PSA PDS4 ARCHIVING GUIDE

Prepared by	S. Martinez, T. Lim, M. Costa, M.S. Bentley, D. Coia
Document Type	TN
Reference	ESDC-PSA-TN-0002
Issue/Revision	2 / 6
Date of Issue	21/12/2022
Status	ISSUED

APPROVAL

PSA PDS4 Archiving Guide	
Issue 2	**Revision** 6
Author S. Martinez, T. Lim, M. Costa, M.S. Bentley, D. Coia	**Date** 21-12-2022
Approved by	**Date**
M.S. Bentley	Mark Bentley Mark Bentley 2022.12.22 15:43:46 +01'00'
R. Docasal	

CHANGE LOG

Reason for change	Issue	Revision	Date
First draft for iteration with missions using PDS4	D	1	13/11/2015
Overview of the archiving process added	D	2	22/12/2015
Name of partially processed collection updated to “data_processed”	D	2	03/02/2016
“miscellaneous_ancillary” collection added to mission and instrument bundles Extension for collection inventory files changed to csv	D	2	04/02/2016
Naming convention for context products updated, following PDS4 DPH 1.4.0	1	0	11/02/2016
Minor updates following comments from ALTEC for ExoMars RSP	1	1	18/10/2016
Removed SPICE Collection, updated context lids	1	2	26/04/2017
Added SPICE Bundle Sections. Updated SPICE references	2	0	18/06/2017
Added policies for data products, more details on labels and specified namespaces. Added requirements and recommendations on Geometry metadata, FITS and CDF.	2	1	26/07/2018
Minor updates following internal review	2	2	18/09/2018
Corrected SPICE Bundle Section	2	3	03/10/2018
Expanded browse product and Modification_History descriptions, general updates	2	4	28/02/2019
Updated SPICE Bundle Section based on ExoMars2016 Bundle development	2	5	28/03/2019
Added additional recommendations based on recent PSA PDS4 discussions	2	5	29/08/2019
Added DOI, schema and pipeline sub-sections in the SPICE Bundle Section	2	5	14/11/2019
Updated: location of PDS4 context products at PDS, CDF recommendations & requirements.	2	6	06/05/2020
General updates following PSA PDS4 discussions	2	6	27/07/2020
Adding details of referencing archived SPICE products	2	6	29/10/2021

CHANGE RECORD

Issue 2	**Revision** 6		
Reason for change	**Date**	**Pages**	**Paragraph(s)**
Naming convention for context products updated, following PDS4 DPH 1.4.0.	18/06/2017	All	All
Minor updates following comments from ALTEC for ExoMars RSP	18/10/2016	6, 16, 17, 18, 28	2, 4.1, 4.3, 4.4, 6.2.2.1
Minor updates in the introduction to justify the use of PDS4	02/08/2017	5	1.1
Added target context rules and host bundle to table 5	30/01/2018	sect 3.2.1, 3.3.1	All
Added policies for data products, more details on labels and specified namespaces	26/06/2018	All	All
Author list and approval list modified	29/06/2018	metadata	metadata
Added guidelines for use of FITS and CDF in PDS4	25/07/2018	sect. 11	All
Added guidelines for Geometry metadata	26/07/2018	sect. 8	All
Minor updates following internal review	18/09/2018	All	All
Corrected SPICE Bundle Section	03/10/2018	sect. 10	All
Minor updates	28/02/2019	All	All
Corrected SPICE Bundle Section	28/03/2019	sect. 10	All
Minor updates to product recommendations	29/08/2019	All	All
Added DOI, schema and pipeline sub-sections in the SPICE Bundle Section	14/11/2019	sect. 10	All
Updated location of PDS4 context products at PDS	20/01/2020	sect. 3.3.1.1	All
Updated CDF recommendations & requirements	06/05/2020	sect. 11.2	All
Minor updates following internal discussions	27/07/2020	All	All
Updated following BepiColombo MTR	29/10/2021	Sect. 4.5.1	All

Table of Contents

1. INTRODUCTION

1.1. Purpose and Scope

This document compiles a set of guidelines, rules, common terminologies and conventions to be followed by all data providers when generating and submitting their science data and associated products to the Mission Science Ground Segment (SGS) for archiving within the Planetary Science Archive (PSA). This guide is also intended as a quick introduction to the PDS4 standards (fully described in [AD.01], [AD.02] and [AD.03]).

The rules and conventions defined in this document are intended to cover all needs at the level of the PSA overall. Specific rules and conventions defined at the level of each mission are provided as appendices to this document. As such, the conventions here-in are expected to remain stable and static for the most part. The dynamic aspects defined for each mission within the appendices will be edited and updated as needed to cover arising needs and requirements.

The use of PDS4 standard should be perceived as a tremendous benefit for the data producer in providing scientific products in a framework that will enhance its usability by the science community (see also RD.04). The benefits are at first for the Planetary Science Archive (PSA) as a multi-mission and multi-instrument archive, and also towards the international community since the PDS4 standard ensure:

- long term preservation of the data products
- easy ingestion of these data products into the PSA
- discovery of these data products through the PSA search interface
- cross mission search of these data products with other planetary missions both through the PSA and other data access protocols

1.2. Applicable Documents

The following documents, of the issue given here-under, are pertinent to the extent specified herein and impose requirements to the SGS or the SGS schedule. They are referenced in the form [AD XX]:

[AD.01] PDS4 Standards Reference (SR)

[AD.02] PDS4 Data Dictionary (DDDB)

[AD.03] PDS4 Information Model Specification (IM)

1.3. Reference Documents

The following documents, of the issue given here-under, although not part of this document, amplify or clarify its contents. If no issue given, the most recent issue should be used. They are referenced in the form [RD.XX]:

[RD.01] PDS4 Data Providers Handbook (DPH)

[RD.02] PDS4 Concepts

[RD.03] PSA Acronyms and Abbreviations

[RD.04] PSA Concept Document (not yet issued)

1.4. Abbreviations and Acronyms

See PSA online Acronyms and Abbreviations [RD.03].

2. OVERVIEW OF THE ARCHIVING PROCESS

This document is both aimed at data providers to the PSA and PSA users who wish to gain an insight into PDS4 data in the archive. The PDS4 data standard is defined at (http://pds.nasa.gov/pds4/) and while this defines file formats and data dictionaries in some detail, the organisation of the data can vary e.g. between NASA and ESA archives. The PSA has defined a common organisation for ESA missions to enable navigation and transparency.

The top level structure for all PDS4 data entities is a bundle. For archiving in the PSA, each mission is required to have a single bundle for each instrument, plus two separate “mission” bundles, one containing mission wide, non-instrument specific data such as spacecraft housekeeping data, and the other mission bundle contains SPICE files. These "mission" bundles plus the instrument bundles are typically sufficient to store all mission data, however in some cases, where the mission is split into separate vehicles, it may be more appropriate to put such data into separate "host" bundles. An example of this is the ExoMars 2020 RSP mission where the Rover and Surface Platform become, to a large extent, separate missions on the surface and in this case information will be generally stored at host level.

