and 'Gas'. |

| *organic_type | The organic_type attribute identifies the organic type to which the specimen belongs. Allowable values are 'Inorganic', 'Organic', and 'Mixture'. |
|--|---|
| *material_type | The material_type attribute indicates the general type of the specimen. See the definition in Section 5 for the list of allowed values. |
| material_subtype | The material_subtype attribute provides for a finer or more detailed classification of material type. This attribute can appear more than once. |
| mineral_type (required if material_type = Mineral) | The mineral_type attribute indicates the mineral class for the specimen. See the definition in Section 5 for the list of allowed values. This attribute can appear more than once in the case of a mixture of minerals. |
| mineral_subtype (optional; allowed if material_type = Mineral) | The mineral_subtype attribute provides for further subdividing the mineral classification. For example, the value could be 'Smectite' if the mineral_type is 'Phyllosilicate'. There is no enumerated list for this attribute. It can appear more than once. |
| rock_type (required if material_type = Rock) | The rock_type attribute indicates the rock type for the specimen. Possible values are 'Igneous', 'Sedimentary', and 'Metamorphic'. |
| rock_subtype (optional; allowed if material_type = Rock) | The rock_subtype attribute provides for further subdividing the rock type. For example, the value could be 'Sandstone' if the rock_type is 'Sedimentary'. There is no enumerated list for this attribute. It can appear more than once. |
| volatile_type | The volatile_type attribute indicates whether the material is volatile-poor (less than 2.0% LOI) or volatile-rich (greater than 2.0% LOI). Possible values are 'Poor', 'Rich', and 'Unknown'. |
| synthetic_processing_description | The synthetic_processing_description attribute describes how a synthetic specimen was generated. The description can be up to 255 characters long. |

The following rules apply to the use of the ${\bf Specimen_Classification}$ class.

| Rule | Description |
|--|--|
| speclib_classification_rule_solid_material | If material_state is Solid, then the attributes |
| | material_type and material_subtype must be |
| | present, and material_subtype must include |
| | either Particulate or Nonparticulate. |
| speclib:classification_rule_organic_material | If material_type is Organic, then the attribute |
| | organic_type must also be Organic. |
| speclib_classification_rule_mineral | If material_type is Mineral, then the attribute |
| | mineral_type must be present. |
| speclib_classification_rule_rock | If material_type is Rock, then the attribute |
| | rock_type must be present. |
| speclib_classification_rule_material_subtype | If the attribute material_subtype is present, then |
| | the attribute material_type must also be present. |

| speclib_classification_rule_mineral_subtype | If the attribute mineral_subtype is present, then |
|---|---|
| | the attribute mineral_type must also be present. |
| speclib_classification_rule_rock_subtype | If the attribute rock_subtype is present, then the |
| | attribute rock_type must also be present. |
| speclib_classification_rule_synthetic | If material_origin is Synthetic, then the attribute |
| | synthetic_type must be present. If |
| | material_origin is not Synthetic, then the |
| | attribute synthetic type must not be present. |

4.4 Class <speclib:Measurement_Parameters>

The Measurement_Parameters class provides information about the characteristics of the measurement. It includes the subclass Measurement_Instrument, which identifies the instrument used to make the measurement. A spectral measurement may be comprised of multiple segments measured by different instruments. The attribute measurement_segments in the Spectral_Library_Product superclass gives the number of segments that make up the spectrum. There is one instance of the Measurement_Parameters class for each segment.

The class is expressed in the label as shown below. This class has one subclass, Measurement_Instrument.

```
<speclib:Spectral Library Product>
   <speclib:Measurement Parameters>
      <speclib:segment number>[which segment this is]/speclib:segment number>
      <speclib:Measurement Instrument>
          <speclib:instrument name>[name]</speclib:instrument name>
          <Internal Reference>
             <lid reference>[Instrument LID] </lid reference>
             <reference type>is instrument</reference type>
          </Internal Reference>
      </speclib:Measurement Instrument>
      <speclib:measurement type>[e.g., Reflectance]/speclib:measurement type>
      <speclib:spectral range parameter name>
          [e.g., Wavelength]
      </speclib:spectral range parameter name>
      <speclib:spectral range min>[minimum]</speclib:spectral range min>
      <speclib:spectral range max>[maximum]</speclib:spectral range max>
      <speclib:spectral range unit>[e.g., nm]</speclib:spectral range unit>
      <speclib:spectral sampling interval min>
          [minimum]
      </speclib:spectral sampling interval min>
      <speclib:spectral sampling interval max>
          [maximum]
      </speclib:spectral sampling interval max>
      <speclib:spectral sampling interval unit>
      </speclib:spectral sampling interval unit>
      <speclib:spectral resolution width min>
          [minimum]
      </speclib:spectral resolution width min>
      <speclib:spectral resolution width max>
          [maximum]
      </speclib:spectral resolution width max>
      <speclib:spectral resolution width unit>
```

```
[unit]
      </speclib:spectral resolution width unit>
      <speclib:measurement reference standard>
          [text]
      </speclib:measurement reference standard>
      <speclib:measurement geometry type>
          [e.g., Bidirectional]
      </speclib:measurement_geometry_type>
      <speclib:incidence angle unit="deg">[value]</speclib:incidence angle>
      <speclib:emission angle unit="deg">[value]</speclib:emission angle>
      <speclib:phase angle unit="deg">[value]</speclib:phase angle>
      <speclib:measurement source description>
      </speclib:measurement source description>
      <speclib:measurement atmosphere pressure>
          [value]
      </speclib:measurement atmosphere pressure>
      <speclib:measurement atmosphere temperature>
          [value]
      </speclib:measurement_atmosphere_temperature>
      <speclib:measurement atmosphere relative humidity>
      </speclib:measurement atmosphere relative humidity>
      <speclib:measurement atmosphere description>
          [description]
      </speclib:measurement_atmosphere_description>
      <speclib:measurement date time>
          [YYYY-MM-DDThh:mm:ss]
      </speclib:measurement date time>
      <speclib:data producer name>
          [who made the measurement? e.g., RELAB]
      </speclib:data_producer_name>
      <speclib:data provider name>
          [who submitted the measurement to the Spectral Library?]
      </speclib:data provider name>
      <speclib:measurement requestor>
          [who requested the measurement?]
      </speclib:measurement requestor>
      <speclib:measurement notes>
          [text]
      </speclib:measurement notes>
   </speclib:Measurement Parameters>
</speclib:Spectral Library Product>
```

The table below describes the components of the **Measurement_Parameters** class. Asterisks (*) indicate required components. More complete definitions are in Section 5.

