

# Origins Spectral Interpretation Resource Identification Security-Regolith Explorer (OSIRIS-REx) Project

## OSIRIS-REx Spectral Processing Derived Data Product Software Interface Specification

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## CM FOREWORD

This document is an OSIRIS-REx Project controlled document. Changes to this document require prior approval of the OSIRIS-REx Configuration Control Board (CCB) and Configuration Management Lead (CML). Proposed changes shall be submitted to the OSIRIS-REx Project CML, along with supportive material justifying the proposed change.

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# OSIRIS-REx Project Spectral Processing Derived Data Product SIS

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DOCUMENT CHANGE LOG

REV/VERSION LEVEL	DESCRIPTION OF CHANGE	APPROVED BY	DATE APPROVED
0.2	Initial SAWG Draft	MKC	12/30/2013
0.3	Draft		
0.4	Changes to processes and data formats		
1.0	Initial Release		07/08/2016
2.0	Update per CR-47		02/26/2019
2.0	Removal of Comments, resolve editorial questions	BEC	02/26/2019
2.0	Ephemeris Time missing in OVIRS L3C, L3E, or L3F, L3G – JY will check on implementation for L3E, L3F, Amy can do L3C?	JYL	02/26/2019
2.0	Reformat of the SPINDEX output file	BEC	02/26/2019
2.0	Clean up Section 5 Table captions. Clean up Section 4 OTEs data tables to be consistent with the SAWG ICD.	BEC, HK	02/26/2019
3.0	Updates to all sections for release of final products to the PDS	MKC	6/16/2023
3.1	Final PDS lien resolution	MKC	5/1/2024

LIST OF TBDs/TDRs

SECTION ID	DESCRIPTION OF TBD/TBR	DATE OF RESOLUTION
4.3.2.5	TBD Table – Binning for Spectral Parameters Maps	06/16/2023
Table 3	Table to be updated spring 2016	06/16/2023
Table 4	TBR Data Volume by Phase	06/16/2023
7.6	Example PDS Labels	01/07/2019

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## 1 Purpose and Scope

The data products described by this Software Interface Specification (SIS) are the OSIRIS-REx spectral processing data products derived from the OSIRIS-REx Thermal Emission Spectrometer (OTES) and the OSIRIS-REx Visible and Infrared Spectrometer (OVIRS). The OSIRIS-REx Science Processing and Operation Center (SPOC) located at the University of Arizona produces these data products in conjunction with the OSIRIS-REx Science Team Spectral Analysis Working Group (SAWG). The SPOC distributes the data products to both the entire OSIRIS-REx Science Team and the Planetary Data System.

The purpose of this document is to provide users of the data products with a detailed description of the product and a description of how it was generated, including data sources and destinations. The document is intended to provide enough information to enable users to read and understand the data products. The users for whom this document is intended are the scientists who will analyze the data, including those associated with the project and those in the general planetary science community.

## 2 Applicable Documents and Constraints

This Data Product SIS is consistent with the following Planetary Data System Documents:

1. Planetary Data System Standards Reference, Version 1.7.0, September 29, 2016.
2. PDS4 Data Dictionary – Abridged – Version 1.7.0.0, September 30, 2016.
3. PDS4 Information Model Specification, V.1.7.0.0, September 29, 2016.

This Data Product SIS is consistent with the following OSIRIS-REx documents:

4. OSIRIS-REx Science Data Management Plan, UA-PLN-9.4.4-004.
5. OSIRIS-REx Science Processing and Operations Center and Planetary Data System Small Bodies Node Interface Control Document, UA-ICD-9.4.4-101, Rev 1.0, October 2013.
6. OSIRIS-REx Science Processing and Operations Center and Spectral Analysis Working Group Interface Control Document UA-ICD-9.4.4-1011.
7. OSIRIS-REx Visual and Infrared Spectrometer (OVIRS) Uncalibrated / Calibrated Data Product Software Interface Specification, UA-SIS-9.4.4-306.
8. OSIRIS-REx Thermal Emission Spectrometer (OTES) Uncalibrated / Calibrated Data Product Software Interface Specification, UA-SIS-9.4.4-304.
9. OSIRIS-REx Map Format Software Interface Specification, UA-SIS-9.4.4-324.
10. OSIRIS-REx Solar Flux Model, UA-HBK-9.4.2-1001

Finally, this SIS is meant to be consistent with the contract negotiated between the OSIRIS-REx Project and the Science Processing and Operations Center.

## 3 Relationships with Other Interfaces

Changes to the data products described in this SIS affect or are affected by the following software, products, or documents:



**Table 1 - Interface Relationships**

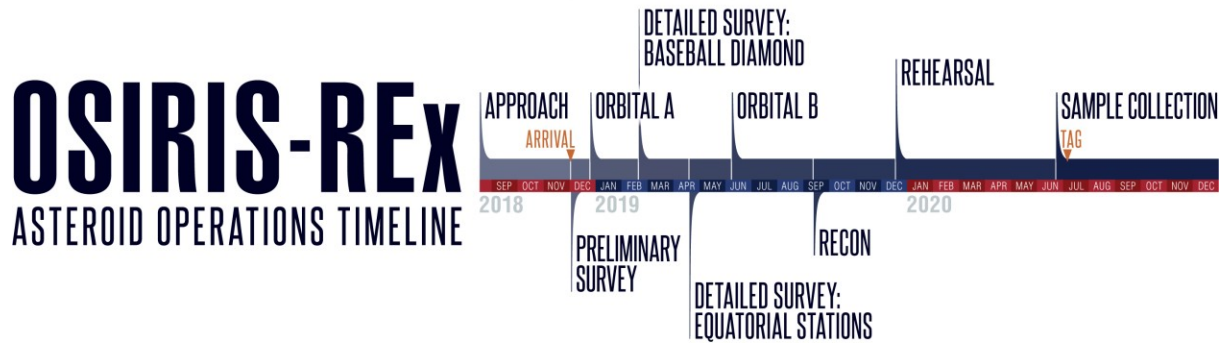
<b>Name</b>	<b>Type</b>	<b>Owner</b>
SPOC Database Schema	Product	SPOC
Rotationally Resolved Spectral Characteristics	Product	SPOC
Spot Emissivity	Product	SPOC
Spot Kinetic Temperature	Product	SPOC
Spot E-T Temperatures	Product	SPOC
Resampled OVIRS Calibrated Radiance Spectra	Product	SPOC
Thermal excess removed OVIRS Spectra	Product	SPOC
Spot I/F spectra	Product	SPOC
Photometrically corrected OVIRS Spectra (REFF)	Product	SPOC
Spot Spectral Indices,	Product	SPOC
Spot Bond Albedo	Product	SPOC
Global and Site-Specific Bond Albedo Maps	Product	SPOC
OTES Calibrated Radiance Spectra	Product	SPOC
OVIRS Calibrated Radiance Spectra	Product	SPOC
SPOC Archive Packager	Software	SPOC
OSIRIS-REx Science Data Management Plan	Document	Project

## **4 Data Product Characteristics and Environment**

### **4.1 Observation Overview**

The data products described in this SIS are Spectral Processing derived data products. These products are derived from the calibrated observational data of the OTES and OVIRS instruments. For information about the calibrated OTES and OVIRS data please refer to Applicable Documents 7 and 8, listed above. OTES and OVIRS data are processed and/or corrected in several ways to yield spectral parameter information for a variety of mineral and chemical species. Data for global data products are acquired during the Detailed Survey mission phase. Data for Site-Specific products are acquired during the Reconnaissance mission phase. The spectral parameter data are used to evaluate the science value of potential sample-sites and to characterize the surface of Bennu. Inferences about the geologic history of Bennu can also be drawn from the spectral parameter maps.