Each bundle is then subdivided into a set of collections. The available collection types are detailed in Chapter 3. Generally the PSA implementation aims to separate data types into an easy to navigate manner so an instrument bundle will contain separate collections for documentation, instrument science data, calibration products etc. For the instrument science data there are actually separate collections for each processing level and this is standardised by PDS4 to four levels: raw, partially processed, calibrated and derived.

The structure of some collections such as documentation are instrument specific so will vary between instruments and missions. However instrument science data does have a cross-mission substructure detailed in Chapter 3 and divisions into mission phase, sub-instrument etc. are defined as being cross-mission for the PSA. This bundle/collection structure can be considered as a set of folders which organise the actual data products of the instrument. When an archive user queries the archive and the results are displayed, this structure will not be immediately apparent. Instead, depending on the query, a set of products matching the query will be displayed. However once a set of products is selected for download, the downloaded entity will be organised as a set of folders matching the bundle structure i.e. as a bundle created on the fly.

The definition of products (both the file formats and the metadata) is tightly constrained by the PDS4 standards and data dictionary (see links in chapter 2). Each product contains at least two files, one for the metadata (always in an XML file) and the other(s) for data with different file types allowed. These file formats include both binary and ASCII tables, multi-dimensional arrays, and can include external formats such as FITS, CDF, and GeoTIFF if certain constraints are followed. Rules regarding the science products are detailed in chapter 5 for product structures and chapter 6 for the metadata. Geometry is dealt with separately in chapter 7. Products are allowed different versions and these are stored internally in the "version ID" commonly referred to as the "VID". Each product also contains a unique logical identifier "LID" which is attached to the version to create a "LIDVID". This identifier makes the product unique not just in the PSA, but in the entire set of federated PDS-compliant archives. The implementation of LIDVIDs used in the PSA is described in chapter 4.

2.1. PDS Standards

All science data delivered to the PSA must be compliant with the NASA's Planetary Data System (PDS) standards. The applicable version of the standards is PDS4, with the precise version determined by each mission at the time of archive definition, and documented accordingly in the appendices. Changes to the applicable version of the PDS standards for any mission will be documented in the relevant appendix.

Further information about PDS4 can be found here: http://pds.nasa.gov/pds4/

2.2. Introduction to XML

As introduced above, PDS4 labels provides all relevant meta-data about a product (document, observational data, calibration file etc.), including references to source products, links to the parent mission and spacecraft, instrument and domain-specific meta-data and, of course, a description of how the file can be opened by PDS4 compatible software. PDS4 labels are written in XML, the eXtensible Markup Language. In contrast to PDS3, this makes the labels easy to produce and parse in standard, open tools. Equally, validation is possible with a wide variety of tools, however the PDS also provide a bespoke software ("validate") for validation of both labels and data content.

XML is a generic markup-language, which provides for an unlimited set of "tags" to describe the associated data. PDS4 defines an "XML application", which constrains the set of available tags for a particular purpose. These constraints are applied by XML schema and Schematron, which together are called PDS4 dictionaries. For those familiar with HTML, the basic structure of an XML document is very similar - data are bracketed by a start tag (e.g. <name>) and a closing tag (e.g. </name>). These tags, and their content, together make an XML element. These elements are arranged in a tree - every element has one parent, with the exception of the root element, which has none and contains all others. In PDS4 the root element defines the product type (e.g. Product_Observational or Product_Document).

XML elements can also have attributes, which further qualify the element. These take the form of name-value pairs, separated by an equals sign and appear inside the start tag. Primarily PDS4 uses XML attributes to define units, for example:

```
<exposure_duration unit="ms">10</exposure_duration>
```

Comments are allowed in XML and are enclosed by <!-- and -->. These can be multi-line, but cannot contain other comments (indeed a double dash ('--') must not appear inside a comment.

Additional processing instructions can be defined in an XML document. These appear outside the root element and are bracketed by <? and ?>. These are not part of the XML markup itself, but are instructions to software reading the XML. These are used in PDS4 to point to the Schematron files (set of rules) which appear in dictionaries, and several <?xml-model…?> statements will usually appear before the root element.

A document which follows the basic XML rules (all tags are closed, there is only one root element etc.) are said to be "well-formed". If not, any processing software will likely stop at this point. A well-formed document does not, however, imply that it is a valid PDS4 label. The associated XML schema are used by processing software (editors, validation tools) to make sure that the label is PDS4-compliant.

2.3. PDS4 Terminology

The terminology described in this section is used in the PDS4 documentation to refer to the elements and structure of a PDS4 label. Note that, although PDS4 labels are XML-formatted files, the terminology used in PDS4 differs from the XML terminology. In particular, PDS4 adopts the software terminology of classes and attributes. Any XML element which no children is termed an attribute, and these attributes are grouped in parent elements called classes. Note that the term attribute is used differently in PDS4 and XML. PDS4 refers to qualifiers such as "unit" in the above example as XML attributes, to distinguish them from PDS4 attributes. Class names in PDS4 all start with a capital letter, whilst attributes names are always lower case. The following examples show both a class and attributes.

Attribute:

```
<attribute>VALUE</attribute>
```

Class: Grouping of attributes and classes.

```
<Class>
    <attribute>VALUE</attribute>
    <attribute>VALUE</attribute>
</Class>
```

PDS4 Requirements for PSA

The combination of the documents listed below give the set of common requirements that apply across PDS.

- The PDS4 Data Dictionary (DDDB) is the fundamental reference for definitions of classes and attributes.
- The PDS4 Information Model (IM) is the fundamental reference for PDS4 structure; its requirements can be validated automatically using eXtensible Markup Language (XML) schemas.
- The PDS4 Standards Reference (SR) is a compilation of policies, rules, and other PDS4 constraints that are not given explicitly in the previous references.

PSA has defined archive-specific requirements detailed in the following sectionds that further constrain — but do not conflict with — the common PDS4 requirements. These specific rules apply to all science data to be ingested and preserved in the Planetary Science Archive. Further constraints to the standards can be applied at mission level, and these are described in the relevant appendix for each mission.

2.3.1. PDS4 schemas

Schema (or Data Dictionary in the PDS context) and Schematron (rules) files are used to set rules on the layout and context of XML files plus the values this can take. Generally the schema files create a list of (metadata) "attributes" and define how these are organised into "classes". The core set of definitions for PDS4 is available on the PDS website and comprises the PDS4 dictionary and the rules associated with these attributes in the PDS4 Schematron. Together these are known as the PDS Information Model.

PDS is organised into a set of discipline nodes and most nodes also maintain a Discipline Dictionary which extends the core dictionary and provides classes and attributes for specialised areas such as atmospheric studies, imaging etc. When a PDS4 product is created the use of the core is mandatory and one or more discipline dictionaries are optional.