| Measurement_Parameters Class | |
|------------------------------|---|
| Component | Description |
| *segment_number | The segment_number attribute identifies which segment of a merged spectrum is described in this Measurement_Parameters class. The first segment is segment_number 1. If the spectrum is not |

| ent_number is 1. easurement_Instrument class identifies instrument made the measurement. easurement_type attribute identifies the f spectroscopy performed on a specimen. See in 5 for the list of allowed values. ectral_range_parameter_name attribute |
|---|
| instrument made the measurement. easurement_type attribute identifies the f spectroscopy performed on a specimen. See n 5 for the list of allowed values. ectral_range_parameter_name attribute |
| easurement_type attribute identifies the f spectroscopy performed on a specimen. See n 5 for the list of allowed values. ectral_range_parameter_name attribute |
| f spectroscopy performed on a specimen. See n 5 for the list of allowed values. pectral_range_parameter_name attribute |
| n 5 for the list of allowed values. pectral_range_parameter_name attribute |
| ectral_range_parameter_name attribute |
| |
| : |
| ies the name of the parameter which |
| nines the sampling interval of the |
| rement. See Section 5 for the list of allowed |
| |
| ectral_range_min attribute identifies the |
| um value at which a given data item was |
| ed. For example, a spectrum that was |
| ired in the 0.4 to 3.5 μm range would have a |
| al_range_min value of 0.4. |
| ectral_range_max attribute identifies the |
| num value at which a given data item was |
| ed. For example, a spectrum that was |
| ired in the 0.4 to 3.5 μm range would have a |
| al_range_max value of 3.5. |
| ectral_range_unit attribute identifies the |
| measure for the values specified by the |
| al_range_min and spectral_range_max. |
| ectral_sampling_interval_min attribute |
| ies the minimum distance between band |
| s in a given spectrum. If all band centers are |
| y spaced, spectral_sampling_interval_min |
| pectral_sampling_interval_max will have the |
| value. |
| ectral_sampling_interval_max attribute |
| ies the maximum distance between band |
| s in a given spectrum. If all band centers are |
| y spaced, spectral_sampling_interval_min |
| ectral_sampling_interval_max will have the |
| value. |
| ectral_sampling_interval_unit attribute |
| ies the unit of measure for the values |
| ed by spectral_sampling_interval_min and |
| al_sampling_interval_max. |
| pectral_resolution_width_min attribute |
| ies the minimum width of a spectral band in |
| n spectrum. If all bands are the same width, |
| al_resolution_width_min and |
| al_resolution_width_max will have the same |
| |
| nkurprkurpfrhpfrhp/pffipfrh |

| spectral_resolution_width_max | The spectral_resolution_width_max attribute identifies the maximum width of a spectral band in a given spectrum. If all bands are the same width, spectral_resolution_width_min and spectral_resolution_width_max will have the same value. |
|------------------------------------|--|
| spectral_resolution_width_unit | The spectral_resolution_width_unit attribute identifies the unit of measure for the values specified by spectral_resolution_width_min and spectral_resolution_width_max. |
| measurement_reference_standard | The measurement_reference_standard attribute describes the standard object on which observations are performed in order to calibrate a measurement. |
| *measurement_geometry_type | The measurement_geometry_type attribute identifies the type of geometry at which a measurement is taken. See Section 5 for the list of allowed values. |
| *incidence_angle | The incidence_angle attribute provides the angle between the local vertical at the intercept point and a vector from the intercept point to the illumination source. The value must be between 0 and 90 degrees, or the attribute may be present with a null value. |
| *emission_angle | The emission_angle attribute provides the angle between the local vertical at the intercept point and a vector from the intercept point to the detector. The value must be between 0 and 90 degrees, or the attribute may be present with a null value. |
| *phase_angle | The phase_angle attribute provides the angle between incidence and emission vectors. The value must be between 0 and 180 degrees, or the attribute may be present with a null value. |
| measurement_source_description | The measurement_source_description attribute identifies the source used for the measurement such as the type of lamp, heating element, laser, or radioactive source. |
| measurement_atmosphere_pressure | The measurement_atmosphere_pressure attribute provides the atmospheric pressure of measurement environment. Allowable units for this attribute are 'Pa', 'bar', 'hPa', and 'mbar'. |
| measurement_atmosphere_temperature | The measurement_atmosphere_temperature attribute provides the temperature of the measurement environment. Allowable units for this attribute are 'K' and 'degC'. |

| *measurement_atmosphere_relative_humidity | The measurement_atmosphere_relative_humidity attribute provides the relative humidity of the measurement environment. The attribute may be present with a null value. | |
|---|--|--|
| measurement_atmosphere_composition | The measurement_atmosphere_composition attribute identifies any gas or gases present in measurement environment. | |
| *measurement_atmosphere_description | The measurement_atmosphere_description attribute describes the atmospheric conditions with which the data was taken. | |
| *measurement_date_time | The measurement_date_time attribute identifies the date and time when the measurement was made. The attribute may be present with a null value. | |
| *data_producer_name | The data_producer_name element provides the name of the creator of the product. | |
| *data_provider_name | The data_provider_name attribute provides the full name of the person who submitted the measurement to the library. | |
| *measurement_requestor | The measurement_requestor attribute provides the full name of the person who requested the measurement to be made. It may appear more than once. The attribute may be present with a null value. | |
| measurement_notes | The measurement_notes attribute contains relevant notes about how a measurement was made, up to 1000 characters. | |

4.5 Class <speclib:Measurement_Instrument>

Measurement_Instrument is a subclass of **Measurement_Parameters**. It identifies the spectrometer that made the measurement by its Logical Identifier (LID).

The class is expressed in the label as shown below. This class has one subclass, **Internal_Reference**, which is defined in the PDS Core Dictionary.

The table below describes the components of the **Measurement_Instrument** class. Asterisks (*) indicate required components. More complete definitions are in Section 5.

| Measurement_Instrument Class | | |
|------------------------------|---|--|
| Component | Description | |
| *instrument_name | The instrument_name attribute provides a descriptive name of | |
| | the instrument that made a spectral measurement. | |
| *Internal_Reference | The Internal_Reference class contains the following two | |
| | attributes that identify the instrument. Note that this class is | |
| | defined in the PDS core data dictionary, not the Spectral Library | |
| | data dictionary (i.e., it lacks the 'speclib:' prefix). | |
| *lid_reference | The lid_reference attribute gives the unique PDS4 Logical | |
| | Identifier (LID) of the instrument that made the measurement. | |
| *reference_type | The reference_type attribute specifies that the LID refers to an | |
| | instrument. The value of this attribute must be 'is_instrument'. | |

4.6 Class < speclib: Ancillary Product>

The **Ancillary_Product** class is optional. A spectral measurement may be accompanied by one or more ancillary products, which may be images of the specimen, plots of the measurement, or other types of measurements of the specimen. This class identifies an ancillary product by its Logical Identifier (LID).

The class is expressed in the label as shown below. This class has one subclass, **Internal_Reference**, which is defined in the PDS Core Dictionary.

