Description of the ChemCam Passive Surface Spectra PDS Archive

Data Specification

Version 5.0

February 3, 2023

Prepared by:

Jeffrey R. Johnson
Johns Hopkins University Applied Physics Laboratory

Jennifer Ward
PDS Geosciences Node
Washington University

Document Change History

Revision Number	Revision Date	Author	Section	Remarks
1.0	10/30/20	J. Johnson J. Ward	All	Initial version.
2.0	12/1/20	J. Johnson	All	Minor updates; doi numbers included.
3.0	2/3/21	J. Johnson	Table 2	Changed filenames to lower case.
3.0	2/3/21	J. Johnson	Table 2	Included explanations of filename convention using original SIS for reference.
3.0	2/3/21	J. Johnson	Introduction	Added explanation to first paragraph of Introduction regarding 400-840 nm restriction.
3.0	2/3/21	J. Johnson	Section 4	Included explanation of urn:nasa:pds:msl_chemcam_psv_calibrated.
3.0	2/3/21	J. Johnson	Page 1	Added note about 400-840 nm restriction to relative reflectance spectra.
3.0	2/3/21	J. Johnson	Introduction	Included ChemCam resolution from Wiens et al. (2013).
4.0	2/3/22	J. Johnson	All	Updates to archive, covering Sols 2077-2934
4.0	2/3/22	J. Johnson	Section 2.2	Added description of rover elevation to metadata table
4.0	2/3/22	J. Johnson	Table 1	Added rover elevation to metadata table
4.0	2/3/22	J. Johnson	2.3	Added caveat regarding artifacts in relative reflectance spectra during high atmospheric opacity
5.0	2/3/23	J. Johnson	Table 1	Added Formation and Member names (when applicable) to metadata table
5.0	2/3/23	J. Johnson	2.2	Added caveat regarding nature of Formation and Member names for some targets

Table of Contents

1. Introduction

The Mars Science Laboratory (MSL) Chemistry and Camera (ChemCam) instrument relative reflectance spectra data set contains derived data from the CCAM instrument on the MSL rover Curiosity. The Laser-Induced Breakdown Spectrometer (LIBS) portion of ChemCam uses three dispersive spectrometers to cover the ultraviolet (UV; 240-342 nm), blue-violet (VIO; 382-469 nm) and visible/near-infrared (VNIR; 474-906 nm) spectral regions at high spectral (< 1 nm) and spatial (0.65 mrad) resolution. In active LIBS mode, light emitted from a laser-generated plasma is dispersed onto these spectrometers and used to detect elemental emission lines (Wiens et al., 2012; Maurice et al., 2012). Johnson et al. (2015) developed a method to calibrate passive radiance measurements (PSV, acquired without the laser) to relative reflectance spectra (400-840 nm) of rocks, dust, soils, and calibration target surfaces. Because VNIR spectrometer responsivity past ~840 nm and VIO spectrometer responsivity below ~400 nm are relatively low, it recommended to restrict analyses of relative reflectance to 400-840 nm. Resolution of ChemCam is 0.15 nm FWHM between 240 and 342 nm; 0.20 nm between 382 and 469 nm; and 0.65 nm between 474 and 906 nm (Wiens et al., 2013).

As part of a Planetary Data Archiving, Restoration, and Tools (PDART) grant (80NSSC19K0415), the work presented here used PSV files obtained from the existing ChemCam mission archive of the Planetary Data System (PDS) for all surface observations for the first 2,934 sols of the MSL mission (doi:10.17189/1519485). (Atmospheric passive observations were not included in this archive.) These data were calibrated to radiance and relative reflectance using software developed under the same PDART. Also included is a spreadsheet of metadata that describes details of each of the ~33,000 measurements, such as target name, type, and illumination conditions using raw file header information and contextual information from publicly available ChemCam Remote Micro-Imager (RMI; doi: 10.17189/1519494) and MSL Mastcam images, as detailed below. Most of these observations were obtained on rocks (76%) and soils (15%), but also on ChemCam calibration targets (8%), and long-distance observations (>500m; 1%).

This archive was produced using the PDS4 archiving standards. An overview of PDS4 is provided in the PDS4 Concepts document (PDS4 Concepts, 2019), and the standards are specified in the PDS4 Standards Reference (PDS4 Standards Reference, 2019).