In addition, the PSA maintains a similar dictionary covering extensions for all missions providing PDS4 data to the PSA; rules and policies relating to the use of this dictionary are described below. The PSA dictionary can be found on the PSA public FTP site at ftp://psa.esac.esa.int/pub/mirror/PSA/psa_bundle/xml_schema.

Finally, a mission team is likely to define mission or instrument metadata which is specific to that mission or instrument. Usually as a minimum a mission level dictionary is required where all these data are stored. For missions with complex instruments the mission team may also elect to create separate instrument dictionaries. Both dictionary types are considered by PDS to be "mission level".

It is understood at PSA level that the creation and maintenance of dictionaries and Schematron is not a straightforward process and therefore, in general, the mission archive scientist will take responsibility of creating these for each instrument team. These dictionaries will then be used by the archive scientist to create template XML label files for the instrument teams to use for the production of their data products.

Note for Data Providers Wishing to Create their own Dictionaries: Please note that PDS are in the process of making the use of LDD Tool to create mission level dictionaries mandatory. As of PDS version 1.11, this tool lacks much of the required functionality and does not even recognise the registered PSA namespace, however any data provider planning to create their own dictionaries should use this tool and aid the PSA in providing feedback to PDS.

2.3.2. Namespaces

Namespaces are the mechanism by which dictionaries and rules files are located within PDS and by which naming conflicts are avoided. Each namespace must be registered within PDS and each URL must resolve. The registration and URL will be handled by the PSA team at ESAC in all cases where the PSA is the archiving authority.

The PSA namespace is:

Namespace	URLs
https://psa.esa.int/psa/v1	• https://psa.esa.int/psa/v1/PDS4_PSA_1101.xml • https://psa.esa.int/psa/v1/PDS4_PSA_1101.xsd • https://psa.esa.int/psa/v1/PDS4_PSA_1101.sch

Mission namespaces must follow the pattern from this example of the ADRON instrument on the ExoMars 2020 Rover:

	Namespace	URLs
Mission (emrsp)	https://psa.esa.int/psa/emrsp/v1	• https://psa.esa.int/psa/emrsp/v1/PDS4_PSA_EMRSP_1000.xml • https://psa.esa.int/psa/emrsp/v1/PDS4_PSA_EMRSP_1000.xsd • https://psa.esa.int/psa/emrsp/v1/PDS4_PSA_EMRSP_1000.sch
Host (rm)	https://psa.esa.int/psa/emrsp/rm/v1	• https://psa.esa.int/psa/emrsp/rm/v1/PDS4_PSA_EMRSP_RM_1000.xml • https://psa.esa.int/psa/emrsp/rm/v1/PDS4_PSA_EMRSP_RM_1000.xsd • https://psa.esa.int/psa/emrsp/rm/v1/PDS4_PSA_EMRSP_RM_1000.sch
Instrument (ADRON)	https://psa.esa.int/psa/emrsp/rm/adr/v1	• https://psa.esa.int/psa/emrsp/rm/v1/PDS4_PSA_EMRSP_RM_ADRON_1000.xml • https://psa.esa.int/psa/emrsp/rm/v1/PDS4_PSA_EMRSP_RM_ADRON_1000.xsd • https://psa.esa.int/psa/emrsp/rm/v1/PDS4_PSA_EMRSP_RM_ADRON_1000.sch

Namespaces used are declared within each product and further details are given below. Note is it permissible, and indeed common at mission level, to have a dictionary (schema) but not a set of rules (Schematron). It is equally possible for a mission to use only Schematron rules, which can be applied to provide additional mission-specific rules on PDS and PSA dictionaries. For example, a mission Schematron could make the inclusion of an optional attribute in a discipline dictionary mandatory for a specific mission.

Prepared by	S. Martinez, T. Lim, M. Costa, M.S. Bentley, D. Coia
Document Type	TN
Reference	ESDC-PSA-TN-0002
Issue/Revision	2 / 6
Date of Issue	21/12/2022
Status	ISSUED

3. DATA ORGANISATION

This section describes the hierarchical structure (generic structure) that must be used to organise the science products resulting from any investigation/mission/instrument. For a detailed description of the data organisation, see section 2 of the PDS4 Std. Reference [AD.01]. The PSA recommended organisation, based on this generic structure, is described in Section 3.2, and should be follow where possible.

The highest level of organisation defined in PDS4 is called “bundle” (top-level directory). Each bundle is organised into a number of “collections” (sub-directories), each collection containing a set of closely related products based on their type and purpose. The types of collections allowed in PDS4 are listed in Table 1.

Products assigned to a collection must be organised into lower level sub-directories, following the most convenient criteria for each type of data.

Collection Type	***Description***	***Typical PDS4 Product Classes in this Collection Type***
data	Contains primary products i.e. scientific data resulting from instrument observations.	Product_Observational
calibration	Contains calibration products used at any stage of the calibration process.	Product_Observational Product_Ancillary Product_Document Product_File_Text
document	Contains documentation and supporting information to assist in understanding and using the primary products.	Product_Document Product_File_Text
geometry	Contains geometry products including pointing, orientation and positioning information typically provided in tables of calculated values. GIS shape files can also be considered for this collection, but discussions on an appropriate format are ongoing. See further information in section 8.2.	Product_Observational Product_Document Product_Ancillary
browse	Contains browse products including overview representations or quick-look plots/reports of the primary products.	Product_Browse Product_Thumbnail

	See further information in section 8.2.	Product_Document
miscellaneous	Contains miscellaneous products including any additional information and documentation products not easily classified as one of the other collections.	Product_Observational Product_Ancillary Product_Document Product_File_Text
context	Contains products that provide descriptions of the mission, spacecraft, instrumentation and targets.	Product_Context
xml_schema	Contains XML Schemas and related products used for generating and validating the products.	Product_XML_Schema
spice_kernels	Contains SPICE ancillary data files "kernels" products used for geometry computations.	Product_SPICE_Kernel