The table below describes the components of the **Ancillary_Product** class. Asterisks (*) indicate required components. More complete definitions are in Section 5.

| Ancillary_Product Class | | | |
|-------------------------|--|--|--|
| Component | Description | | |
| *Internal_Reference | The Internal_Reference class contains the following two | | |
| | attributes that identify the ancillary product. Note that this class | | |
| | is defined in the PDS core data dictionary, not the Spectral | | |
| | Library data dictionary (i.e., it lacks the 'speclib:' prefix). | | |
| *lid_reference | The lid_reference attribute gives the unique PDS4 Logical | | |
| | Identifier (LID) of an ancillary product related to this product. | | |
| *reference_type | The reference_type attribute specifies that the LID refers to an ancillary product. The value of this attribute must be | | |
| | | | |
| | 'data_to_ancillary'. | | |
| *ancillary_product_type | The ancillary_product_type attribute gives the type of data in | | |
| | the ancillary product. See Section 5 for the list of allowed values. | | |
| | Additional values may be added to the dictionary. | | |

5 Definitions

Complete definitions of Spectral Library classes and attributes are given here in alphabetical order.

| Ancillary_Product (class) | |
|-----------------------------|--|
| Definition | The Ancillary_Product class identifies an ancillary measurement related to a Spectral Library specimen. RELAB NOTES: This is most commonly a photograph (image) of the specimen taken by RELAB personnel or idependently-measured chemical data for the specimen provided by the measurement requestor. |
| Min/max occurences in label | 0 1 |

| ancillary_product_type (attribute) | | | |
|------------------------------------|---|---|--|
| Definition | The ancillary_product_type element provides the type of data found in an ancillary product. | | |
| PDS4 data type | UTF8_Short_String_Collapsed | | |
| Min/max occurences in class | 1 | 1 | |
| Nillable? | no | | |
| Allowed values | Attenuated Total Reflectance Spectroscopy | IR spectroscopic technique in which placing a sample next to a high refractive index crystal causes total internal reflection resulting in an evanescent wave that samples shallow properties of the sample | |
| | Image | An image of the sample | |
| | Chemical Composition | Elemental or oxide | |
| | | abundances for samples | |
| | Differential Scanning | Technique in which the sample | |
| | Calorimetry | is heated and temperature is | |

| | monitored to evaluate exothermic and endothermic reactions that are indicative of composition |
|--------------------|--|
| Electron Micropro | be Analysis Microprobe technique in which the sample is bombarded with electrons, with resultant X-ray emission spectra indicative of sample composition |
| Modal Mineralogy | Sample mineral abundances defined as weight or volume percentages |
| Raman Spectrosco | py Spectroscopic technique based on based on inelastic scattering of monochromatic light, usually from a laser source |
| Reflectance Spectr | oscopy Spectroscopic technique based on measuring the spectral properties of light scattered from samples |
| Thermogravimetric | c Analysis Technique in which sample mass is measured as its temperature is increased |
| Transmission Spec | troscopy Spectroscopic technique based on measuring the spectral properties of light transmitted through samples |
| X-ray Diffraction | X-rays diffracted by a sample as a function of incident angle are used to determine sample crystal structure |
| X-ray Fluorescence | Spectroscopic technique in which the sample is bombarded by high-energy X-rays or gamma rays, with fluorescent X-ray emission spectra indicative of sample composition |

| data_producer_name (attribute) | |
|--------------------------------|---|
| Definition | The data_producer_name element provides the name of the creator of the product. RELAB NOTES: For products in RELAB, the value of data_producer_name is always "RELAB". |
| PDS4 data type | UTF8_Short_String_Collapsed |

| Min/max occurences in class | 1 | 1 |
|-----------------------------|-----|---|
| Nillable? | no | |
| Min/max characters | 1 | |
| Allowed values | any | |

| data_provider_name (attribute) | | |
|--------------------------------|-----------------------------|--|
| Definition | - - | vider_name element provides the full name of the ubmitted the product to the Spectral Library. |
| PDS4 data type | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 1 | 1 |
| Nillable? | no | |
| Min/max characters | 1 | 255 |
| Allowed values | any | |

| emission_angle (attribute) | | |
|-----------------------------|--|----|
| Definition | The emission_angle element provides the angle between the local vertical at the intercept point and a vector from the intercept point to the sensor. | |
| PDS4 data type | ASCII_Real | |
| Min/max occurences in class | 1 | 1 |
| Nillable? | yes | |
| Min/max values | -90 | 90 |

| incidence_angle (attribute) | | |
|-----------------------------|---|----|
| Definition | The incidence_angle element provides the angle between the local vertical at the intercept point and a vector from the intercept point to the detector. | |
| PDS4 data type | ASCII_Real | |
| Min/max occurences in class | 1 | 1 |
| Nillable? | yes | |
| Min/max values | -90 | 90 |

| instrument_name (attribute) | | |
|-----------------------------|---|-----|
| Definition | The instrument_name element provides a descriptive name of the instrument that made a spectral measurement. | |
| PDS4 data type | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 1 1 | |
| Nillable? | no | |
| Min/max characters | 1 | 100 |
| Allowed values | any | |

material_common_name (attribute)

| Definition | The material_common_name element gives the specific name of the specimen material, as specifically as it is known. For example, if a specimen is pure olivine, put "Olivine". If a specimen is a mixture of kaolinite and opal, put "Kaolinite/Opal". Indicate if "Unidentified". | |
|-----------------------------|---|-----|
| PDS4 data type | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 0 1 | |
| Nillable? | no | |
| Min/max characters | 1 | 100 |
| Allowed values | any | |

| material_origin (attribute) | | | |
|-----------------------------|--|--|--|
| Definition | The material_origin element identifies whether the specimen is | | |
| | natural or synthetic. | | |
| PDS4 data type | UTF8_Short_String_Collapsed | | |
| Min/max occurences in class | 1 | 1 | |
| Nillable? | no | | |
| Allowed values | Natural | The Natural value indicates | |
| | | that the specimen was not | |
| | | made in a laboratory. | |
| | Synthetic | The Synthetic value indicates | |
| | | that the specimen <u>or some</u> | |
| | | portion of a specimen was | |
| | | made in a laboratory. A | |
| | | synthetic sample could be | |
| | | either a physical mixture of | |
| | | natural materials or a | |
| | | laboratory synthesized | |
| | | material. A synthetic material | |
| | | could also be a natural | |
| | | material that has been altered | |
| | | in some way (e.g., heated) in a | |
| | | <u>laboratory.</u> | |
| | | RELAB NOTES: Natural | |
| | | materials that have only been | |
| | | ground and/or dry-sieved for | |
| | | RELAB measurements are still | |
| | | considered 'natural', as are | |
| | | specimens that have been | |
| | | magnetically separated or | |
| | | washed with water. | |
| | | Specimens that are | |
| | | synthesized mixtures of solely natural materials are | |
| | | | |
| | | considered 'synthetic'. | |
| | | Specimens that have been | |
| | | altered in some way <u>other</u> | |