2. Data Product Overview

Archived data products comprise three types described in sections 2.1-2.2.

2.1. Data Product Types: ChemCam Spectra

2.1.1. Radiance files

The radiance (RAD) files were produced using the technique described in section 2.3 and represent values of $W/m^2/sr/\mu m$.

2.1.2. Relative reflectance files

The relative reflectance files were created using the technique describe in section 2.3 and represent values of reflectance (0 to 1) relative to that of the sol 76 observation of the white paint on the ChemCam calibration target. Only data between 400 nm and 840 nm are intended for use, with a gap in the region between channels 4077-4110 (~468-477 nm) where the VIO-VNIR detector gap exists.

2.2. Data Product Types: Metadata Table

Because of the large number of passive spectra acquired by ChemCam, it was important to document for each spectrum the instrumental and observation conditions relevant to interpreting specific targets of interest. **Table 1** presents a summary listing of the metadata elements that were collected for each spectrum by using a combination of keyword headers available in the raw data product label files. This includes the Sol number (referred to with the PLANET_DAY_NUMBER keyword), the Sequence Identifier (listed within the file name, e.g., CCAM01076), the LOCAL_TRUE_SOLAR_TIME keyword (LTST), and the instrument temperature (available via the BU_CCD_UV_A keyword in the INSTRUMENT_TEMPERATURE group). The Group keywords designated by the "DERIVED GEOMETRY DATA ELEMENTS: SITE FRAME" contain the instrument and solar azimuth and elevation values, from which the incidence, emission, and phase angle of each spectrum were computed for each spectrum. The distance to the target was recorded in the PSV data products from the PDS, along with the exposure time.

The elevation of the rover during each target acquisition was determined by using the localization tables available from the PLACES Data Products on the PDS, as described in this document: https://pds-imaging.jpl.nasa.gov/data/msl/MSLPLC_1XXX/DOCUMENT/PLACES_PDS_SIS.PDF
Elevation values are referenced to the Mars Observer Laser Altimeter (MOLA) areoid.

The target name, location number within a raster, and determination of laser activity prior to or after passive spectra acquisition made use of the target name list archived in the PDS here: http://pds-geosciences.wustl.edu/msl/msl-m-chemcam-libs-4_5-rdr-v1/mslccm_1xxx/document/msl_ccam_obs.csv

In combination with the above, we used publicly available RMI images, annotated RMI mosaics provided by http:/msl-chemcam.com and/or by the MSL Curiosity Analyst's Notebook (https://an.rsl.wustl.edu/msl/mslbrowser/default.aspx) via the PDS (Stein et al., 2018), and context Mastcam images provided by the PDS to categorize each target type using these classes for Target Type (shot specific):

1) *Sand*
2) *Soil*
3) *Bedrock*
4) *Float rock*
5) *Meteorite (Fe-Ni)*
6) *Vein*
7) *Other Diagenetic features*
8) *Long distance*
9) *Drill tailings*
10) *Drill hole*
11) *Calibration target (with numbered cal target as shown in Johnson et al*. 2015)
12) *Shadow*

By viewing the RMI images acquired nearly simultaneously with the ChemCam passive spectra measurements, each location was also classified regarding whether it was shadowed during acquisition of the spectrum.

The Group, Formation, and Member names represent the rover position at the time of the observation, but not necessarily the correct designation for the specific target. For example, some Float Rocks or Long-distance target designations may not be correct.

Table 1. Metadata table populated for each ChemCam passive spectrum.

Sol	EDR Filename	Type of Product
Target	Sequence	Distance (m)
# of Shots	Shots Averaged	Exposure (msec)
LMST	LTST	Type of Observation
Target Type	Raster Location #	SOLAR ELEVATION (deg)
INSTRUMENT ELEVATION (deg)	INSTRUMENT AZIMUTH (deg)	SOLAR AZIMUTH (deg)
Incidence (deg)	Emission (deg)	Phase (deg)
Inst. Temp (C)	LIBS before or after passive	Atmospheric opacity (t)
Target Type (shot specific)	Rover Elevation (m)	Group, Formation, Member name