Figure 1. Mission Phases



## 4.2 Data Product Overview

This SIS describes the derived Spectral Processing data products produced for the OSIRIS-REx mission. In general, Spectral Processing data products are produced as either FITS or HDF5 format files with associated header information. Most products are produced at several stages in the mission, with the first release at a lower fidelity, with subsequent releases at higher resolutions. Specific details for each product can be found in Section 5. The data products described in this SIS are:

1. Spot Emissivity – This data product is a set of OTES observation spot temperatures and emissivity spectra (as a function of wavenumber) derived from emissivity-temperature separation. The spot temperatures calculated here have a dependence on the blackbody information chosen during temperature/emissivity separation.
2. Spot Kinetic Temperatures – This data product is a set of single OTES observation spot temperature values. These temperature values do not have blackbody model dependence.
3. Resampled Spectra – This data product is a set of OVIRS spot radiance spectra that have been resampled to a common energy scale.
4. I/F Spectra – This data product is a set of OVIRS spot radiance spectra that have had thermal emission removed, and that have been divided by the spectral Solar irradiance for conversion to units of Radiance Factor (RADF or I/F).
5. Site-Specific Spectral Parameter Maps – This data product is a map of a specific spectral parameter referenced to a potential sample site topographic map.
6. Global Spectral Parameter Maps – This data product is a global map of a specific spectral parameter referenced to the asteroid shape model.

## 4.3 Data Processing

All OSIRIS-REx mission science data processing is performed at the University of Arizona Science Processing and Operations Center (SPOC). OTES and OVIRS science and housekeeping telemetry are received by the SPOC via the Lockheed Martin Mission Support Area and the Deep Space Network. Telemetry data are reconstructed and stored in the SPOC data repository. Raw data (OREx Level 0) are retrieved from the data repository and fed into the OTES- and OVIRS-specific data processing pipelines. The pipelines produce calibrated

OTES and OVIRS spectral and housekeeping data products. Generally, OTES spectra are stored in binary table format, OVIRS spectra are stored in FITS file format, and housekeeping in a binary table format. Production rates of spectra vary over the course of the mission based on specific science goals of each mission phase. Spectral Processing uses calibrated OTES and OVIRS radiance data to derive emissivity, temperature, thermal-excess removed radiance, I/F, photometrically-corrected reflectance, and spectral slope or band strength of the surface of Bennu.

### 4.3.1 Data Processing Level

Table 2 shows the OSIRIS-REx data processing levels of all science data products described by this SIS. Correlation to NASA and CODMAC data processing levels and definitions can be found in Appendix 7.2.

**Table 2. Data Processing Levels**

Spectral Processing Product	NASA Product Level	OSIRIS-REx Processing Level	Description
OTES Spot Emissivity	Level - 5	L3	Emissivity spectrum of individual OTES observation
OTES Spot Temperatures	Level - 5	L3	Temperatures fit to individual OTES observations in the course of emissivity-temperature separation.
OTES Spot Kinetic Temperature	Level - 5	L3	Temperature calculated from individual OTES observations.
OVIRS Spot Resampled Radiance	Level - 5	L3	OVIRS Spot calibrated radiance resampled on to a standard sampling axis.
OVIRS Spot I/F	Level - 5	L3	Thermal tail removed, solar flux calibrated OVIRS spectra, in units of Radiance Factor, RADF = I/F.
Site-Specific Spectral Parameter Maps	Level - 5	L4	Spectral parameter maps of potential sample sites
Global Spectral Parameter Maps	Level - 5	L4	Spectral parameter maps of the surface of Bennu

### 4.3.2 Data Product Generation

As mentioned previously, all OSIRIS-REx science data processing is completed at the SPOC located at the University of Arizona. The decision was made early in the mission lifecycle that all processing would be centralized to facilitate the relatively quick turn-around needed by the science and operations teams to make tactical decisions about sample site selection.

#### 4.3.2.1 OTES Spot Emissivity and Temperature

Because the field of view (FOV) of each OTES observation includes surfaces with different temperatures, the OTES radiance spectra are really weighted mixtures of the radiance emitted from those surfaces. To determine the thermal infrared emissivity of the surface within each spot, the temperature component of the measured radiance must be removed by model the blackbody emission from the mixture of temperatures within the field of view and dividing it out of the measured radiance. The approach used with OTES data fits a mixture of blackbody radiance functions to each calibrated radiance spectrum using a linear least-squares methodology similar to that documented and widely used for spectral mixture analyses of emissivity spectra [e.g. *Ramsey and Christensen, 1998; Rogers and Aharonson, 2008*].

This approach uses weighted mixtures of Planck functions with two basic assumptions: 1) the emitted radiance is the linear summation of the radiances from each temperature component, weighted by the fraction of the OTES FOV covered by that component; and 2) the absorption features are shallow and narrow relative to the broad shape of the Planck functions and do not significantly affect the Planck function fits. OTES radiance spectra of Bennu were fit using a library of Planck functions for temperatures of 100-440 K in 10 K increments. Prior to fitting, the data were filtered using a variable-width filter whose kernel increased with increasing instrument noise and varied in width from 1 to 11 spectral samples. This method reduces the radiometric noise at the extreme wavenumber ends of the spectra where the signal is low but preserving the spectral information in regions where the signal-to-noise ratio is high. The spectral fits were performed over the spectral range from 100-1700  $\text{cm}^{-1}$ . Extending the wavenumber range or not filtering the data results in the tendency for the fitting algorithm to include extreme high or low temperature components to better fit spectral regions where the signal-to-noise ratio is low. For determining the asteroid emissivity and composition an exact determination of the spectral radiance is unnecessary – all that is required is that an appropriate blackbody radiance spectrum can be computed, regardless of the exact temperature and abundance of each component.

The emissivity-temperature separation algorithm described above is applied to OTES calibrated radiance spectra and results in an emissivity spectrum (emissivity vs. wavenumber, where emissivity is a unitless quantity ranging from 0-1) and a set of up to five temperature values required to fit the calibrated radiance. Each OTES calibrated radiance spectrum is divided by the best-fit mixed-temperature radiance spectrum to yield the emissivity spectrum. The fitted temperatures and their abundances are recorded in the `mt_temp` and `mt_tconc` elements of the HDF structure.

The emissivity-temperature separation algorithm (`mt_emissivity`) processing includes:

1. Reading the OTES calibrated radiance spectra into Davinci (<http://davinci.asu.edu/>)
2. Running Davinci routine `mt_emissivity()` using OTES calibrated radiance spectra as input; options include (not a comprehensive listing):
  - filter size for determining maximum brightness temperature
  - optional maximum emissivity (e.g., 0.95 instead of default of 0.97)
  - optional starting wavenumber for brightness temperature calculation
  - optional ending wavenumber for brightness temperature calculation

3. Save output HDF5 structure containing identifying information for input calibrated radiance spectrum and wavenumber axis, derived temperatures and their fractional contributions to the fit, the emissivity spectra, optional parameter values, and ancillary geometric information.

The HDF5 output is ingested into the SPOC Data Repository to ensure access by the entire OSIRIS-REx Science Team. The Spectral Analysis Working Group uses spot emissivity spectra as inputs to derive mineral and chemical abundances on the surface of Bennu.