| than simple grinding and/or | | |
|-----------------------------|-----|--|
| sieving (e.g., heating, | | |
| interaction with solvents) | are | |
| considered 'synthetic'. | | |

| material_state (attribute) | | |
|-----------------------------|---|--|
| Definition | The material_state element identifies the physical state of the specimen. | |
| PDS4 data type | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 1 | 1 |
| Nillable? | no | |
| Allowed values | Solid | The Solid value indicates that the specimen is in the solid state. |
| | Liquid | The Liquid value indicates that the specimen is in the liquid state. |
| | Gas | The Gas value indicates that the specimen is in the gas state. |

| material_subtype (attribute) | | |
|------------------------------|---|-----|
| Definition | The material_subtype element identifies a material subtype of the specimen. | |
| PDS4 data type | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 0 10 | |
| Nillable? | no | |
| Min/max characters | 1 | 255 |
| Allowed values | any | |

| material_type (attribute) | | |
|-----------------------------|---|---|
| Definition | The material_type element indicates the general type of the specimen. | |
| PDS4 data type | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 0 1 | |
| Nillable? | no | |
| Allowed values | Amorphous | Sample without crystalline structure or long range order, e.g., glass |
| | Consolidated Mixture | Sample that is cemented or otherwise aggregated into a solid mass |
| | Element | Sample composed of a single element such as metallic iron |

| Ice | Solid sample composed of gas or liquid (e.g., water vapor or water) now in solid form |
|------------------------|--|
| Mineral | Sample with a given composition within a defined range of compositions and that exhibits a defined crystalline structure |
| Organic | Sample composed of organic materials |
| Rock | Solid sample composed of one or more minerals |
| Single Particle | Sample composed of a single particle |
| Unconsolidated Mixture | Sample of loose or disaggregated material that is a mixture of various minerals and/or other compounds |

| measurement_atmosphere_composition (attribute) | | |
|--|---|--|
| Definition | The measurement_atmosphere_composition element identifies any gas(es) present in measurement environment. | |
| PDS4 data type | UTF8_Text_Preserved | |
| Min/max occurences in class | 0 1 | |
| Nillable? | yes | |
| Min/max characters | 1 1000 | |
| Allowed values | any | |

| measurement_atmosphere_description (attribute) | | | |
|--|------------|---|--|
| Definition | | The measurement_atmosphere_description describes the atmospheric conditions through which the data was taken. | |
| PDS4 data type | UTF8_Text_ | UTF8_Text_Preserved | |
| Min/max occurences in class | 1 | 1 1 | |
| Nillable? | no | | |
| Min/max characters | 1 | 1000 | |
| Allowed values | any | | |

| measurement_atmosphere_pressure (attribute) | | | |
|---|--------------------|--|--|
| Definition | The measurement_ | The measurement_atmosphere_pressure element provides the | |
| | atmospheric pressu | atmospheric pressure of the measurement environment. | |
| PDS4 data type | ASCII_Real | | |
| Min/max occurences in class | 0 | 1 | |
| Nillable? | yes | | |
| Min/max values | unlimited | unlimited | |

| PDS4 unit type | Units_of_Pressure | |
|----------------|-------------------|--|
|----------------|-------------------|--|

| measurement_atmosphere_relative_humidity(attribute) | | | |
|---|------------|---|--|
| Definition | | The measurement_atmosphere_relative_humidity element provides the relative humidity of the measurement environment. | |
| PDS4 data type | ASCII_Real | | |
| Min/max occurences in class | 1 | 1 | |
| Nillable? | yes | | |
| Min/max values | 0 | 100 | |

| measurement_atmosphere_temperature (attribute) | | |
|--|---|-----------|
| Definition | The measurement_atmosphere_temperature element provides the temperature of the measurement environment. | |
| PDS4 data type | ASCII_Real | |
| Min/max occurences in class | 0 | 1 |
| Nillable? | yes | |
| Min/max values | unlimited | unlimited |
| PDS4 unit type | Units_of_Temperatu | ire |

| measurement_date_time (attribute) | | |
|-----------------------------------|---|--|
| Definition | The measurement_date_time element identifies the date and | |
| | time of the observation and measurement. | |
| PDS4 data type | ASCII_Date_Time_YMD | |
| Min/max occurences in class | 1 1 | |
| Nillable? | yes | |
| Allowed values | Formation rule <i>yyyymmddThh:mm:ss.nnnnnnZ</i> . The value may be truncated on the right as far as the year. The Z (UTC time indicator) is optional. | |

| measurement_geometry_type (attribute) | | |
|---------------------------------------|---|---|
| Definition | The measurement_geometry_type element identifies the type of lighting and viewing geometry at which a measurement is taken. | |
| PDS4 data type | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 1 1 | |
| Nillable? | no | |
| Allowed values | Bidirectional | Measurement taken when light is sent in to the specimen at a narrow angular range and received over a narrow angular range. RELAB NOTES: This corresponds to the RELAB bi- |

| | directional (BDR) |
|-----------------------------|------------------------------------|
| | spectrometer. |
| Directional Hemispherical | Measurement taken when |
| | light is sent in to the specimen |
| | at a certain direction and |
| | received in all directions |
| | (perhaps in an integrating |
| | sphere). |
| Hemispherical Hemispherical | Measurement taken when |
| | light is sent in to the specimen |
| | at all directions and received in |
| | all directions (perhaps in an |
| | integrating sphere). |
| Biconical | Measurement taken when |
| | light is sent in to the specimen |
| | at a certain direction and in a |
| | cone-like shape and received |
| | at a certain direction and in a |
| | cone-like shape. |
| | RELAB NOTES: This typically |
| | corresponds to measurements |
| | made with the diffuse |
| | reflectance attachments in |
| | the FTIR spectrometer. |
| Unknown | The measurement geometry is |
| | unknown. |

| Measurement_Instrument (class) | |
|--------------------------------|--|
| Definition | The Measurement_Instrument class identifies which instrument |
| | made the measurement described in the |
| | Measurement_Parameters class. |
| Min/max occurences in class | 1 per Measurement_Parameters class |

| measurement_notes (attribute) | | | |
|-------------------------------|---|------|--|
| Definition | The measurement_notes element contains relevant notes about | | |
| | how a measurement was made. | | |
| PDS4 data type | UTF8_Text_Preserved | | |
| Min/max occurences in class | 0 1 | | |
| Nillable? | no | | |
| Min/max characters | 1 | 1000 | |
| Allowed values | any | | |

| Measurement_Parameters (class) | |
|--------------------------------|---|
| Definition | The Measurement_Parameters class contains attributes relevant |
| | to a single measurement of a specimen. |

| Min/max occurences in class | Value given by attribute measurement_segments |
|-----------------------------|---|
|-----------------------------|---|