Table 1: PDS4 Collection Types

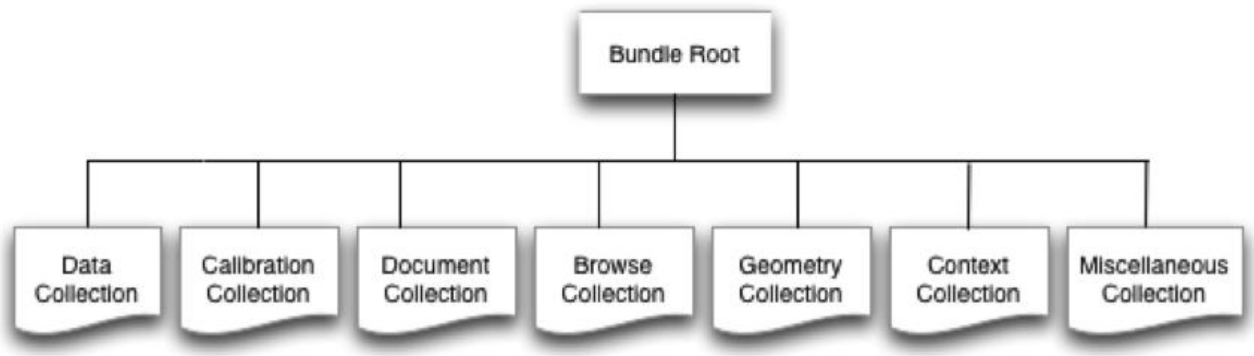


Figure 1 PDS4 bundle structure

3.1. Bundle Contents and Organisation Rules

The physical (on-disk) structure of a typical bundle (top-level directory) is described in this section and summarised in Table 2. Please note that this "Contents and Rules" discussion does not apply to the SPICE Bundle. For more information on the SPICE bundle Contents and Organisation see Section 10. Multiple collections of the same type are allowed in a bundle (unless specifically stated in Table 2 , see column "No. Of Occurrences"). If a bundle contains multiple collections of the same type, the name of the sub-directories must be formed by adding a suffix with a brief descriptive title after the collection type (i.e. <collection_type>_<title>, see collection types in Table 1). The corresponding mission annex typically provides additional guidelines for each mission.

- **bundle.xml** file: This is an inventory file that describes the bundle contents listing references to all the collections included in the bundle.
- **readme.txt** file: This file provides a general overview of the bundle contents and organisation in human readable format. This file is described in the bundle.xml label.

- **data** sub-directory: Contains primary products (main science data results). Products in a data collection are often organised into lower level sub-directories according to processing level, target, instrument mode, etc. and further split into ranges of orbits/dates, etc.
    - **collection_data.xml/.csv** files: Each data collection must contain an inventory file (table format) listing all the products inside the collection, with the corresponding XML label.
- **calibration** sub-directory: Contains calibration products used at any stage of the calibration process, as instrument bundles contain data from raw to derived this collection should always be populated.
    - **collection_calibration.xml/csv** files (required): Calibration collection inventory file (table format) and corresponding XML label.
- **browse** sub-directory (recommended): Contains browse representations (quick-look, thumbnails) of the primary products. Browse products are often organised into lower level sub-directories following the same criteria as for the primary products.
    - **collection_browse.xml/csv** files (required; if browse collection present): Browse collection inventory file (table format) and corresponding XML label.
- **document** sub-directory (**required**): Contains all documents (and related information e.g. figures, tables, etc.) deemed useful for understanding, interpreting and using other collections in the bundle.
    - **collection_document.xml/csv** files (required): Document collection inventory file (table format) and corresponding XML label.
- **geometry** sub-directory (optional): Contains geometry products describing the observing geometry of the primary products, including illumination, pointing, orientation and positioning information typically provided in tables of calculated values.
    - **collection_geometry.xml/csv** files (required; if geometry collection present): Geometry collection inventory file (table format) and corresponding XML label.
- **miscellaneous** sub-directory (optional): Contains any supplementary products that does not fit within the scope of the other collections.
    - **collection_miscellaneous.xml/csv** files (required; if miscellaneous collection present): Miscellaneous collection inventory file (table format) and corresponding XML label.
- **context** sub-directory (**required**): This collection contains a set of products describing the mission, the spacecraft, the instruments and any relevant target. All products in this collection must be included by reference to the mission's master context collection generated and managed by the relevant SGS. Therefore, no physical copies of the products need to be included in the bundle.
    - **collection_context.xml/csv** files (required): Context collection inventory file (table format) and corresponding XML label.

- **xml_schema** sub-directory (**required**): Contains all XML Schema and Schematron files (dictionaries) referenced by the labels in the bundle used for generating and validating the products. Mission level dictionaries should always be in the xml_schema collection of the mission bundle. Instrument dictionaries will either appear in the mission or instrument collect - consult the mission archive scientist for the conventions applicable to a given mission. When referencing schema in a different bundle (e.g. referencing the mission schema from an instrument bundle), the collection inventory should declare these products as secondary - they should not be physically duplicated in the collection, only referenced from the inventory.
    - **collection_xml_schema.xml/csv** files (required): XML Schema collection inventory file (table format) and corresponding XML label.

IMPORTANT: Delivery of data may be in the form of either products or bundles. If the data provider is delivering bundles, then complete bundles are expected, including all of the bundle and collection inventory files (i.e. bundle.xml and collection_*.xml/csv). In the case of the delivery of products such as the ExoMars 2016 and BepiColombo missions, then only products are delivered to the PSA, and the bundle and collection inventory filed are created within the PSA.

IMPORTANT: Each mission archive will contain a unique "context" collection and "xml_schema" collection that will contain all context products and XML schemas used by the mission. These products must be included in each instrument bundle by reference (i.e. Instrument Teams do not need to provide these products when delivering the data).

Products inside the collections described above must reside in lower level sub-directories. Exceptions may be made for collections containing only a few products, in which case the products can be stored directly in the collection sub-directory.

3.1.1. Mandatory and Optional Collections

Data Organisation	*Number of Occurrences*	*Naming Convention*
<bundle_identifier>/		
bundle.xml	1	fixed
readme.txt	1	fixed
data[_title]	1..n	fixed prefix
collection_data[_title].xml/.csv	1	fixed prefix
calibration[_title]	1..n	fixed prefix
collection_calibration[_title].xml/.csv	1	fixed prefix
browse[_title]	0..n	fixed prefix
collection_browse[_title].xml/.csv	1	fixed prefix
document[_title]	1..n	fixed prefix
collection_document[_title].xml/.csv	1	fixed prefix
geometry[_title]	0..n	fixed prefix
collection_geometry[_title].xml/.csv	1	fixed prefix
miscellaneous[_title]	0..n	fixed prefix

collection_miscellaneous[_title].xml/.csv	1	fixed prefix
context (*)	1	fixed
collection_context.xml/.csv	1	fixed
xml_schema (**)	1	fixed
collection_xml_schema.xml/.csv	1	fixed

Table 2: Data organisation and content requirements of a PSA bundle

(*) All products are secondary members i.e. products are added by reference, no physical copies of the products are required to be present in the bundle.

(**) In many cases all products are secondary members, but if instrument dictionaries are included in the instrument collection, these will be primary members.

3.2. Bundle Organisation Criteria

The following rules define the number of bundles and collections to be used by a mission to organise the data. Other organisations are possible and may be used in exceptional cases (e.g. more convenient structure for a specific type of data or instrument). Data organisation and naming conventions must be simple, intuitive and self-explanatory, and must facilitate manual browsing of the contents to the end-users.

IMPORTANT: This is a recommended standard that should be followed where possible. Exceptions should be discussed and agreed within a mission's DHAWG in coordination with PSA personnel. For example, it may be necessary to add additional derived data collections where data are provided from different teams, and in this case the collection names may be data_derived_alpha, data_derived_beta for example.