#### **4.3.2.2 OVIRS Spot Resampled Calibrated Radiance Spectra**

Before the OVIRS calibrated radiance spectra (OVIRS L2 science data product) are used for further scientific processing, they will be "resampled" onto a standard sampling axis such that each channel of the OVIRS spectra will have a fixed position in the wavelength dimension. The OVIRS Calibrated Radiance spectra will be resampled at 2-nm spacing from 0.392 to 2.4 microns and 5-nm spacing from 2.4 - 4.34 microns, as defined by the SAWG. The product is a spectrum with radiance units of  $W/cm^2/\mu m/sr$  per spectral element. The resampling is achieved using a weighted average for each level 2 pixel's wavelength from the bin center. The resultant spectra are stored (see Section 5.2.5) as double precision floating-point arrays of 1393 x 3 elements (radiance, uncertainty, quality flag) x N (number of spectra, where N is determined by the processing implemented by the SPOC) as the first header data unit (HDU, also commonly called an extension) of a FITS file. The second HDU is a 1-dimensional array of 1393-elements that contains the standard wavelength axis as described above. For additional information on the OVIRS instrument and/or the OVIRS Calibrated Radiance Spectra please see the OVIRS instrument paper (Reuter et al., 2018, <https://doi.org/10.1007/s11214-018-0482-9>) or the OVIRS SIS (<urn:nasa:pds:orex.ovirs:document:ovirsis>)

#### **4.3.2.3 I/F OVIRS Spectra**

The OVIRS I/F algorithm is applied to OVIRS calibrated radiance spectra to obtain the surface reflectance, scaled to account for the solar flux as a function of distance to Bennu. The first step in this process is to "resample" the OVIRS calibrated radiance spectra onto a standard wavelength axis (as described above).

The next step in processing is thermal-tail removal. OVIRS radiance spectra include contributions from both reflected solar radiation and emitted thermal radiation. At any temperature expected for Bennu, the thermal component is negligible for wavelengths shorter than 2 microns. For these wavelengths valid reflectance comparisons among observations may be obtained using the directly observed calibrated OVIRS data. To compare reflectance spectra of observations of surface regions having differing temperatures at longer wavelengths, it is desirable to use calibrated OVIRS spectra with the thermal component removed. The thermal tail removal relies on the OTES-derived surface temperature at the time and location of the OVIRS measurement to determine the radiance contribution from thermal emission that must be subtracted from the OVIRS spectrum. The surface reflectance is then obtained as the ratio of the OVIRS resampled, thermal-tail removed, calibrated radiance spectrum to the standard solar radiance spectrum being used by the OSIRIS-REx

mission (See Appendix 7.3). The solar radiance spectrum will be convolved with the OVIRS spectral instrument function at each OVIRS wavelength.

To remove the thermal tail, the following procedure is used:

1. Read in the one-dimensional OVIRS radiance spectrum and surface temperature from a corresponding OTES measurement.
2. Calculate the Planck function ( $W/m^2/nm$ ) at OVIRS wavelengths using the OTES-derived spot kinetic temperature.
3. Perform chi-squared minimization of the Planck function to best match the vertical scaling of the OVIRS spectrum and the observed thermal excess.
4. Subtract thermal flux from OVIRS spectra to leave only the reflectance component of the OVIRS spectrum.
5. Save outputs of (1) OVIRS spectrum with the thermal excess removed and (2) calculated thermal contribution as extensions to the OVIRS calibrated radiance spectra FITS file. Add thermal excess removal method and an OTES spectrum identifier with temperature to the FITS header of the output spectrum with thermal excess removed. Uncertainties calculated in this operation are stored as an extension in the FITS file.

Once the thermal tail is removed from the OVIRS Spectrum, the I/F calculation is performed as follows:

1. Read in OVIRS thermal-tail removed calibrated radiance spectra.
2. Run IDL routine I/F using selected OVIRS radiance spectra as input
  - a. Divide the OVIRS radiance spectrum by the solar flux spectrum corrected for distance.
3. Save output spectrum as an extension to the OVIRS FITS file with I/F reflectance spectrum with optional parameter values, and ancillary geometric information updated in the FITS header. Filenames will follow established SPOC convention.

The Spectral Analysis Working Group uses the resulting OVIRS I/F spectra as inputs to the photometric modeling and photometric correction, and ultimately for the spectral index comparisons made with a program named “Spindex”, described in Kaplan et al., 2020 (<https://doi.org/10.1111/maps.13461>).

#### **4.3.2.4 Global and Site-Specific Spectral Parameters**

Global and Site-Specific Spectral Parameter maps are the numerical display of the spatial distribution of spectral features of interested identified on the surface of Bennu. These maps are derived from binned and averaged values obtained from parameterized OTES emissivity and OVIRS photometrically corrected reflectance spectra.

OTES spot emissivity and OVIRS spot photometrically corrected reflectance spectra are retrieved from the SPOC. The generation of OTES specific spectral parameters and map products is described in detail in Hamilton et al. 2021, <https://doi.org/10.1051/0004->

6361/202039728. The parameters were developed during OTES data analysis to highlight specific spectral features of interest. OVIRS spectral parameters for minerals and chemicals also are obtained using spectral parameter calculations. The spectral parameter algorithms for OVIRS data analysis are written in IDL and are based primarily on indices defined in the visible and near infrared spectroscopy literature. The OSIRIS-REx geometric projection software produces longitude, latitude, and radius data for each spot observation. Spot abundances of minerals and chemicals or spectral parameter values are tabulated for each observation sequence. The size of the data product will depend on the number of spectra in each observation sequence. The generation of OVIRS spectral indices are described in Kaplan et al. 2020, <https://doi.org/10.1111/maps.13461>. The generation of OVIRS map products is described in Simon et al., 2020, <https://doi.org/10.1051/0004-6361/202039688>.

Mineral and chemical maps are produced by processing OTES and OVIRS spot values for the abundance and/or parameter strength of each mineral or chemical (along with appropriate uncertainties) by binning and/or averaging individual abundances or parameter strengths, and uncertainties using pre-computed longitude and latitude values (or shape model facet (plate) numbers) for each spot observation. Per spectra geometry is calculated using standard SPICE processes and included in calibrated data product metadata. Maps are produced for the species of interest identified in

Table 3. The method of map production is similar for all maps. For global maps, a project-approved triangular facet shape model file defining the shape of the asteroid Bennu has been provided to the spectral processing group. The calculation of the shape model is documented in the Altimetry SIS, and can also be found in Seabrook *et al.*, 2022, *Planet. Sci. J.* **3** 265, DOI 10.3847/PSJ/aca011. The specific shape model used for each map produced is indicated in the Shape\_Data\_Source metadata class in the product label obj\_file attribute. The obj files are (will be) archived in the OSIRIS-REx Altimetry archive bundle.

The spectral data are registered to the shape model. Multiple spectral observations that fall in a single shape model facet are combined to yield a single value and associated error term. These values are recorded in an Ancillary Map Data FITS File (see Applicable Document 9), containing an ASCII table with columns for facet number, center latitude, center longitude, center radius, map value, and error of the species of interest. A similar process is used for site-specific or local maps. Again, individual spot data are combined resulting in an Ancillary Map Data FITS File for the species of interest. The format of map products is described in Section 5.2.10.

Each map is also accompanied by a test file names similarly to the map that contains the spacecraft clock (sclk) string, value (band depth) and error value for each observation included in the mapped data product. These observations are mapped to shape model facets using the Make Maps algorithm described by Ferrone et al., 2021, <https://doi.org/10.1029/2019EA000613>. Observations mapped to the same shape model facet are combined using the algorithm specified in the maps\_readme files but are most likely combined using a weighted average. Observations to be included in the map product are chosen using criteria identified in the maps\_readme files. The combination of the individual observations on to the shape model facets results in a single index value for each shape model facet.