| measurement_reference_standa | ard (attribute) | | |
|------------------------------|---|---|--|
| Definition | standard object to calibrate a RELAB NOTES pressed halo | The measurement_reference_standard element identifies the standard object on which observations are performed in order to calibrate a measurement. RELAB NOTES: For the bi-directional spectrometer this is either pressed halon powder or a small Spectralon ™ panel. For FTIR measurements this is most commonly diffuse gold. | |
| PDS4 data type | UTF8_Text_P | reserved | |
| Min/max occurences in class | 0 | 1 | |
| Nillable? | no | | |
| Min/max characters | 1 | 1000 | |
| Allowed values | any | | |

| measurement_requestor (attribu | re) | |
|--------------------------------|--|--|
| Definition | The measurement_requestor element identifies the individual or laboratory who requested the measurement. It may occur more than once. RELAB NOTES: For RELAB measurments the three middle letters of the specimen ID are typically the initials of the primary measurement requestor. | |
| PDS4 data type | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 1 Unlimited | |
| Nillable? | yes | |
| Min/max characters | 1 255 | |
| Allowed values | any | |

| measurement_segments (attribut | e) | |
|--------------------------------|---|-----------|
| Definition | The measurement_segments element gives the number of measurement segments that were combined to create the spectrum. If the spectrum is not merged from multiple segments, then the value of measurement_segments is 1. | |
| PDS4 data type | ASCII_NonNegative_Integer | |
| Min/max occurences in class | 1 | 1 |
| Nillable? | no | |
| Min/max values | 1 | Unlimited |

| measurement_source_description (attribute) | | |
|--|---|--|
| Definition | The measurement_source_description element identifies the | |
| | source used for the measurement such as the type of lamp, | |
| | heating element, laser, or radioactive source. | |
| PDS4 data type | UTF8_Short_String_Collapsed | |

| Min/max occurences in class | 0 | 1 |
|-----------------------------|-----|-----|
| Nillable? | no | |
| Min/max characters | 1 | 255 |
| Allowed values | any | |

| measurement_type (attribute) | | |
|------------------------------|---|---|
| Definition | The measurement_type element identifies the type of | |
| | spectroscopy performed on a sp | pecimen. |
| PDS4 data type | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 1 | 1 |
| Nillable? | no | |
| Allowed values | Reflectance | The Reflectance value indicates reflectance |
| | | spectroscopy, the study of |
| | | light as a function of |
| | | wavelength that has been |
| | | reflected or scattered from a |
| | | material. |
| | Emission | The Emission value indicates emission spectroscpy, which examines the wavelengths emitted by atoms or molecules during their transition from an excited state to a lower energy state. |
| | Raman | The Raman value indicates Raman spectroscopy, which determines information about a material by studying the Raman scattering of monochromatic light off the material. |
| | X-Ray Fluorescence | The X-Ray Fluorescence value indicates x-ray flourescence spectroscopy, which examines the emission of x-rays from a material previously bombarded with high energy x-rays or gamma rays. |
| | X-Ray Diffraction | The X-Ray Diffraction value indicates x-ray diffraction spectroscopy, which studies the diffraction patterns of x-rays scattered off a material. |
| | LIBS | LIBS (Laser-Induced Breakdown Spectroscopy) uses |

| | a highly energetic laser pulse |
|------------------------------|---------------------------------|
| | as its excitation source to |
| | produce emission spectra. |
| Transmission | The Transmission value |
| | indicates transmission |
| | spectroscopy, the study of |
| | light as a function of |
| | wavelength that has been |
| | transmitted through a |
| | material. |
| Attenuated Total Reflectance | Attenuated total reflectance |
| | (ATR) is a sampling technique |
| | used in conjunction with |
| | infrared spectroscopy which |
| | enables samples to be |
| | examined directly in the solid |
| | or liquid state without further |
| | |
| | preparation. |

| mineral_subtype (attribute) | | | |
|-----------------------------|---|---|--|
| Definition | specimens iden be 'Smectite' if enumerated list | The mineral_subtype element provides for further subdividing of specimens identified as minerals. For example, the value could be 'Smectite' if the mineral_type is 'Phyllosilicate'. There is no enumerated list for mineral_subtype. The element may appear more than once. | |
| PDS4 data type | UTF8_Short_String_Collapsed | | |
| Min/max occurences in class | 0 | 10 | |
| Nillable? | no | | |
| Min/max characters | 1 | 255 | |
| Allowed values | any | | |

| mineral_type (attribute) | | |
|-----------------------------|--|--|
| Definition | The mineral_type element identifies the type of mineral to which the specimen belongs. | |
| PDS4 data type | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 0 Unlimited | |
| Nillable? | no | |
| Allowed values | Arsenate | |
| | Borate | |
| | Carbonate | |
| | Chromate | |
| | Cyclosilicate | |
| | Halide | |
| | Hydroxide | |
| | Inosilicate | |

| Iodate | |
|------------------|--|
| Native Element | Native element or alloy |
| Neosilicate | |
| Nitrate | |
| Organic Compound | |
| Oxide | |
| Phosphate | |
| Phyllosilicate | |
| Sorosilicate | |
| Sulfate | |
| Sulfide | |
| Tectosilicate | |
| Unclassified | For a specimen that doesn't fit into any of the categories, but is still a mineral |
| Vanadate | |

| organic_type (attribute) | | | |
|-----------------------------|------------------------|---|--|
| Definition | The organic_type eleme | The organic_type element identifies the organic type to which | |
| | the specimen belongs. | the specimen belongs. | |
| PDS4 data type | UTF8_Short_String_Coll | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 1 | 1 | |
| Nillable? | no | | |
| Allowed values | Organic | The Organic value indicates | |
| | | the specimen is an organic | |
| | | material. | |
| | Inorganic | The Inorganic value indicates | |
| | | the specimen is not an organic | |
| | | material. | |
| | Mixture | The Mixture value indicates | |
| | | the specimen is a mixture of | |
| | | organic and inorganic material. | |
| | | RELAB NOTES: This may | |
| | | correspond to a natural | |
| | | sample that is particularly | |
| | | enriced in organics, such as a | |
| | | tar sand or oil-rich sandstone. | |
| | | It may also correspond to | |
| | | synthetic mixtures of | |
| | | inorganic and organic | |
| | | materials. | |

| phase_angle (attribute) | |
|-------------------------|--|
| Definition | The phase_angle element provides the angle between incidence |
| | and emission vectors. |

| PDS4 data type | ASCII_Real | |
|-----------------------------|----------------|-----|
| Min/max occurences in class | 1 | 1 |
| Nillable? | yes | |
| Min/max values | -180 | 180 |
| PDS4 unit type | Units_of_Angle | |

| processing_description (attribute) | | |
|------------------------------------|--|--|
| Definition | The processing_description element provides information about how measurement(s) for a particular product were made, in addition to the information given in the Measurement Parameters class. In the case of a product created by merging multiple measurements, this element describes how the merge was done. | |
| PDS4 data type | UTF8_Text_Preserved | |
| Min/max occurences in class | 0 1 | |
| Nillable? | no | |
| Min/max characters | 1 Unlimited | |
| Allowed values | any | |