3.2.1. Types of Bundles and associated Collections

LID Formation Rule *(see section 4)*	*File Name*	*Directory Name*	**Bundle Entries** **(Collections)**
PSA Bundle			
urn:esa:psa	bundle_psa.xml	psa	• context • xml_schema
Mission Bundle			
urn:esa:psa:<mission_name>	bundle_<mission_acronym>.xml	<mission_name>	• context • document • miscellaneous[_...] • xml_schema
Host Bundle *(optional)*			

urn:esa:psa:<mission_name>_<host_name>	bundle_<mission_acronym>_<host_acronym>.xml	<host_name>	• context • document • miscellaneous[_...] • xml_schema
Instrument Bundle			
urn:esa:psa:<bundle_identifier>	<bundle_identifier>.xml	<bundle_identifier>	• data_raw • data_partially_processed • data_calibrated • data_derived • browse • browse_raw • browse_partially_processed • browse_calibrated • browse_derived • calibration_files • calibration_raw • calibration_partially_processed • geometry • miscellaneous[_...] • document • context (S) • xml_schema (S)
SPICE Bundle			
urn:esa:psa:<mission_acronym>_spice	bundle_<mission_acronym>_spice.xml	<mission_acronym>_spice	• document • miscellaneous • document • spice_kernels

Table 3: Data organisation and content according to the type of bundle

(S) This is a secondary member collection i.e. all products are added by reference, no physical copies of the products are required to be present in the bundle.

Where:

<bundle_identifier> = <mission_acronym>[_<host_acronym>]_<instrument_id>

(see section 4.1 for details on the formation rule for bundle identifier)

Collections

LID Formation Rule	*File Name*	*Directory Name*
urn:esa:psa:<bundle_identifier>:<collection_identifier>	collection_<collection_identifier>.<ext> where: <ext> = xml, csv	<collection_identifier>

Table 4: Naming conventions for collections

Where:

<collection_identifier> = <collection_type>_[<collection_descriptor>]

(see section 4.2 for details on the formation rule for bundle identifier)

3.2.2. PSA Bundle Organisation Criteria

- One mission bundle
- One bundle per instrument host (e.g. orbiter or lander), if required
- One SPICE bundle per mission
- One bundle per instrument (instrument bundle)
    - Data collections (primary data) within the instrument bundle are organised as follows:
        - One or more data collections for each processing level (named e.g. data_raw, data_calibrated)
        - Products inside each "data" collection must be organised in sub-directories according to the following criteria:
            - mission phase
                - sub-unit or sensor (when applicable)
                - other criteria e.g. experiment type, observation type, instrument mode or purpose of the data

Example:

data_<processing_level>/<mission_phase>/

- [<sensor>]
    - [experiment type or observation type]
        - Range of orbits (e.g. ORBIT_00100_00199)
        - Range of days (e.g. YYYYMMDD_YYYYMMDD)

- Supplementary collections (i.e. browse, calibration, document, geometry, miscellaneous, etc.) are organised in sub-directories according to the purpose of their products. Browse, calibration and geometry collections where products are one-to-one related to the primary products (in a data collection) must be organised following the same directory structure followed by the data collection. To this end, browse collections should follow the same convention as data (e.g. browse_raw, browse_calibrated).
- There is no restriction on the number of bundles and collections that can be delivered, with the exception of the rules defined in section 3.1.
- Data organisation and naming conventions must be simple, intuitive and self-explanatory, and must facilitate manual browsing of the contents to the end-users. Directory and file naming conventions applicable to each mission are as defined in the appendices to this document.

3.3. Context Products

Context products describe the mission, the spacecraft, the instruments and any relevant target. Context products are placed in the mission's bundle context collection, generated and managed by the relevant SGS. These products will be included by reference in the instrument bundles i.e. no physical copies of the products are required to be included in the bundle. The different types of context products are described in the table below, with naming conventions for the logical identifiers and filenames.

Type	*LID / Filename*	*Context Area*	*Reference Type*
Agency	urn:esa:psa:context:agency:agency.esa PDS4_agency_ESA.xml		is_agency
Investigation	urn:esa:psa:context:investigation:mission.<mission_id> PDS4_mission_<mission_name>.xml	Investigation_Area	is_investigation
Instrument Host	urn:esa:psa:context:instrument_host:spacecraft.<instrument_host_id> PDS4_host_<instrument_host_id>.xml	Observing_System	is_instrument_host
Instrument	urn:esa:psa:context:instrument:<instrument_id>.<instrument_host_id> PDS4_inst_<instrument_id>__<instrument_host_id>.xml	Observing_System	is_instrument
Target	urn:nasa:pds:context:target:<target_type>.<target_name> (LID, if under PDS governance) urn:esa:psa:context:target.<target_name> (LID, if under PSA governance) PDS4_target_<target_name>.xml	Target_Identification	data_to_target
Personnel	urn:esa:psa:context:personnel:personnel.<person_id> PDS4_personnel_<person_id>.xml		
Resource	urn:esa:psa:context:resource:resource.<resource_id> PDS4_resource_<resource_id>.xml		

Table 5: Context file naming conventions

3.3.1. Use of Target Context

Currently the use of Target Context files are optional within the PDS standard and their adoption by NASA missions is varied. For the PSA we aim, as a multi-mission archive, to have consistency in their use, hence the set of policies outlined below are adopted.

3.3.1.1. General Rules

- For missions studying one or more bodies in the Solar System that body should by default be the target for all products. For example JUICE will have observations at Jupiter and at Ganymede. When at Jupiter all observations of Jupiter should have target Jupiter and when at Ganymede, the target is Ganymede.
- If the body is not in the PDS target list, a request will be made to PDS to include this and a temporary measure will be made of adding the target to the PSA bundle.
- Any PSA targets adopted by PDS will be deprecated.
- The PSA will not allow duplicate target files. Duplicates will be resolved via use of an alias list within the context product.
- If an occultation observation is being made the target should be the body the spacecraft is pointing at, for example solar occultation measurements made to study the atmosphere of Mars, the target should be Sun.
- For landers and rovers, the PDS target should almost always be the body the rover or lander has landed on.
- For rovers, where local targets are required e.g. named rocks or sample numbers, a local target context will be produced and stored in the appropriate mission or host bundle. This level must be used for all cross-instrument targets. The use of local target context files for local targets identified by these types of experiments is mandatory for missions in the PSA.
- A second level of local targets is permissible at instrument level and these will be stored in the instrument bundle. For example the ExoMars Rover close up imager instrument will image a small part of the Martian surface identified by a local mission target. However features within this image may be labelled as local targets at the instrument level.
- For new generic targets (e.g. we may add Plasma), names will be agreed by the PDS4 Archive Scientist team before adoption.