2.3. Data Processing

Each ChemCam spectrometer records 2048 spectral channels, thus providing 6144 total channels per observation (Wiens et al., 2012; Maurice et al., 2012). The spectral resolution varies with each spectrometer: 0.15 nm (UV), 0.20 nm (VIO), and 0.61 nm (VNIR). For every LIBS point measurement acquired by ChemCam with its laser, a 3 msec exposure passive ("dark") measurement was acquired without the laser for calibration purposes. As shown by Johnson et al. (2015) these "dark" measurements were of sufficient quality to be used as passive radiance

spectra when acquired on sunlit surfaces. Longer exposure ("dedicated") measurements at 30 msec, 400 msec, and (for data acquired in the first 1,160 sols) 5000 msec were acquired when possible for specific targets of interest to increase the signal to noise ratio (SNR) in each of the three detectors.

Calibration of such measurements to relative reflectance followed procedures similar to those established for field spectroscopy in which a scene radiance spectrum is divided by a calibration target radiance spectrum. We used observations acquired at 3, 30, 400, and 5000 msec exposures on Sol 76 of the white paint of the ChemCam calibration target holder to minimize dark current variations between scene and calibration targets. We converted the PDS raw data (already corrected for wavelength variations as a function of instrument temperature by the ChemCam team) to radiance using the methods described by Johnson et al. (2015), covering the full ChemCam spectral region of 240-905 nm. The required instrument response function for ChemCam is available on the PDS (GAIN_MARS.TAB on http://pds-geosciences.wustl.edu/msl/msl-m-chemcam-libs-4_5-rdr-v1/mslccm_1xxx/document/).

The ratio of the scene and calibration target radiance measurements, multiplied by the known laboratory reflectance of the calibration target material (Wiens et al., 2013), provided an estimate of relative reflectance. Johnson et al. (2015) estimated that the radiance absolute calibration uncertainty was 6-8%. They noted that even with moderate relative reflectance uncertainties (e.g., 20-30%), the band positions and shapes were resilient to calibration errors and ultimately useful in constraining compositions and/or mineral detections.

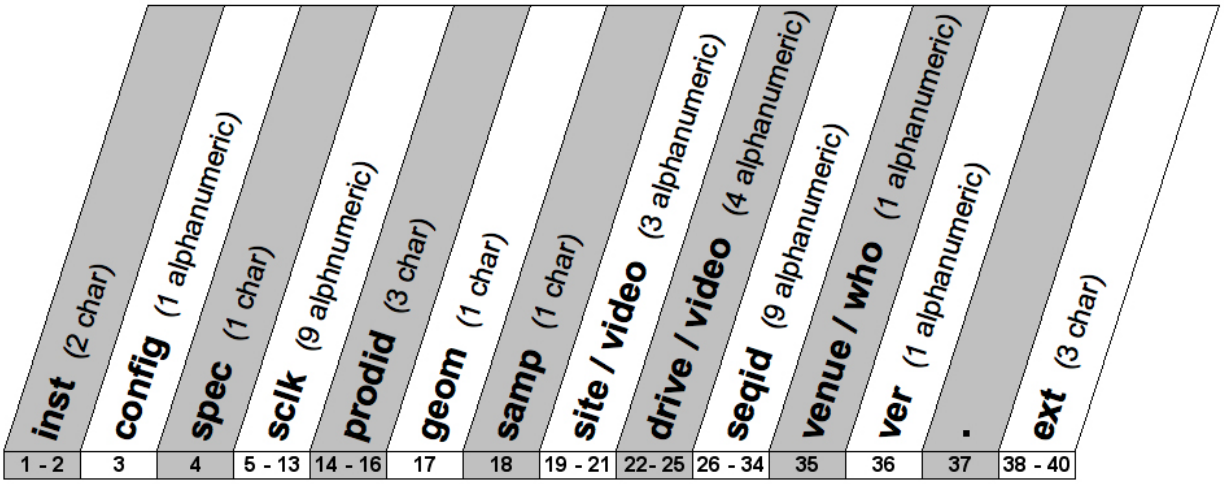
Because the white paint calibration target material has near-zero reflectance at wavelengths <400 nm, the UV spectrometer data cannot be calibrated to relative reflectance using the methods described here. In addition, VNIR spectrometer response past ~840 nm and VIO spectrometer response below ~400 nm are relatively low. As such, typical relative reflectance analyses are most useful in the 400-840 nm region. However, future researchers may find the radiance calibrated UV data valuable.