| rock_subtype (attribute) | | |
|-----------------------------|---|--|
| Definition | The rock_subtype element provides for further subdividing of specimens identified as rocks. For example, the value could be 'Sandstone' if the rock_type is 'Sedimentary'. There is no enumerated list for rock_subtype. The element may appear more than once. | |
| PDS4 data type | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 0 10 | |
| Nillable? | no | |
| Min/max characters | 1 255 | |
| Allowed values | any | |

| rock_type (attribute) | |
|-----------------------|--|
| Definition | The rock_type element identifies the type of rock the specimen is. RELAB NOTES: For meteorites (and lunar rocks), material_type = rock, thus rock_type is required to be defined. The designation of a rock type is not entirely straightforward for some samples. Chondrite meteorites are generally regarded as sedimentary rocks and are defined as such. For simplicity, lunar basalts and other basalts (e.g., eucrites) are commonly defined as igneous even when they are brecciated. Specimens that are primarily regoligh breccias or impact-generated mixtures of various lithologies (e.g., howardites) are defined as sedimentary, though the individual components may all have a primary igneous origin. In general, the RELAB database |

| | considers impact gardening/brecciation to be a sedimentary process that results in the formation of sedimentary rocks. The exception, which is common amongst certain extraterrestrial samples, is when the resulting breccia is dominated by a single lithology. Thus brecciated eucrites are considered igneous, primitive achondrites may be considered as having resulted from igneous processes, and various lunar basalts may be considered igneous in origin (though many are heavily | |
|-----------------------------|--|--|
| | brecciated/fractured). Sp | pecimens identified as more complex, |
| | | preccias are defined as sedimentary. |
| PDS4 data type | UTF8_Short_String_Colla | |
| Min/max occurences in class | 0 | 1 |
| Nillable? | no | |
| Allowed values | Igneous | The Igneous value indicates that the specimen is volatile-poor and was formed by the cooling of magma or lava. |
| | Sedimentary | The Sedimentary value indicates that the specimen was formed by sedimentary processes (e.g., lithification of unconsolidated material, direct chemical precipitation). |
| | Metamorphic | The Metamorphic value indicates that the specimen was formed by metamorphic processes (e.g., increased temperature and/or pressure conditions that altered the rock composition without melting) |
| | Unknown | The Unknown value indicates that there is not enough information about the specimen to assign it a rock type |

| segment_number (attribute) | | |
|-----------------------------|--|--|
| Definition | The segment_number element identifies which segment of a merged spectrum is described by a Measurement_Parameters class. The first segment is segment number 1. If the spectrum is not merged from multiple segments, then the value of segment number is 1. | |
| PDS4 data type | ASCII_NonNegative_Integer | |
| Min/max occurences in class | 1 1 | |
| Nillable? | no | |

| Min/max values 1 Unlimited |
|----------------------------|
|----------------------------|

| source_specimen_id (attribute) | | | |
|--------------------------------|--|---|--|
| Definition | The source_specimen_id e | The source_specimen_id element identifies the source specimen | |
| | from which the observed specimen is derived, if any. | | |
| PDS4 data type | UTF8_Short_String_Collapsed | | |
| Min/max occurences in class | 0 | 1 | |
| Nillable? | yes | | |
| Min/max characters | 1 | 255 | |
| Allowed values | any specimen_id value | | |

| Specimen_Classification (class) | | |
|---------------------------------|--|---|
| Definition | The Specimen_Classification Class how a specimen has been classification physical state. | • |
| Min/max occurences in class | 1 | 1 |

| specimen_collection_location (attribute) | | |
|--|---|-----|
| Definition | The specimen_collection_location element provides the place where the specimen was collected. | |
| PDS4 data type | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 1 | 1 |
| Nillable? | yes | |
| Min/max characters | 1 | 255 |
| Allowed values | any | |

| specimen_description (attribute) | | | |
|----------------------------------|--------------|--|--|
| Definition | • | The specimen_description element provides an optional short description of the specimen. | |
| PDS4 data type | UTF8_Text_Pr | eserved | |
| Min/max occurences in class | 0 | 1 | |
| Nillable? | no | | |
| Min/max characters | 1 | 1000 | |
| Allowed values | any | | |

| specimen_id (attribute) | |
|-------------------------|--|
| Definition | The specimen_id element uniquely identifies the specimen within the Spectral Library. Note that this identifier is not a PDS LID (Logical Identifier), as specimens are not PDS products. RELAB NOTES: For RELAB measurments the three middle letters of the specimen_ID are typically the initials of the primary measurement requestor. |
| PDS4 data type | UTF8_Short_String_Collapsed |

| Min/max occurences in class | 1 | 1 |
|-----------------------------|-----|-----|
| Nillable? | no | |
| Min/max characters | 1 | 255 |
| Allowed values | any | |

| specimen_max_size (attribute) | | |
|-------------------------------|--|-----------|
| Definition | The specimen_max_size element identifies the maximum particle size of the observed specimen. | |
| PDS4 data type | ASCII_Real | |
| Min/max occurences in class | 1 | 1 |
| Nillable? | yes | |
| Min/max values | 0 | Unlimited |
| PDS4 unit type | Units_of_Length | |

| specimen_min_size (attribute) | | |
|-------------------------------|--|-----------|
| Definition | The specimen_max_size element identifies the minimum particle size of the observed specimen. | |
| PDS4 data type | ASCII_Real | |
| Min/max occurences in class | 1 | 1 |
| Nillable? | yes | |
| Min/max values | 0 | Unlimited |
| PDS4 unit type | Units_of_Length | |

| specimen_name (attribute) | | |
|-----------------------------|--|-----|
| Definition | The specimen_name element identifies the specimen as it is named where it is being kept. | |
| PDS4 data type | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 0 | 1 |
| Nillable? | no | |
| Min/max characters | 1 | 255 |
| Allowed values | any | |

| specimen_owner_location (attribute) | | | |
|-------------------------------------|---|-----|--|
| Definition | The specimen_owner_location element provides the institution or laboratory name where the specimen resides. | | |
| PDS4 data type | UTF8_Short_String_Collapsed | | |
| Min/max occurences in class | 1 | 1 | |
| Nillable? | yes | | |
| Min/max characters | 1 | 255 | |
| Allowed values | any | | |

specimen_owner_name (attribute)

| Definition | The specimen_owner_name element identifies the individual or | |
|-----------------------------|--|-----|
| | laboratory to whom the specimen belongs. | |
| PDS4 data type | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 1 | 1 |
| Nillable? | yes | |
| Min/max characters | 1 | 255 |
| Allowed values | any | |

| Specimen_Parameters (class) | | |
|-----------------------------|---------------------------------|------------------------------|
| Definition | The Specimen_Parameters class p | provides information about a |
| | specimen for which measuremen | ts have been made. |
| Min/max occurences in class | 1 | 1 |