For information:

- PDS Target Context Products are available at: https://pds.nasa.gov/data/pds4/context-pds4/
  - and mirrored at PSA under: ftp ://psa.esac.esa.int/pub/mirror/pds/context/target
- PSA Target Context Products (to be deprecated if adopted by PDS): ftp://psa.esac.esa.int/pub/mirror/PSA/psa_bundle/context/target

Solar System Bodies Naming Conventions

- The Sun exists as a separate target within PDS
    - but will shortly be moved to the "star" class of targets - this document will be updated when this happens
- PDS also contains context files for all Solar System planets, these just use their name.
- All solar system dwarf planet context files should use number_name.
- Pluto is the allowed exception where only the name is used.
- Currently only 136108_Haumea and 136472_Makemake are hosted by PDS.
- Currently PDS has duplication in satellite target files with both the satellite name and number in one file and just the name in the other e.g. PDS4_target_M1_PHOBOS and PDS4_target_PHOBOS.
    - If available the file with the name and number should be used by the PSA missions as only the number is unambiguous.
    - The exception to this rule is the Moon, where the file only contains the name.
    - Unassigned satellites may use their discovery designation until numbered, once numbered the context file should be deprecated and replaced by the number file.
    - The discovery designation should be retained as an alias.
- Jupiter Saturn Neptune and Uranus all have generic Rings target context files in PDS in form PDS_target_PlanetInitial_RINGS, these should be used for Rings observations in the PSA.
- Similarly all asteroid files should be named PDS_target_number_asteroid. Currently there are no asteroids in the PDS4 list, so for now all files will be local
- *No policy is yet in place for comets*

3.3.1.2. Calibration Targets

Observations of dark sky should use the PDS_target_DARK_SKY. Hence the following, similarly names files should not be used:

- Deep Space
- Black Sky
- Space
- Skyflat
- Sky
- Flatfield
- Bias

As much as possible, specific targets relating to internal calibration sources should be avoided, instead one of the following are encouraged:

- Cal_Target – to be used for internal calibration targets
- Internal_Source – to be used for all illumination sources
- Dark – internal darks
- Rover
- Lander
- Spacecraft_deck

The following PDS files should not be used:

- Test_image
- Plaque
- Responsivity
- CalImage
- Calibration
- Cal_Lamps
- FF_Lamp
- Stim_Lamp
- Cal

When an observation is made where no target is specified the Non_Science target file should be used. This includes checkout observations hence the “Checkout” target should never be used.

Unknown targets are not allowed in the PSA, we will form a temporary name if necessary.

3.3.1.3. Celestial Targets

- All Celestial targets should have a target context file. If the file is not in PDS a file will be generated in the PSA bundle and a request will be made to PDS to include this.
- By convention calibration stars with local target context files in the PSA will be named via their HD number. *PDS is currently investigating using the SIMBAD name, but this name is often not in common use.*

- All celestial target files produced for the PSA will include an alias list with all alternate identifiers from SIMBAD included.
- For objects without an HD number the PSA will use the SIMBAD name.
- No convention is established for the naming of star clusters or Galaxies, it is expected for most the Messier identification will be adopted.
- For nebulae and fainter objects the NGC catalogue is preferred.
- All Celestial Targets should be named hence generic PDS files are excluded. Currently within PDS two such generic names exist, and should never be used in the PSA:
    - Starfield
    - OB_Star

3.3.1.4. Other Targets

The PSA allows the following alternative targets:

- Dust
- Interstellar_Particles
- Solar_Wind
- Io_Plasma_Torus

Additional alternative targets are likely to be added to this list. These will be added by agreement with the PDS4 Archive Scientist team.

LOGICAL IDENTIFIERS

Every product (including bundles and collections) in PDS is assigned an identifier that allows it to be uniquely identified across the system. This identifier is referred to as Logical Identifier (LID). Logical identifiers are constructed as four fields (for a bundle), five fields (for a collection) or six fields (for a basic product), as defined below, with colons delimiting the fields.

Logical Identifiers	
bundle	urn:esa:psa: ***<bundle_identifier>***
collection	urn:esa:psa:<bundle_identifier>: ***<collection_identifier>***
product	urn:esa:psa:<bundle_identifier>:<collection_identifier>: ***<product_identifier>***

Table 6: Logical Identifiers Formation Rules

Bundle, collection and product identifiers are formed according to the conventions described in the following sections with the exception of the SPICE Bundle, collection and product identifiers which are described in Section 9

A version identifier (VID) may be appended to the logical identifier (separated by a double colon i.e. ::<version_id>), allowing different versions of the same product to be referenced uniquely.

urn:esa:psa:<bundle_identifier>***::<version_id>***

urn:esa:psa:<bundle_identifier>:<collection_identifier>***::<version_id>***

urn:esa:psa:<bundle_identifier>:<collection_identifier>:<product_identifier>***::<version_id>***

The combination of a logical identifier and a version identifier is known as Versioned Logical Identifier (LIDVID).

3.4. Bundle Identifiers Formation Rule

A unique logical identifier shall be assigned to every bundle generated by a mission. Bundle logical identifiers shall be based on the following definition:

```
urn:esa:psa:<bundle_identifier>
```

where <bundle_identifier> shall take the form of :

```
<mission_id>[_<instrument_host_id>]_<instrument_id>[_<descriptor>]
```

where:

- ***<mission_id>*** is a fixed part used for all bundles delivered by a mission. The value to be used for each mission is defined in the relevant mission appendix. Where a mission comprises more than one spacecraft, the value should be of the form ***<mission_id>_<instrument_host_id>*** , for example **bc_mpo** for BepiColombo Mercury Planetary Orbiter;
- ***<instrument_id>*** is the instrument identifier (when applicable). Instrument identifiers are defined by each mission's SGS and listed in the appendices.
- ***<descriptor>*** details on bundle types/structure and naming conventions are provided in the corresponding mission appendix.

3.5. Collection Identifiers Formation Rule

A unique logical identifier shall be assigned to every collection generated by a mission. Collection logical identifiers shall be based on the following definition:

<collection_type>[_<descriptor>]

where:

<collection_type> is the collection type (see Table 1).

<descriptor> , details on collection types/structure and naming conventions are provided in the corresponding mission appendix.