The temperature of the ChemCam spectrometers also influences the detectors' signal-to-noise ratio. Typical operating temperatures for ChemCam (determined by the "BU_CCD_UV_A" onboard sensor reading listed in the data product header) range from -10° C to 5°C, but can exceed 10°C for late-afternoon observations. At such temperatures, increases in noise can dominate the UV and VIO portion of the spectrum and noticeably affect the VNIR portion of the spectrum at shorter wavelengths. These temperatures have been documented in the metadata described below. RMI images were acquired as part of all ChemCam observations, from which accurate locations for the individual points within a raster were placed (Wiens et al., 2012, 2015; Maurice et al., 2012; Le Mouélic et al., 2015). Comparison to Mastcam M-100 images acquired as part of the ChemCam observations also provided context images for interpreting the passive spectra. The 0.65 mrad FOV of the spectra corresponds to a ~2 mm spot size at an observation distance of 3 m. We used a combination of RMI images available on the PDS and the published RMI mosaics (available on http:/msl-chemcam.com and the MSL Analyst's Notebook) that include accurate annotated raster locations to help determine the metadata described below.

The Sol 76 observation of the white paint on the calibration target holder was acquired when the atmospheric opacity was ~0.71. Users should note that data acquired under vastly different atmospheric opacities (e.g., during dust storms when opacities > 2 occurred) will result in artifacts such as enhanced reddening of the relative reflectance spectra.

3. Data Product Formats

Data that comprise this archive are formatted in accordance with PDS specifications (see References 1-4). This section provides details on the formats used for each of the products included in the archive. Filenames follow the examples shown in Table 2. As per the ChemCam MSL Camera and ChemCam EDR/RDR Data Product SIS (https://pds-geosciences.wustl.edu/msl/msl-m-chemcam-libs-2-edr-v1/mslccm_0xxx/document/msl_camera_sis.pdf), the filename convention follows this scheme:



ChemCam LIBS ("CL")	"**0**" - "**9**"	For ChemCam passive spectra, the types are: 0 = 1-D Average Spectra, no laser 1 = 1-D Single Spectra, no laser 9 = Spectra Stats (all), no laser
underscore	"_"	separator
Spacecraft Clock Start Count, in units of seconds	9 alphanumeric	9 alphanumeric
Product Type identifier	3 characters	PSV = Passive EDR RAD = Radiance REF = Relative reflectance
Geometry type	1 alphanumeric	"_" = Compression mode is for the first instance of the product data processed on the ground
Sample type	1 character	"f" = Full Frame raster data, full resolution
Site location count, from the Rover Motion Counter (RMC)	3 alphanumeric	Range 000 thru 999 – "000", '"001", … "999"
Drive (position-within-Site) location count, from the RMC	4 alphanumeric	Range 0000 thru 9999 – "0000", '"0001", … "9999"
Sequence identifier	9 alphanumeric:	Composed of a 4-char subfield ("ccam") and a 5-digit numeric subfield representing the 6-bit "Category" and 14-bit numeric components of the commanded Sequence ID, respectively

Venue and Product Producer ID	1 character	P = Flight Model Rover; original produced by LANL (Los Alamos, NM)
Version identifier	1 alphanumeric	Range 1 thru 9 – "1", "2", …"9"
Product type extension	3 characters	"tab" = data file "xml" '= xml file "lbl" = label file"

Table 2. File naming convention of output files (example).

Input File (from PDS)	cl9_404236313psv_f0050104ccam01076p3.tab
Output Radiance File	cl9_404236313**rad**_f0050104ccam01076p3.tab
Output Relative Reflectance File	cl9_404236313**ref**_f0050104ccam01076p3.tab

3.1. Spectral Data Format

3.1.1. RAD files

PSV files processed to radiance (RAD files) follow the format of the ingested PSV files, with an embedded header comprising the first 29 lines, followed by 2-column ASCII data representing the wavelength and radiance value (in $W/m^2/sr/\mu m$).

3.1.2 REF files

RAD files processed to relative reflectance (REF files) using the technique described above are 2-column ASCII data representing the wavelength and relative reflectance.