| specimen_type (attribute) | | | |
|-----------------------------|--------------------------------------|--|--|
| Definition | The specimen_type element given | The specimen_type element gives one or more terms that | |
| | classify the origin of the specimen. | | |
| PDS4 data type | UTF8_Short_String_Collapsed | | |
| Min/max occurences in class | 1 | Unlimited | |
| Nillable? | no | | |
| Allowed values | Terrestrial Sample | The Terrestrial value means | |
| | | the specimen is a terrestrial | |
| | | sample originating on Earth. | |
| | Lunar Meteorite | The Lunar Meteorite value | |
| | | means the specimen is a | |
| | | sample from a lunar | |
| | | meteorite. | |
| | Mars Meteorite | The Mars Meteorite value | |
| | | means the specimen is a | |
| | | sample from a Mars meteorite. | |
| | Other Meteorite | The Other Meteorite value | |
| | | means the specimen is a | |
| | | sample from a meteorite that | |
| | | is not a lunar or Mars | |
| | Datum addum an Canada | meteorite. | |
| | Returned Lunar Sample | The Returned Lunar Sample | |
| | | value means the specimen is a lunar sample returned by a | |
| | | mission. | |
| | Returned Asteroid Sample | The Returned Asteroid Sample | |
| | Retained Asteroid Sample | value means the specimen is | |
| | | an asteroid sample returned | |
| | | by a mission. | |
| | Synthetic Sample | The Synthetic Sample value | |
| | -, | means the specimen is a | |
| | | laboratory-generated sample. | |
| | | / 0 | |

| RELAB NOTES: This includes |
|-----------------------------------|
| mixtures of natural terrestrial |
| or extraterrestrial materials |
| that were made in a |
| laboratory (e.g., basalt and |
| clay mixtures, meteorite and |
| organic mixtures). |
| · |

| Spectral_Library_Product (class) | | |
|----------------------------------|-------------------------------------|--------------------------------|
| Definition | The Spectral_Library_Product clas | s provides information about a |
| | data product in the Spectral Librar | ry. |
| Min/max occurences in class | 1 | 1 |

| spectral_range_max (attribute) | | |
|--------------------------------|-------------------------------|-------------------------------------|
| Definition | at which a given data item wa | in the 0.4 to 3.5 um spectral range |
| PDS4 data type | ASCII_Real | |
| Min/max occurences in class | 1 | 1 |
| Nillable? | no | |
| Min/max values | 0 | Unlimited |

| spectral_range_min (attribute) | | |
|--------------------------------|---|-----------|
| Definition | The spectral_range_min element identifies the minimum value at which a given data item was sampled. For example, a spectrum that was measured in the 0.4 to 3.5 um spectral range would have a spectral_range_min value of 0.4. | |
| PDS4 data type | ASCII_Real | |
| Min/max occurences in class | 1 | 1 |
| Nillable? | no | |
| Min/max values | 0 | Unlimited |

| spectral_range_parameter_name (attribute) | | |
|---|---|---|
| Definition | The spectral_range_parameter_name element identifies the name of the parameter which determines the sampling interval of the measurement. | |
| PDS4 data type | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 1 | 1 |
| Nillable? | no | |
| Allowed values | Wavelength | The spectrum is a function of wavelength. |
| | Frequency | The spectrum is a function of frequency. |

| Wa | evenumber | The spectrum is a function of wavenumber. |
|-----|-----------|---|
| Tim | ne | The spectrum is a function of |
| | | time. |
| Ang | gle | The spectrum is a function of |
| | | angle. |
| Ene | ergy | The spectrum is a function of |
| | | energy. |

| spectral_range_unit (attribute) | | |
|---------------------------------|---|-----|
| Definition | The spectral_range_unit element identifies the unit of measure for the values specified by spectral_range_min and spectral_range_max. | |
| PDS4 data type | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 1 | 1 |
| Nillable? | no | |
| Min/max characters | 1 | 255 |
| Allowed values | any | |

| spectral_resolution_width_max (attribute) | | |
|---|---|--|
| Definition | The spectral_resolution_width_max element identifies the maximum width of a spectral band in a given spectrum. If all bands are the same width, spectral_resolution_width_min and spectral_resolution_width_max will have the same value. | |
| PDS4 data type | ASCII_Real | |
| Min/max occurences in class | 0 1 | |
| Nillable? | yes | |
| Min/max values | 0 Unlimited | |

| spectral_resolution_width_min (attribute) | | |
|---|---|--|
| Definition | The spectral_resolution_width_min element identifies the minimum width of a spectral band in a given spectrum. If all bands are the same width, spectral_resolution_width_min and spectral_resolution_width_max will have the same value. | |
| PDS4 data type | ASCII_Real | |
| Min/max occurences in class | 0 1 | |
| Nillable? | yes | |
| Min/max values | 0 Unlimited | |

| spectral_resolution_width_unit (attribute) | |
|--|--|
| Definition | The spectral_resolution_width_unit element identifies the unit |
| | of measure for the values specified by |
| | spectral_resolution_width_min and |
| | spectral_resolution_width_max. |

| PDS4 data type | UTF8_Short_String_Collapsed | |
|-----------------------------|-----------------------------|-----|
| Min/max occurences in class | 0 | 1 |
| Nillable? | yes | |
| Min/max characters | 1 | 255 |
| Allowed values | any | |

| spectral_sampling_interval_max | (attribute) | | |
|--------------------------------|---|--|--|
| Definition | maximum distance betwall band centers are equal spectral_sampling_inter | The spectral_sampling_interval_max element identifies the maximum distance between band centers in a given spectrum. If all band centers are equally spaced, spectral_sampling_interval_min and spectral_sampling_interval_max will have the same value. | |
| PDS4 data type | ASCII_Real | | |
| Min/max occurences in class | 0 | 1 | |
| Nillable? | yes | | |
| Min/max values | 0 | Unlimited | |

| spectral_sampling_interval_min (a | ttribute) | |
|-----------------------------------|--|--|
| Definition | The spectral_sampling_interval_min element identifies the minimum distance between band centers in a given spectrum. If all band centers are equally spaced, spectral_sampling_interval_min and spectral_sampling_interval_max will have the same value. | |
| PDS4 data type | ASCII_Real | |
| Min/max occurences in class | 0 1 | |
| Nillable? | yes | |
| Min/max values | 0 Unlimited | |

| spectral_sampling_interval_unit (attribute) | | | | |
|---|---|--|--|--|
| Definition | The spectral_sampling_interval_unit element identifies the unit | | | |
| | of measure for the values specified by | | | |
| | spectral_sampling_interval_min and | | | |
| | spectral_sampling_interval_max. | | | |
| PDS4 data type | UTF8_Short_String_Collapsed | | | |
| Min/max occurences in class | 0 1 | | | |
| Nillable? | yes | | | |
| Min/max characters | 1 255 | | | |
| Allowed values | any | | | |