3.6. Product Identifiers Formation Rule

A unique logical identifier (LID) shall be assigned to every product generated by a mission. Logical identifiers are based on the following formation rule:

```
urn:esa:psa:<bundle_identifier>:<collection_identifier>:<product_identifier>::<versio
n_id>
```

The <product identifier> is based on the following convention:

```
<instrument_acronym>_[<processing_level>]_[<type>]_[<subunit>]_<descriptor>
```

[ ] = optional fields

where:

- ***<instrument_acronym>*** , see table further below
- ***<processing_level>:*** Allowed values: raw | par | cal | der (mostly only applicable to primary products: data)
- ***<type>***

  - for primary products, possible split is: hk | sc
  - for supplementary products, specify type: calib | browse | thumb | geo | doc | misc (list controlled by SGS)
- ***<subunit>*** is the sensor / detector / sub-unit identifier (when applicable), see table further below
- ***<descriptor>:*** additional information e.g.
  - observation id
  - observation type
  - measurement type
  - start / stop date (<YYYYMMDDThhmmss> or <YYYYMMDDThhmmss>_<YYYYMMDDThhmmss>
    - UTC time of the first (and last) measurement in the data product
  - orbit number (<NNNNN> or <NNNNN>_<MMMMM>
    - orbit number of the first (and last) measurement in the data product, padded with zeroes

For all products generated by an instrument team, the label filename (without the extension) and the product identifier should be identical. Differences in case **are**, however, allowed. It is recommended that the PDS product files (minus the extension) also match the LID and label filename, as shown in the following examples:

LID	Label and data filename
urn:esa:psa:bc_mpo_mag:data_raw:mag_raw_sc_ob_s2_urf_00000_20181215	mag_raw_sc_ob_s2_urf_00000_20181215.[xml/tab]
urn:esa:psa:bc_mpo_berm:data_raw:ber_raw_hk_report_20181214	ber_raw_hk_20181214.[xml/fit]
urn:esa:psa:bc_mpo_mertis:data_raw:mer_raw_hk_default_20181113t105244_20181113t235959	mer_raw_hk_default_20181113T105244_20181113T235959.[xml/dat]
urn:esa:psa:em16_tgo_acs:geometry:acs_geo_mir_nir_20201029t033933-20201029t034634	acs_geo_mir_nir_20201029t033933-20201029t034634[.xml/.dat/.tab]
urn:esa:psa:em16_tgo_nmd:browse_calibrated:nmd_cal_sc_browse_20190331t234006-20190331t235619-i-uvis	nmd_cal_sc_browse_20190331T234006-20190331T235619-i-uvis[.png]

where there is more than one data file per product (i.e. one label and several data files), it is recommended that the data files share the same filename (minus extension) as the label/LID but that a suffix is used to indicate their purpose, for example a product could comprise these files:

- ber_raw_hk_20181214.xml
- ber_raw_hk_20181214_data.fits

- ber_raw_hk_20181214_ancillary.dat

Note also that while it may be convenient to include a time in the LID, if the spacecraft clock time correlation changes over the mission, this could result in the LID changing - essentially creating an entirely new product. Thus this should be done with caution, and in consultation with the mission archive scientist.

IMPORTANT:

- PDS product labels will have extension ".xml"
- PDS product file extension will depend on the format of the data they contain (".tab", ".fit", ".cdf", ".img")
- Orbit and date may be applicable to certain types of products
- Version is inside the label, follows PDS4 versioning scheme described in section 4.4
- Product identifiers will be used as product filenames (except for context products) as above
- Logical identifiers shall be lowercase. This restriction does not apply to filenames; PDS4 is case insensitive for filenames.

3.7. Version Numbers

The PDS4 versioning scheme is defined in detail in the PDS4 Standards Reference [AD.01]. Rules specific to the implementation of the versioning scheme in PSA are listed below.

- Bundle, collection, and product version identifiers will be sequential, and of the form M.n (with M initialised to “1”, and n initialised to “0”)
- 0.n will be used until the first official delivery to the PSA (e.g. for test/sample data, during data preparation or archive development)
    - where n is an integer with no padding, i.e. 0.1, 0.99, 0.100 are acceptable, 0.01 is not
- Version identifiers will be incremented every time there is a delivery to the PSA.
- Version identifiers are not included in the product filename (i.e. the product filename does not change)

For **observational products** (and supplementary products e.g. geometry products, browse products) typically generated with a pipeline:

- M will be incremented for major changes/updates, n will be incremented for minor updates (following a criteria similar to the versioning of the data processing software)
- Version numbers will increment independently of the software version e.g. when using different input parameters / files.

- In order to keep the traceability of a given version of a product to the software version and the input parameters / files, this information will be included in the label of the product.
    - *Details of the required metadata for this purpose will be included in a future version of the document.*
- All versions of a product will be available in the archive for retrieval (i.e. no limitation on the number of versions to keep available to the users by default). If this becomes unmanageable for a specific mission / case, a limit will be defined and applied to that particular case.

For **bundles and collections**:

- Each time a product is updated / added to a collection, the applicable collection and bundle versions will be incremented. The current policy at PSA is to increase major version once a month and minor version once a week.
- Bundle and collection versions will not be exposed to the users through the user interface, but will be used by the SGS/SOC to track which product versions have been delivered in a given delivery package
- When the delivery package to the PSA contains only individual products (typical case for systematic deliveries), the corresponding bundle and collection products are produced by the "bundle generation" software, that will increment the version numbers accordingly
- A criteria for incrementing major/minor numbers shall be defined to avoid large numbers (e.g. increment M monthly, following the public release schedule)

3.8. Internal references

LIDs or LIDVIDs are also heavily used in PDS4 to make links between products in the archive. As a result, it is possible to link data and browse products, to link a derived product (e.g. a high level map) with source products, to link calibrated data to both raw data and calibration files etc. Such references are typically used in the Reference_List class of a PDS4 label and have the form:

```
<Reference_List>


    <Internal_Reference>
        <lid_refererence> or <lidvid_reference>
        <reference_type>
        <comment>
    </Internal_Reference>


    <Source_Product_Internal>
        <lidvid_reference>
        <reference_type>
        <comment>
    </Source_Product_Internal>


</Reference_List>
```

Two types of reference to archived products can be made - a more generic internal reference, and one specifically for referencing source products. In both cases the comment attribute is optional. For Internal_Reference only one of lid_reference or lidvid_reference are needed (depending on whether it is necessary to link to a specific version of a product). The reference_type attribute has different allowed values, depending on where it is used. The allowed types can be found in the PDS4 Data Dictionary. For example, in a Product_Observational label, the following types are commonly used for Internal_Reference:

- data_to_calibration_document
- data_to_calibrated_product
- data_to_derived_product
- data_to_geometry
- data_to_document
- data_to_browse
- data_to_ancillary_data

Many of these links can be made in both directions - for example a Product_Observational is linked to its corresponding browse product via an internal reference of type data_to_browse_product, whilst the browse product can be associated back to its data product by a link of type browse_to_data. In the PSA the use of Internal_Reference is important since it allows the user interface of the PSA website to know which documents to download, or which browse products to display.

The Reference_List can also include the more specific Source_Product_Internal class "contains input data for the creation of this product". In this case a LIDVID is required, and the reference_type has to be one of:

- data_to_calibrated_source_product
- data_to_derived_source_product

- data_to_partially_processed_source_product
- data_to_raw_source_product
- data_to_telemetry_source_product

Note that currently the only way for the PSA to link products is by using the Reference_List/Internal_Reference class. Source_Product_* and psa:Processing_Input_Information are not actually used for that purpose. Furthermore, psa:Processing_Input_Identification/type=PDS product will likely soon be deprecated as PDS products should be referenced using PDS standard classes.