A summary of species of interest for Global and Site-Specific Mapping are tabulated below:

**Table 3. Band Depths of Interest**

TIR	
Band Depth / Index Name	Description
R987/814	The ratio of the emissivity at 987 $\text{cm}^{-1}$ to that at 814 $\text{cm}^{-1}$ , defined as the average of OTES (level 3 x-axis) channels [113:115] divided by the average of channels [93:95].
BD440	Band depth at $\sim 440 \text{ cm}^{-1}$ , defined as the average emissivity of OTES channels [60:62] plus the average emissivity of OTES channels [43:45] divided by two, divided by the average emissivity in channels [50:51].
BD350	Band depth at $\sim 350 \text{ cm}^{-1}$ , defined as the average emissivity of OTES channels [34:35] plus the average emissivity of OTES channels [44:45] divided by two, divided by the average emissivity in channels [40:41].
VNIR	
BandArea3200to3600nm	Absorption area between 3200 and 3600 nm (3.2 and 3.6 microns) diagnostic of carbonates and/or organics, calculated on un-ratioed spectra
OH2700nm	Hydration feature band depth at 2740 nm (2.74 microns) with continuum points at 2.6 and 3 microns calculated on un-ratioed spectra.
Pyroxene920nm	Band depth at 920 nm (0.92 microns) with continuum points at 0.807 and 0.984 microns calculated on spectra ratioed to a global average spectrum.
Ref1550nm	The reflectance (I/F) at 550 nm (0.55 microns) calculated on un-ratioed, pipeline values from spindex
Slope1polyfit	Polynomial (1st order) fit to the spectrum between 0.5 and 1.5 microns calculated on spectra ratioed to a global average spectrum using a stand-alone version of spindex.
Slope2polyfit	Polynomial (1st order) fit to the spectrum between 1.0 and 2.2 microns calculated on spectra ratioed to a global average spectrum using a stand-alone version of spindex.

### 4.3.3 Data Flow

Spectral Analysis data products are derived from input data products stored in the SPOC data repository. Input products such as the Bennu shape model, OTES calibrated spectral radiance, and OVIRS calibrated spectral radiance are retrieved from the SPOC data repository and fed into the Spectral Processing data processing algorithms. Data products are produced and returned to the SPOC data repository for storage and retrieval by the rest of the



OSIRIS-REx Science Team. Specifics of each data processing algorithm are discussed in Section 4.3.2.

#### 4.3.4 Labeling and Identification

OSIRIS-REx science data products are named according to the OSIRIS-REx Naming Conventions Document (UA-HBK-9.4.4-905). The following paragraphs are excerpts of this document that describe how Spectral Processing files are named. The generalized file naming convention is:

Coverage Type “\_” + “\_” Ground Sample Distance+ “mm”+ “\_” + SDP Area + “\_” + Description + “\_” + “Center Location”+ “\_” + “v” + Version + “.” + PDS Type

Coverage Type is either G for Global or L for Local.

The Ground Sample Distance (Resolution) is expressed in millimeters plus the appended units indicator of "mm". For example, a 1000mm global map at the equator (since it's an Equirectangular map) will be: g\_1000mm

The SDP Area is one of:

ALT = Altimetry – OSIRIS- REx Laser Altimeter

AST = Astronomy

IP = Image Processing

RD = Regolith Development

RS = Radio Science

SP = Spectral Processing

SPC = Altimetry – Stereophotoclinometry

SPO = Altimetry – Stereophotoclinometry and OSIRIS-REx Laser Altimetry

SS = Sample Site

TA = Thermal Analysis

Description gives SPOC Global Specification identifier for the product type. This is a free form field that may give instrument, mission phase, product (map) type or other information,

Center Location is an optional name component that describes latitude and longitude in the center location of the data product. The format is “LatitudeLongitude”, where latitude is 4 digits and longitude is 5 digits.

Version is a three-character version identifier.

An example of a named product that holds a global map of the would be:

l\_1600mm\_sp\_ovirs\_reca\_refl550nm\_allsites\_wavc\_0000n00000

### 4.4 Standards Used in Generating Data Products

#### 4.4.1 PDS Standards

All data products described in this SIS conform to PDS4 standards as described in the PDS Standards document noted in the Applicable Documents section of this SIS. Prior to public

release, all data products will have passed both a data product format PDS peer review and a pre-release PDS peer review to ensure compliance with applicable standards.

#### **4.4.2 Time Standards**

Time Standards used by the OSIRIS-REx mission conform to PDS time standards. The spacecraft clock (SCLK) reference is 1/1/2000 12:00:00 UTC, with a minimum range date from 1/1/2010 to 1/1/2030. Onboard time tagging is the standard 32-bit seconds and 16-bit subseconds. OSIRIS-REx data products contain both the spacecraft clock time of data acquisition and a conversion to UTC to facilitate comparison of data products. All spatial quantities are derived from mid-observation time in UTC. In the case of TAGCAMS spacecraft clock time is given at the start of the acquisition. Data may also contain Ephemeris Time (ET) and/or Ground Receive Time (GRT) to facilitate processing.

#### **4.4.3 Coordinate Systems**

All coordinate systems used by the OSIRIS-REx mission conform to IAU standards. A complete discussion of the coordinate systems and how they are deployed in the mission can be found in the document “OSIRIS-REx Coordinate System Plan” found in the archive documents collection.

#### **4.4.4 Data Storage Conventions**

Data is stored according to the FITS 3.0 standard, or the HDF5 standard.

### **4.5 Data Validation**

The SPOC has a comprehensive Verification and Validation Plan for all software used at or developed by the SPOC. All software is configuration controlled and any changes made follow the SPOC Configuration Control Plan, which includes substantive testing of changes. During day-to-day production of L0 data products from telemetry, check sums and spot checks are used to validate that software is producing data products correctly.

In addition to software types of verification and validation, each OSIRIS-REx data product has been peer reviewed for both PDS data format acceptability and scientific usefulness. No changes are expected to data formats after peer review. The SPOC Configuration Control Plan governs any changes, should they be needed.

## **5 Detailed Data Product Specifications**

The following sections provide detailed data product specifications for each Spectral Processing derived data product. These specifications provide sufficient detail, so that data product users can read and interpret the products.

### **5.1 Data Product Structure and Organization**

The OSIRIS-REx archive is organized into bundles for each detector (OCAMS, OTES, OVIRS, OLA, REXIS), TAGSAM, SPICE, and higher-order data products. The higher-order data products are bundled by scientific working groups. These bundles include Astrometry, Altimetry, Image Processing, Spectral Processing, Radio Science, and Thermal Analysis.

Each higher-order bundle contains data and document collections, with the possibility that some bundles may contain a calibration or geometry collection. Within the data collections, data products are divided into sub-directories for each mission phase in which data was collected.

Spectral Processing (note: we use spectral processing and spectral analysis interchangeably to mean the data products produced for analysis by the Spectral Analysis Working Group) derived data products are natively formatted either as FITS files with associated header information or as HDF5 files. However, both FITS and HDF5 products are labeled according to PDS4 standards, which allow access to the data within the products in a generic way. As instrument observations are planned to support sample site selection and sample collection activities, not all instruments collect data in all mission phases. In turn, not all mission processing elements produce derived data products in all mission phases. In these cases, there will be no data products for that processing element assigned to the mission phase.

The bundle/collection organization for the Spectral Analysis bundle is as follows:

- SAWG Bundle – urn:nasa:pds:orex.spectral\_analysis
  - Document collection - urn:nasa:pds:orex.spectral\_analysis:document
  - Resampled spectra collection -  
urn:nasa:pds:orex.spectral\_analysis:data\_vnir\_resampled\_spectra
  - IOF spectra collection -  
urn:nasa:pds:orex.spectral\_analysis:data\_vnir\_iof\_spectra
  - Temperature/emissivity collection -  
urn:nasa:pds:orex.spectral\_analysis:data\_tir\_tmp\_emissivity
  - OVIRS band depth maps collection -  
urn:nasa:pds:orex.spectral\_analysis:data\_vnir\_maps
  - OTES band depth maps collection -  
urn:nasa:pds:orex.spectral\_analysis:data\_tir\_maps

## **5.2 Data Format Descriptions**

The following sections specify the exact file formats for each of the Spectral Processing data product types.

### **5.2.1 OTES Spot Temperature and Emissivity**

The spot temperature and emissivity data products are natively formatted as an HDF5 file containing 17 data elements. This file can be read by any HDF5 reader or API, or data can be accessed using the detached PDS4 label that describes the 17 array, numeric, or text type data element within the file. Note that the order of the elements is listed by byte-offset in the PDS4 label and in the table below, however an HDF5 reader may display the arrays in alternate order (e.g. alphabetical).