3.1.3 Metadata Table Format

The metadata table is in CSV format. Table 1 shows the headings used.

4. Bundle Organization

This bundle is organized into 4 collections: a data_ref collection, a data_rad collection, a data_table collection, and a document collection. The data collections contain the RAD and REF data products, organized by sol. The metadata table is in a separate data_table collection.

The bundle LID is urn:nasa:pds:msl_chemcam_psv_calibrated, where msl_chemcam_psv_calibrated is the <bundle ID>. The collection LIDs are formed by appending a collection specific ID to the collection's parent bundle LID: urn:nasa:pds<bundle ID>:<collection ID>, e.g. urn:nasa:pds:msl_chemcam_psv_calibrated:data_ref. The product LIDs are formed by appending a product specific ID to the product's parent collection LID: urn:nasa:pds<bundle ID>:<collection ID>:<productID>, e.g. urn:nasa:pds:msl_chemcam_psv_calibrated:data_ref:cl9_490966957ref_f0482470ccam01053p3.

The document collection contains the document you are currently reading.

Each product in the bundle is accompanied by a PDS4 label. PDS4 labels are ASCII text files written in the eXtensible Markup Language (XML). Product labels are detached from the files they describe (with the exception of the Product_Bundle label). There is one label for every

product. A PDS4 label file has the same name as the data product it describes, but always with the extension ".xml".

The information in the PDS4 labels includes complete software-readable descriptions of data file formats, so that users may write custom software to read the products if desired. Data may also be accessed and viewed with the PDS4 viewer available at http://sbndev.astro.umd.edu/wiki/PDS4_Viewer.

Please see References 1-4 for additional information about archive organization, identifiers, and naming conventions in PDS4.

5. References

This Specification references the following documents:

1. Planetary Data System Standards Reference, Version 1.13.0, October 24, 2019.
2. PDS4 Data Dictionary Document, Version 1.13.0.0, September 25, 2019.
3. Planetary Data System (PDS) PDS4 Information Model Specification, Version 1.13.0.0, Sept. 25, 2019.
4. Data Providers' Handbook: Archiving Guide to the PDS4 Data Standards, Version 1.13.0, Oct. 23, 2019.
5. Johnson, J.R., et al., ChemCam Passive Reflectance Spectroscopy of Surface Materials at the Curiosity Landing Site, Mars, Icarus, 249, 74–92, DOI: 10.1016/j.icarus.2014.02.028, 2015.
6. Le Mouélic S., Gasnault O., Herkenhoff K.E., Bridges N.T., Langevin Y., Mangold N., Maurice S., Wiens R.C., Pinet P., Newsom H.E., Deen R.G., Bell III J.F., Johnson J.R., Rapin, W., Barraclough B., Blaney D.L., Deflores L., Maki J., Malin M.C., Pérez R., and Saccoccio M., The ChemCam Remote Micro-Imager at Gale crater : review of the first year of operations on Mars, Icarus, 249, 93-107, 2015.
7. Maurice, S., et al. (2012), The ChemCam instrument suite on the Mars Science Laboratory (MSL) rover: Science objectives and mast unit description, Space Sci. Rev., 170, 95–166, doi:10.1007/s11214-012-9912-2.
8. Stein, T. C., R. E. Arvidson, W. Rapin, K. L. Wagstaff, D. Delapp, R. C. Wiens, and O. Gasnault, PDS Analyst's Notebook: Curiosity ChemCam RMI Mosaic and Mars Target Encyclopedia Integration and Interface Updates, In Lunar and Planetary Science Conference, #1248, 2018.
9. Wiens, R. and 80 others (2012) The ChemCam Instrument Suite on the Mars Science Laboratory (MSL) Rover: Body Unit and Combined System Performance, Space Sci Rev., 170, 167-227.
10. Wiens, R. C., et al. (2013) Pre-flight calibration and initial data processing for the ChemCam laser-induced breakdown spectroscopy instrument on the Mars Science Laboratory rover, Spectrochimica Acta Part B: Atomic Spectroscopy 82, 1-27.
11. Wiens, R.C., S. Maurice, and the MSL Science Team (2015) ChemCam: Chemostratigraphy by the first Mars microprobe, Elements, 11(1):33-38, doi:10.2113/gselements.11.1.33.