| synthetic_processing_description (attribute) | | | |
|--|--|---|--|
| Definition | The synthetic_processing_description element describes how a | | |
| | synthetic specimen has been processed. | | |
| PDS4 data type | UTF8_Short_String_Collapsed | | |
| Min/max occurences in class | 0 | 1 | |

| Nillable? | no | | |
|--------------------|-----|-----|--|
| Min/max characters | 1 | 255 | |
| Allowed values | any | | |

| synthetic_type (attribute) | | |
|-----------------------------|--|--|
| Definition | The synthetic type element identifies the process by which the | |
| | specimen was produced synthetically. | |
| PDS4 data type | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 0 | 1 |
| Nillable? | no | |
| Allowed values | Entirely Synthetic | The sample is entirely human- |
| | | made. <u>If a mixture, no</u> |
| | | component in the mixture was |
| | | <u>natural.</u> |
| | Natural and Synthetic | The sample is a mixture of |
| | | human-made and naturally |
| | | occurring components. |
| | | RELAB NOTES: An example |
| | | would be a mixture of a |
| | | natural rock sample (e.g., |
| | | shale) and a synthetic orgnic |
| | | compound that was measured |
| | | to understand detection limits |
| | From Not and | of certain organic compounds. |
| | From Natural | A natural product chemically |
| | | or mineralogically altered by a |
| | | laboratory treatment (e.g., heating). Does <u>not</u> include size |
| | | and magnetic separates of |
| | | natural samples or washing by |
| | | water. |
| | | RELAB NOTES: As an example, |
| | | a mixture that is composed of |
| | | several minerals, all of which |
| | | were found in nature, would |
| | | be considered a synthetic |
| | | mixture that is 'From Natural'. |
| | | If one of the components had |
| | | been altered in some way in |
| | | the lab (e.g., heated) then the |
| | | mixture would be considered |
| | | 'Natural and Synthetic'. |
| | Hardware | Portions of an instrument, e.g., |
| | | portions of a spectrometer |
| | | that contribute to a |
| | | spectroscopic signature and |
| | | thus need to be characterized. |

| volatile_type (attribute) | | | |
|-----------------------------|---|--|--|
| Definition | The volatile_type element indicates whether the material was volatile-poor (less than 2.0% LOI) or volatile-rich (greater than 2.0% LOI). | | |
| PDS4 data type | UTF8_Short_String_C | UTF8_Short_String_Collapsed | |
| Min/max occurences in class | 0 | 1 | |
| Nillable? | yes | | |
| Allowed values | Poor | The Poor value indicates the specimen had less than 2.0% LOI. | |
| | Rich | The Rich value indicates the specimen had greater than 2.0% LOI. | |
| | Unknown | The Unknown value indicates the specimen's volatile type is unknown. | |

6 Example

The example below shows the Spectral Library part of a label for an actual product, with attribute and class names in blue text, attribute values in black text, and attribute qualifiers in orange and brown.

```
<?xml version="1.0" encoding="UTF-8"?>
<?xml-model . . . ?>
<?xml-model . . . ?>
<Product Observational . . . >
  <Identification Area>
 </Identification_Area>
  <Observation Area>
    <Discipline Area>
       <speclib:Spectral Library Product>
           <speclib:Specimen Parameters>
               <speclib:specimen id>RM-REM-137/speclib:specimen id>
               <speclib:specimen name>
                    Hisingerite 70080 Gillinge < 45 um</speclib:specimen name>
               <speclib:specimen description>
                    Silicate (Phyllo) , Hisingerite, Vis-NIR and XRD study
                    of clay minerals on Mars (MDAP)
               </speclib:specimen description>
               <speclib:specimen min size unit="micrometer">
                    0</speclib:specimen min size>
               <speclib:specimen max size unit="micrometer">
                    45</speclib:specimen max size>
               <speclib:specimen collection location>
                    Gillinge, Sweden</speclib:specimen collection location>
               <speclib:specimen owner location>
                    Brown University</speclib:specimen owner location>
```

```
<speclib:specimen owner name xsi:nil="true" nilReason="unknown"/>
</speclib:Specimen Parameters>
<speclib:Specimen Classification>
   <speclib:specimen type>Terrestrial Sample/speclib:specimen type>
    <speclib:material origin>Natural</speclib:material origin>
    <speclib:material state>Solid</speclib:material state>
    <speclib:organic_type>Inorganic
   <speclib:material_type>Mineral</speclib:material_type>
   <speclib:material_subtype>Particulate</speclib:material_subtype>
   <speclib:material subtype>
        Particulate Ground Sorted</speclib:material subtype>
   <speclib:mineral type>Phyllosilicate/speclib:mineral type>
</speclib:Specimen Classification>
<speclib:measurement segments>1</speclib:measurement segments>
<speclib:Measurement Parameters>
    <speclib:segment number>1</speclib:segment number>
    <speclib:Measurement Instrument>
       <speclib:instrument name>
            RELAB Bidirectional Spectrometer</speclib:instrument name>
        <Internal Reference>
           <lid reference>
               urn:nasa:pds:context:instrument:facility.bd-vnir.relab
            </lid reference>
            <reference type>is instrument</reference type>
        </Internal Reference>
   </speclib:Measurement Instrument>
   <speclib:measurement type>Reflectance</speclib:measurement type>
   <speclib:spectral range parameter name>
        Wavelength</speclib:spectral range parameter name>
   <speclib:spectral range min>300</speclib:spectral range min>
    <speclib:spectral_range_max>2600</speclib:spectral range max>
   <speclib:spectral_range_unit>nm</speclib:spectral_range_unit>
   <speclib:measurement geometry type>
       Bidirectional</speclib:measurement geometry type>
   <speclib:incidence angle unit="deg">30</speclib:incidence angle>
   <speclib:emission angle unit="deg">30</speclib:emission angle>
   <speclib:phase angle unit="deg">30</speclib:phase angle>
   <speclib:measurement atmosphere relative humidity xsi:nil="true"</pre>
        nilReason="unknown"/>
    <speclib:measurement atmosphere description>
       Ambient</speclib:measurement atmosphere description>
    <speclib:measurement date time>
        2012-12-14</speclib:measurement date time>
   <speclib:data producer name>RELAB</speclib:data producer name>
   <speclib:data provider name>RELAB</speclib:data provider name>
   <speclib:measurement requestor>REM</speclib:measurement requestor>
   <speclib:measurement requestor>RM</speclib:measurement requestor>
</speclib:Measurement Parameters>
<speclib:Ancillary Product>
   <Internal Reference>
        d reference>
         urn:nasa:pds:relab:data ancillary image:RM-REM-137 On9mmDish
       </lid reference>
        <reference type>data to ancillary</reference type>
   </Internal Reference>
    <speclib:ancillary_product_type>
         Image</speclib:ancillary_product_type>
</speclib:Ancillary Product>
```