Table 4. Spot Temperature/Emissivity

<b>Structure #</b>	<b>Structure</b>	<b>Description</b>
1	Sclk – array of observation times	Spacecraft clock time at the start of an OTES mirror scan (seconds )
2	Sclk_sub – array of observation times	Sub-second part of sclk. Each count represents 1/(2 <sup>16</sup> ) seconds
3	Quality- array of observation quality flags	0 - Space observations spaced less than 400 seconds apart 1 - Space observations spaced more than 400 seconds but less than 800 apart 2 - Space observations spaced more than 800 seconds apart 3 - No space observations in the sequence
4	kinetic_temp – array of observation kinetic temperatures	The effective kinetic temperature of the surface derived from the brightness temperature spectrum.
5	kinetic_temp_uncertainty – array of observation kinetic temperature uncertainties.	Uncertainty value associated with derived kinetic_temp.
6	total_temperature_uncertainty – array of observation total temperature uncertainties	Root sum of squares uncertainty of brightness temperature and kinetic temperature uncertainties.
7	kinetic_temp_wave – array of observation kinetic temperature wave numbers.	The wavenumber at which the kinetic_temp was identified.
8	ot_emissivity_version – array of observation version numbers.	OTES temperature emissivity separation software version number.
9	mt_temp – 2d array of temperature x observation	The temperature(s) used in the E-T fit and separation (up to five per spectrum)
10	mt_tconc -2d array of temperature fraction x observation	The fraction of each Multi-Temperature contribution to the modeled radiance.
11	mt_emissivity – 2d array of emissivity spectrum x observation	The emissivity spectra obtained from the multiple-temperature fits to the measured spot calibrated radiances (unitless).
12	xaxis_L3 – 208 element array of wavenumbers.	The x-axis wavenumbers of the emissivity spectrum.
13	sma_version - array of software version numbers	spectral mixing algorithm (sma) software version (in Davinci software) number for each observation.
14	sma_algorithm – text stream	Description of the sma (spectral mixing algorithm) type used – always non-negative least squares
15	max_emiss – array of observation maximum emissivities	The maximum emissivity assumed in fitting the measured calibrated radiance.

<i>Structure #</i>	<i>Structure</i>	<i>Description</i>
16	tes_wavel – array of wavenumbers	Starting wavenumber for emissivity calculation.
17	tes_wave2 – array of wavenumbers	Ending wavenumber for emissivity calculation.

## 5.2.2 OVIRS Spot Resampled Calibrated Radiance Spectra

The OVIRS resampled calibrated radiance spectra are formatted as a spectrum with radiance units of W/cm<sup>2</sup>/μm/sr per spectral element. The spectra are stored as double precision floating-point arrays of 1393 x 3 elements (radiance, uncertainty, quality flag) x N (number of spectra, where N is determined by the processing implemented by the SPOC) as the first header data unit (HDU, also commonly called an extension) of a FITS file. The second HDU is a 1-dimensional array of 1393 elements that contains the wavelength axis.

**Table 5. OVIRS Resampled Calibrated Radiance**

Attribute Name	FITS Keyword	Units	Description
element_array.data_type	BITPIX		number of bits per data pixel
axes	NAXIS		number of data axes in array
axis_array.sequence_number	NAXIS1		Length of FITS data axis 1 equivalent to sample. Detector pixels (512)
axis_array.sequence_number	NAXIS2		Length of FITS data axis 2 equivalent to line. Number of lines in ROI
axis_array.sequence_number	NAXIS3		Length of FITS data axis 3 equivalent to frames. Number of frames in observation sequence. If absent, the array is a 2d-array representing a single frame's data.
n/a - FITS specific	EXTEND		FITS dataset may contain extensions
element_array.value_offset	BZERO		offset data range to that of unsigned short
element_array.scaling_factor	BSCALE		default scaling factor
investigation_area.name	MISSION		Mission name: OSIRIS-REx
observing_system.name	HOSTNAME		Spacecraft hostname
observing_system.component.name	INSTRUME		Instrument name: OSIRIS-REx OVIRS
mission_area.utc	DATE_OBS		The UTC time of the instrument clock on readout
mission_area.mid_obs	MIDOBS		Spacecraft mid-exposure time, UTC [Cal d] (DATE_OBS - .5*EXPTIME).
mission_area.expo_ms	EXPTIME	ms	Exposure time in milliseconds
mission_area.exposure	EXPOSEC	s	Exposure time in seconds
mission_area.mid_obs_et	ET		The ephemeris time of the mid-exposure time, mid_obs
mission_area.mid_obs_sclk	MID_SCLK		The SCLK string of the mid-exposure time, mid_obs
mission_area.bore_flag	BS_FLAG		Boresight flag: 0-Boresight does not intersect surface of asteroid; 1-Boresight intersects surface of asteroid

Attribute Name	FITS Keyword	Units	Description
mission_area.fov_fill_flag	FOV_FLAG		Field of view flag: 0-Entire FOV images empty space; 1-Entire FOV image s asteroid surface; 2-Portion of FOV images empty space
mission_area.bore_angle	BS_ANGLE	deg	Angle between boresight and origin of Bennu in planetocentric Cartesian coordinates
mission_area.latitude	LAT	deg	Planetocentric latitude of boresight intersection with the surface. Allowed range +90.0 to -90.0. If Boresight Flag is not equal to 1, then value shall be -9999.
mission_area.longitude	LON	deg	Planetocentric longitude of boresight intersection with the surface. Allowed range 0 to 360. If Boresight Flag is not equal to 1, then value shall be -9999.
mission_area.boresight_range	RANGE	km	Range from spacecraft to the closest boresight intersection to spacecraft. Must be positive number. If Boresight Flag is not equal to 1, then value shall be -9999.
mission_area.boresight_x	BS_X	km	X coordinate of boresight intersection with surface in planetocentric Cartesian coordinates. Allowed range 0 to 1000.0. If Boresight Flag is not equal to 1, then value shall be -9999.
mission_area.boresight_y	BS_Y	km	Y coordinate of boresight intersection with surface in planetocentric Cartesian coordinates. Allowed range 0 to 1000.0. If Boresight Flag is not equal to 1, then value shall be -9999.
mission_area.boresight_z	BS_Z	km	Z coordinate of boresight intersection with surface in planetocentric Cartesian coordinates. Allowed range 0 to 1000.0. If Boresight Flag is not equal to 1, then value shall be -9999.
mission_area.incidence_angle	INCIDANG	deg	Incidence angle. The angle between the vector normal to the surface at the location of the boresight intersection with the surface and the vector pointing at the Sun. If Boresight Flag is not equal to 1, then value shall be -9999. Allowed range is 0.0 to 90.0
mission_area.emission_angle	EMISSANG	deg	Emission angle. The angle between the vector normal to the surface at the location of the boresight intersection with the surface and the vector pointing to the Spacecraft. If Boresight Flag NE 1, then value shall be -9999. Allowed range is 0.0 to 90.0
mission_area.phase_angle	PHASEANG	deg	Phase Angle. The angle between the vector pointing to the Sun and the vector pointing to the Spacecraft. If Boresight Flag is not equal to 1, then value shall be -9999. Allowed range is 0.0 to 180.0

Attribute Name	FITS Keyword	Units	Description
mission_area.fov_fill_factor	FILL_FAC	frac	Fill Factor. If FOV Flag = 2, describes the fraction of the FOV that intersects the asteroid surface. If FOV Flag = 0, value shall be 0.0. If FOV Flag = 1, value shall be 1.0. Allowed range is 0.0 to 1.0
mission_area.semimajor axis	SMJAX	m	Semi-major axis of FOV ellipse on surface
mission_area.semiminor axis	SMNAX	m	Semi-minor axis of FOV ellipse on surface
mission_area.sun_range	SUN RNG	km	Range from Sun to center of target body
mission_area.target_range	TRGTRNG	km	Range from S/C to target body center
mission_area.right_ascension	RA	deg	Boresight Right Ascension (RA) in J2000 frame.
mission_area.declination	DEC	deg	Boresight Declination (DEC) in J2000 frame
mission_area.bennu_ra	BENNURA	deg	Right Ascension of the vector, expressed in the Earth Mean Equator of the J2000 Epoch, from the ORX spacecraft toward the target named in FITS keyword BENNURDT (typically Bennu); see also BENNURDQ for a statement of the quality of this value
mission_area.bennu_dec	BENNUDEC	deg	Declination of the vector, expressed in the Earth Mean Equator of the J2000 Epoch, from the ORX spacecraft toward the target named in FITS keyword BENNURDT (typically Bennu); see also BENNURDQ for a statement of the quality of this value
mission_area.bennu_radec_target	BENNURDT		Target for the BENNURA, BENNUDEC, BENNUNX1 and BENNUNX2 FITS keywords; typically BENNU; may be NONE if the calculation failed. Target is not required to be in the field of view.
mission_area.bennu_radec_quality	BENNURDQ		(Quality: provenance) for the BENNURA, BENNUDEC, BENNUNX1, BENNUNX2 FITS keywords. This will be one of three values: (BEST: SPK), meaning the geometry was obtained from SPICE SP-Kernels; (POOR: osculating elements; +/- 1E6km), meaning the geometry was obtained from osculating orbital elements of Bennu w.r.t the Sun, and will have uncertainties of order 1E6km; (NONE: FAILURE), meaning both the SPK and elements methods failed; the parentheses, (), are only delimiters here and not part of the quality:provenance values.
array_2d_resampled_radiance			Array: Plane 1 of FITS 3d array, resampled calibrated radiance values of frame
array_2d.uncertainty			Array: Plane 2 of FITS 3d array, Uncertainty of the resampled radiance value.
array_2d.quality			Array: Plane 3 of FITS 3d array, quality indicator of the resampled calibrated frame.
array_2d.wavelen			Array: Wavelengths of the resampled cube

### 5.2.3 I/F OVIRS Spectra

Resampled, thermal-tail removed, OVIRS calibrated radiance spectra are divided by the range-corrected reference solar flux (see Appendix 7.3) to produce the I/F Spectra. Input OVIRS radiance and solar flux units are W/cm<sup>2</sup>/micron/sr and W/m<sup>2</sup>/nm, respectively. I/F uncertainty is computed using standard error propagation.

**Table 6. OVIRS I/F Spectra**

Attribute Name	FITS Keyword	Units	Description
element_array.data_type	BITPIX		number of bits per data pixel
axes	NAXIS		number of data axes in array
axis_array.sequence_number	NAXIS1		Length of FITS data axis 1 equivalent to sample. Detector pixels (512)
axis_array.sequence_number	NAXIS2		Length of FITS data axis 2 equivalent to line. Number of lines in ROI
axis_array.sequence_number	NAXIS3		Length of FITS data axis 3 equivalent to frames. Number of frames in observation sequence. If absent, the array is a 2d-array representing a single frame's data.
n/a - FITS specific	EXTEND		FITS dataset may contain extensions
element_array.value_offset	BZERO		offset data range to that of unsigned short
element_array.scaling_factor	BSCALE		default scaling factor
investigation_area.name	MISSION		Mission name: OSIRIS-REx
observing_system.name	HOSTNAME		Spacecraft hostname
observing_system.component_name	INSTRUME		Instrument name: OSIRIS-REx OVIRS
mission_area.utc	DATE_OBS		The UTC time of the instrument clock on readout
mission_area.mid_obs	MIDOBS		Spacecraft mid-exposure time, UTC [Cal d] (DATE_OBS - .5*EXPTIME).
mission_area.expo_ms	EXPTIME	ms	Exposure time in milliseconds
mission_area.exposure	EXPOSEC	s	Exposure time in seconds
mission_area.mid_obs_et	ET		The ephemeris time of the mid-exposure time, mid_obs
mission_area.mid_obs_sclk	MID_SCLK		The SCLK string of the mid-exposure time, mid_obs
mission_area.boresight_flag	BS_FLAG		Boresight flag: 0-Boresight does not intersect surface of asteroid; 1-Boresight intersects surface of asteroid
mission_area.fov_fill_flag	FOV_FLAG		Field of view flag: 0-Entire FOV images empty space; 1-Entire FOV image s asteroid surface; 2-Portion of FOV images empty space
mission_area.boresight_angle	BS_ANGLE	deg	Angle between boresight and origin of Bennu in planetocentric Cartesian coordinates



Attribute Name	FITS Keyword	Units	Description
mission_area.latitude	LAT	deg	Planetocentric latitude of boresight intersection with the surface. Allowed range +90.0 to -90.0. If Boresight Flag is not equal to 1, then value shall be -9999.
mission_area.longitude	LON	deg	Planetocentric longitude of boresight intersection with the surface. Allowed range 0 to 360. If Boresight Flag is not equal to 1, then value shall be -9999.
mission_area.boresight_range	RANGE	km	Range from spacecraft to the closest boresight intersection to spacecraft. Must be positive number. If Boresight Flag is not equal to 1, then value shall be -9999.
mission_area.boresight_x	BS_X	km	X coordinate of boresight intersection with surface in planetocentric Cartesian coordinates. Allowed range 0 to 1000.0. If Boresight Flag is not equal to 1, then value shall be -9999.
mission_area.boresight_y	BS_Y	km	Y coordinate of boresight intersection with surface in planetocentric Cartesian coordinates. Allowed range 0 to 1000.0. If Boresight Flag is not equal to 1, then value shall be -9999.
mission_area.boresight_z	BS_Z	km	Z coordinate of boresight intersection with surface in planetocentric Cartesian coordinates. Allowed range 0 to 1000.0. If Boresight Flag is not equal to 1, then value shall be -9999.
mission_area.incidence_angle	INCIDANG	deg	Incidence angle. The angle between the vector normal to the surface at the location of the boresight intersection with the surface and the vector pointing at the Sun. If Boresight Flag is not equal to 1, then value shall be -9999. Allowed range is 0.0 to 90.0
mission_area.emission_angle	EMISSANG	deg	Emission angle. The angle between the vector normal to the surface at the location of the boresight intersection with the surface and the vector pointing to the Spacecraft. If Boresight Flag NE 1, then value shall be -9999. Allowed range is 0.0 to 90.0
mission_area.phase_angle	PHASEANG	deg	Phase Angle. The angle between the vector pointing to the Sun and the vector pointing to the Spacecraft. If Boresight Flag is not equal to 1, then value shall be -9999. Allowed range is 0.0 to 180.0
mission_area.fov_fill_factor	FILL_FAC	frac	Fill Factor. If FOV Flag = 2, describes the fraction of the FOV that intersects the asteroid surface. If FOV Flag = 0, value shall be 0.0. If FOV Flag = 1, value shall be 1.0. Allowed range is 0.0 to 1.0
mission_area.semimajor_axis	SMJAX	m	Semi-major axis of FOV ellipse on surface
mission_area.semiminor_axis	SMNAX	m	Semi-minor axis of FOV ellipse on surface

Attribute Name	FITS Keyword	Units	Description
mission_area.sun_range	SUN_RNG	km	Range from Sun to center of target body
mission_area.target_range	TRGTRNG	km	Range from S/C to target body center
mission_area.right_ascension	RA	deg	Boresight Right Ascension (RA) in J2000 frame.
mission_area.declination	DEC	deg	Boresight Declination (DEC) in J2000 frame
mission_area.bennu_ra	BENNURA	deg	Right Ascension of the vector, expressed in the Earth Mean Equator of the J2000 Epoch, from the ORX spacecraft toward the target named in FITS keyword BENNURDT (typically Bennu); see also BENNURDQ for a statement of the quality of this value
mission_area.bennu_dec	BENNUDEC	deg	Declination of the vector, expressed in the Earth Mean Equator of the J2000 Epoch, from the ORX spacecraft toward the target named in FITS keyword BENNURDT (typically Bennu); see also BENNURDQ for a statement of the quality of this value
mission_area.bennu_radec_target	BENNURDT		Target for the BENNURA, BENNUDEC, BENNUNX1 and BENNUNX2 FITS keywords; typically BENNU; may be NONE if the calculation failed. Target is not required to be in the field of view.
mission_area.bennu_radec_quality	BENNURDQ		(Quality: provenance) for the BENNURA, BENNUDEC, BENNUNX1, BENNUNX2 FITS keywords. This will be one of three values: (BEST: SPK), meaning the geometry was obtained from SPICE SP-Kernels; (POOR: osculating elements; +/- 1E6km), meaning the geometry was obtained from osculating orbital elements of Bennu w.r.t the Sun, and will have uncertainties of order 1E6km; (NONE: FAILURE), meaning both the SPK and elements methods failed; the parentheses, (), are only delimiters here and not part of the quality:provenance values.
array_2d.iof_spectrum			Array: I/F values of frame
array_2d.wavelen			Array: Wavelengths of the resampled cube

## 5.2.4 Map Data Products

All Spectral Analysis Working Group (SAWG) produced maps will conform to the OSIRIS-REx Map Format Software Interface Specification, UA-SIS-9.4.4-324. Specifically, the SAWG produced maps conform to section 5.2.1 OBJ + Ancillary File. The SAWG will produce Ancillary FITS files conforming to this standard based on the project supplied OBJ shape files. Note that the Map Formats SIS indicates that NaNs will be treated as IEEE754 NaNs, however this treatment is not PDS4 compliant. SAWG produced maps will use -9999 as the NaN value convention.

Map products to be produced are:

1. Site-Specific Spectral Parameter Maps – This data product is a map of a specific mineral or chemical species referenced to a potential sample site.
2. Global Spectral Parameter Maps – This data product is a global map of a specific mineral or chemical species referenced to the asteroid shape model.

### **5.3 Label and Header Descriptions**

All data products are labeled with PDS4 compliant detached XML labels. These labels describe the content and format of the associated data product. Labels and products are associated by file name with the label having the same name as the data product except that the label file has an .xml extension.

Labels are constructed with the PDS4 Product Class, `Product_Observational` sub-class. The `Product_Observational` sub-class describes a set of information objects produced by an observing system. A hierarchical description of the contents of `Product_Observational` products is:

`Product_Observational`

`Identification_Area` - attributes that identify and name an object.

`Logical_Identifier` - name/location of file

`Version_ID` - version of product

`Title` - Name of file

`Information_model_version` - version of PDS4 information model used to create product

`Product_Class` - attribute provides the name of the product class (`Product_Observational`)

`Modification_History` - attributes describing changes in data product

`Observation_Area` - attributes that provide information about the circumstances under which the data were collected.

`Time_Coordinates` - time attributes of data product

`Primary_Results_Summary` - high-level description of the types of products included in the collection or bundle

`Investigation_Area` - mission, observing campaign or other coordinated, large-scale data collection attributes

`Observing_System` - observing system (instrument) attributes

`Target_Identification` - observation target attributes

`Mission_Area` - mission specific attributes needed to describe data product

`File_Area_Observational` - describes a file and one or more tagged\_data\_objects contained within the file.

`File` - identifies the file that contains one or more data objects

Information in the preceding paragraphs was distilled from the PDS4 Information Model provided by PDS. Additional information on PDS4 product labels can be found by selecting “How to Approach a PDS4 Data Set” on the Small Bodies Node web site at <http://sbn.pds.nasa.gov>.

Each Spectral Processing data product has an associated detached PDS4 compliant XML label. This label contains enough information for a user to understand and interpret the data product and the circumstances of data collection.

Many of the Spectral Processing data products are produced as FITS files with associated headers. The headers are keyword = value in format. The information contained in the header is duplicated in the detached PDS XML label.

## **6 Applicable Software**

The following sections describe display software that may be used to examine, display, or analyze the Spectral Processing data products.

### **6.1 Utility Programs**

At the current time, the OSIRIS-REX project has no plans to release any mission specific utility programs. As most Spectral Processing data products are FITS or HDF5 files, any viewer with the capability of reading FITS or HDF5 can be used to view the data products. Some examples of these viewers are IDL, J-Mars (<http://jmars.asu.edu/download>), and Davinci ([http://davinci.asu.edu/index.php/Main\\_Page](http://davinci.asu.edu/index.php/Main_Page)). HDF5 files can be read in any HDF5 viewer. Some examples of these include IDL, J-Mars (<http://jmars.asu.edu/download>), and Davinci ([http://davinci.asu.edu/index.php/Main\\_Page](http://davinci.asu.edu/index.php/Main_Page)). Additionally, PDS4 compliant data products can be viewed in the PDS4 Data Viewer ([https://sbnwiki.astro.umd.edu/wiki/PDS4\\_Viewer](https://sbnwiki.astro.umd.edu/wiki/PDS4_Viewer))

### **6.2 Applicable PDS Software Tools**

The PDS supplies a number of software tools that can be used in conjunction with PDS data products. Please refer to the PDS4 software website (<http://pds.nasa.gov/pds4/software/index.shtml>) for additional information on these tools.

### **6.3 Software Distribution and Update Procedures**

As the OSIRIS-REx project will not be providing software, this section is not applicable.

## 7 Appendices

### 7.1 References

- Blackburn et al. 2010. Solar Phase Curves and Phase Integrals for the Leading and Trailing Hemispheres of Iapetus from the Cassini Visual Infrared Mapping Spectrometer. *Icarus* 209, 738-744.
- Blackburn, DG, Buratti, BJ, and Ulrich, R. 2011. A Bolometric Bond Albedo Map of Iapetus from Cassini VIMS and ISS and Voyager ISS. *Icarus* 212, 329-338.
- Christensen, P.R. et al. (2018). The OSIRIS-REx Thermal Emission Spectrometer (OTES) Instrument. *Space Science Reviews* doi:10.1007/s11214-018-0513-6.
- Ferrone, S. et al. (2021). Analysis of Projection Effects in OSIRIS-REx Spectral Mapping Methods: Recommended Protocols for Facet-Based Mapping. *Earth and Space Science* doi:10.1029/2019EA000613.
- V. E. Hamilton, P. R. Christensen, H. H. Kaplan, C. W. Haberle, A. D. Rogers, T. D. Glotch, L. B. Breitenfeld, C. A. Goodrich, D. L. Schrader, T. J. McCoy, C. Lantz, R. D. Hanna, A. A. Simon, J. R. Brucato, B. E. Clark and D. S. Lauretta: Evidence for limited compositional and particle size variation on asteroid (101955) Bennu from thermal infrared spectroscopy, *A&A*, Volume 650, June, 2021.
- Helfenstein et al. 1996. Galileo Photometry of Asteroid 243 Ida. *Icarus* 120, 48-65.
- Howett, CJA, Spencer, JR, Pearl, J., and Segura, M. 2010. Thermal Inertia and Bolometric Bond Albedo Values for Mimas, Enceladus, Tethys, Dione, Rhea, Iapetus, as Derived from Cassini/CIRS Measurements. *Icarus* 206, 573-593.
- Kaplan, H.H., Hamilton, V.E., Howell, E.S., Scott Anderson, F., Barrucci, M.A., Brucato, J., Burbine, T.H., Clark, B.E., Cloutis, E.A., Connolly, H.C., Jr., Dotto, E., Emery, J.P., Fornasier, S., Lantz, C., Lim, L.F., Merlin, F., Praet, A., Reuter, D.C., Sandford, S.A., Simon, A.A., Takir, D. and Lauretta, D.S. (2020), Visible–near infrared spectral indices for mapping mineralogy and chemistry with OSIRIS-REx. *Meteorit Planet Sci*, Vol 55, 744-765.
- Li, J.Y., Helfenstein, P., Buratti, B., Takir, D. and Clark, B.E. (2015) Asteroid Photometry. In *Asteroids IV*, Univ of Arizona Press. pp. 129-150.
- Pitman, KM, Buratti, BJ, and Mosher, JA, 2010. Disk-integrated Bolometric Bond Albedos and Rotational Light Curves of Saturnian Satellites from Cassini VIMS. *Icarus* 206, 537-560.
- Ramsey, M. S., and P. R. Christensen (1998), Mineral abundance determination: Quantitative deconvolution of thermal emission spectra, *J. Geophys. Res.*, 103, 577-596.
- D.C. Reuter, A.A. Simon, J. Hair, A. Lunsford, S. Manthripragada, V. Bly, B. Bos, C. Brambora, E. Caldwell, G. Casto, Z. Dolch, P. Finneran, D. Jennings, M. Jhabvala, E. Matson, M. McLelland, W. Roher, T. Sullivan, E. Weigle, Y. Wen, D. Wilson, and D.S. Lauretta (2018), The OSIRIS-REx Visible and InfraRed Spectrometer (OVIRS): Spectral Maps of the Asteroid Bennu, *Space Sci Rev*, 214:54.
- Rogers, A. D., and O. Aharonson (2008), Mineralogical composition of sands in Meridiani Planum determined from Mars Exploration Rover data and comparison to orbital measurements, *J. Geophys. Res.*, 113(E06S14), doi:10.1029/2007JE002995.

Ruff, S.W and P.R. Christensen (2002), Bright and Dark Regions on Mars: Particle size and mineralogic characteristics based on Thermal Emission Spectrometer data, *J. Geophys. Res.*, 107, NO. E12, 5127, doi:10.1029/2001JE001580.

Simon, A. A., H. H. Kaplan, E. Cloutis, V. E. Hamilton, C. Lantz, D. C. Reuter, D. Trang, S. Fornasier, B. E. Clark and D. S. Lauretta, Weak spectral features on (101995) Bennu from the OSIRIS-REx Visible and InfraRed Spectrometer, *A&A*, Volume 644, December, 2020

Takir, D., B.E. Clark, C. d’Aubigny, C.W. Hergenrother, J.Y. Li, D.S. Lauretta, R.P. Binzel (2015) Photometric Models of disk-integrated observations of the OSIRIS-REx Target Asteroid (101955) Bennu. *Icarus* 252, 393-399.

## 7.2 Definitions of Data Processing Levels

OSIRIS-REx	NASA	CODMAC	Description
	Packet data	Raw - Level 1	Telemetry data stream as received at the ground station, with science and engineering data embedded.
Level 0 - Raw	Level 0	Edited - Level 2	Instrument science data (e.g., raw voltages, counts) at full resolution, time ordered, with duplicates and transmission errors removed.
Level 1- Uncalibrated	Level 1A	Calibrated - Level 3	NASA Level 0 data that have been located in space and may have been transformed (e.g., calibrated, rearranged) in a reversible manner and packaged with needed ancillary and auxiliary data (e.g., radiances with the calibration equations applied).
Level 2 - Calibrated	Level 1B	Resampled - Level 4	Irreversibly transformed (e.g., resampled, remapped, calibrated) values of the instrument measurements (e.g., radiances, magnetic field strength).
Level 3 - Processed	Level 1C	Derived - Level 5	NASA Level 1A or 1B data that have been resampled and mapped onto uniform space-time grids. The data are calibrated (i.e., radiometrically corrected) and may have additional corrections applied (e.g., terrain correction).
Level 4 - Derived	Level 2	Derived - Level 5	Geophysical parameters, generally derived from Level 1 data, and located in space and time commensurate with instrument location, pointing, and sampling.

Level 4 - Derived	Level 3	Derived - Level 5	Geophysical parameters mapped onto uniform space-time grids.
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<b>Level</b>	<b>Definition</b>	
<b>Low-Level Products</b>	Any data product assigned to OSIRIS-REx Level 0 through Level 2	
	OREx Level 0	<i>Telemetry.</i> Raw instrument data reconstructed from telemetry with header and ancillary information appended. Appended header and ancillary data is data necessary for further processing.
	OREx Level 1	<i>Uncalibrated.</i> Data in one of the fundamental structures. This data will be archived to the PDS.
	OREx Level 2	<i>Reversibly calibrated.</i> Data in units proportional to physical units. Since PDS allows offsets and scaling factors in its array and table structures, this would be the minimum level capable of satisfying the “in physical units” requirement. This data will be archived to the PDS
<b>High-Level Products</b>	Any product assigned to an OSIRIS-REx data product level above Level 2.	
	OREx Level 3	<i>Irreversibly processed.</i> Higher-level products from a single source that cannot be losslessly converted back to the lower-level products from which they were derived. These might also satisfy the “in physical units” requirement. Data products of this processing level will be archived to the PDS according to DMP-Table 19
	OREx Level 4	<i>Derived data.</i> Products created by combining data from more than one source (instrument, observer, etc.). Data products of this processing level will be archived to the PDS according to DMP-Table 19

### 7.3 OSIRIS-REx Solar Flux Model

The following is a description of the OSIRIS-REx Solar Flux Model. The corresponding data product is found in the calibration collection of this archive bundle with the filename of OrexSolarOVIRS.csv. This file is equivalent to the “OrexSolarOVIRS.2015\_03\_02.txt” referred to below.

Solar Flux Model - Composite of Thuillier 2004 and Rieke 2008, compiled by Dr. Mike Nolan:

“To make a composite spectrum, I divided the spectrum from Thuillier et al. 2004 by 1.01400000 and rescaled the axis units to those of Rieke 2008. I then concatenated the portion of the Thuillier et al. 2004 spectrum longward of 0.2 microns with the portion of the Rieke 2008 spectrum longer than 2.398 microns.

The result is a spectrum that is everywhere higher resolution than the OVIRS instrumentation (perhaps by quite a bit too much over most of the spectrum). It has the solar constant of Rieke 2008, but the spectral shape and sampling of Thuillier et al. 2004. I rescaled by a small factor (0.2 %) to make the solar constant (integral over the whole hi-res spectrum) come out to 1367 exactly (to simplify – because the solar constant varies from year to year by one part in a thousand).

(Note: The definition of "solar constant" is not spelled out in the literature, but it's intended to be at 1 AU above the Earth's atmosphere. The exact value varies among authors, usually +/- 2 in the last digit, but with a recent value as different as 1361. I adopted 1367 W/m<sup>2</sup> as a nominal value. When the Solar Flux model is used, it must be scaled for distance (proportional to 1/r<sup>2</sup>.)

I then convolved the spectrum with a Gaussian to the approximate OVIRS resolution and then resampled at 2-nm spacing from 0.39 to 2.4 microns and 5 nm spacing from 2.4 - 4.37 microns. There are a few places where this spacing doesn't quite double-sample (from about 0.4 to 0.5 and 2.4 to 2.5 microns). The Gaussian FWHM was taken from an estimate from Dennis Reuter. The Gaussian width was linearly interpolated and/or extrapolated in wavelength space using the given sampling and the start and end points for the ~linear strip regions at 1100, 1800, and 2900 nm.

Error bars are from Thuillier et al. 2004, 3% from 0.4 to 2.4 microns, and from Rieke 2008, 2% above 2.4 microns.

The four columns in the data file “OrexSolarOVIRS.2015\_03\_02.txt” are wavelength (microns), spectral energy density (W m<sup>-2</sup> nm<sup>-1</sup>), uncertainty (W m<sup>-2</sup> nm<sup>-1</sup>, assumed to be the absolute uncertainty reported for the underlying high-res spectrum), and smoothing resolution ( $\lambda / \Delta \lambda$  FWHM).”