3.8.1. Referencing SPICE products

All planetary missions use the SPICE framework for the calculation of geometry, conversion of spacecraft clock values to UTC etc. It is therefore important that the SPICE kernels (input data files) used to make these calculations are referenced in the data products to ensure that the end user has traceability. However, there are several types of kernels in use - typically early data products are produced with operational kernels which are not yet ingested in the archive. Conventions vary per mission and the mission archive scientist will advise data providers, but the following scenarios are possible:

Data product does NOT include geometry, but only uses SPICE for SCLK → UTC conversion (using operational SPICE kernels)

In this case the psa:Processing_Context class can be used. Either the specific kernels needed for the time conversion should be included, or else a versioned meta-kernel.

```
<psa:Processing_Context>
    <psa:processing_software_title>mcam_tm2raw</psa:processing_software_title>
    <psa:processing_software_version>1.4.8</psa:processing_software_version>
    <psa:Processing_Inputs>
       <psa:Processing_Input_Identification>
           <psa:type>SPICE kernel</psa:type>
           <psa:file_name>bc_ops_v281_20211028_001.tm</psa:file_name>
       </psa:Processing_Input_Identification>
    </psa:Processing_Inputs>
</psa:Processing_Context>
```

Data product does NOT include geometry, but only uses SPICE for SCLK → UTC conversion (using archived SPICE kernels)

In this case the archived kernels can be referenced using the Internal_Reference class in the Reference_List. Either the specific kernels needed for the time conversion should be included, or else a versioned meta-kernel.

```
<Reference_List>
    <Internal_Reference>
        <lid_reference>urn:esa:psa:em16_spice:spice_kernels:mk_em16</lid_reference>
        <reference_type>data_to_spice_kernel</reference_type>
    </Internal_Reference>
</Reference_List>
```

Data product includes geometry, using operational SPICE kernels

In this case the geometry discipline dictionary should be used to declare the SPICE kernels in use. Again, this can be via a list of kernels, or a versioned meta-kernel. The latter case is shown here for simplicity:

```
<geom:Geometry>
    <geom:SPICE_Kernel_Identification>
        <geom:SPICE_Kernel_Files>
            <geom:spice_kernel_file_name>bc_ops_v281_20211028_001.tm</geom:spice_kernel
_file_name>
        </geom:SPICE_Kernel_Files>
        <geom:comment>Calculations were performed using the operational SPICE kernels
for BepiColombo corresponding to the listed versioned meta-kernel</geom:comment>
    </geom:SPICE_Kernel_Identification>

    ... other geometry classes go here ...

</geom:Geometry>
```

Data product includes geometry, using archive SPICE kernels

In this case the geometry dictionary should be used, but the kernels should be referenced by name AND by their LID or LIDVID:

```
<geom:Geometry>
    <geom:SPICE_Kernel_Identification>
        <geom:SPICE_Kernel_Files>
            <geom:spice_kernel_file_name>em16_v003.tm</geom:spice_kernel_file_name>
            <Internal_Reference>
                <lidvid_reference>urn:esa:psa:em16_spice:spice_kernels:mk_em16::3.0</li
dvid_reference>
                <reference_type>data_to_spice_kernel</reference_type>
            <Internal_Reference>
        </geom:SPICE_Kernel_Files>
        <geom:comment>Calculations were performed using the archive SPICE kernels for
ExoMars 2016 corresponding to the listed versioned meta-kernel</geom:comment>
    </geom:SPICE_Kernel_Identification>

    ... other geometry classes go here ...

</geom:Geometry>
```

This last case cannot be considered until the SPICE kernels have been reviewed and archived, and so this is typically handled during data re-processing. Currently it is foreseen that a single SPICE bundle is used per mission.

There may be other scenarios besides these (e.g. an product lists highly specific geometric meta-data not available in the geometry dictionary, and references these in the Reference_List) and these should be discussed with the mission archive scientist.

4. PRODUCTS

A PDS4 product is composed of an XML-formatted label file with metadata and one or more files containing the actual data (organised into “objects” a.k.a. data structure extensions). For example, a planetary image, the histogram of its pixel values, a table with housekeeping information, and the descriptions of their structure could be organised as a product.

The terminology used in the PDS4 documentation to classify the different types of products is outlined in Table 7.

PDS4 Product Classification		***PDS4 Product Class***
Basic	*Observational*	Product_Observational
	Supplementary	Product_Browse
		Product_Ancillary
		Product_Thumbnail
		Product_Document
		Product_File_Text
		Product_Context
		Product_SPICE_Kernel
		Product_XML_Schema
Aggregate		Product_Bundle
		Product_Collection

Table 7: PDS4 Product Classification

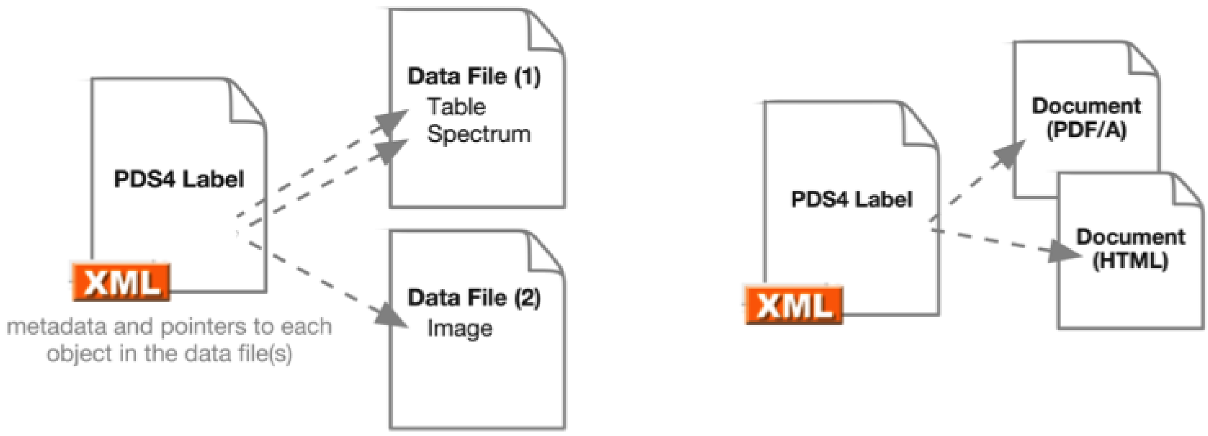


Figure 2: Illustration of a PDS4 Product_Observational and a PDS4 Product_Document

4.1. Fundamental Rules

This section provides a summary of the fundamental rules (see the PDS4 Data Provider's Handbook [RD.01]) that should be taken into account when creating PDS4 products. For a full description of the applicable rules, see the PDS4 Standards Reference [AD.01], section 4.

Objects must be formatted in one of the data structures listed in Table 7.

Each object must be contained in a single file (i.e. an object cannot be spread over multiple files).

A file may contain multiple objects if the objects belong to the same product (except for documents, in which case each object must be in a separate file).

Objects within a file are not required to use the same data structure (e.g. a product can be composed of a header, formatted as a parsable structure, and an image, formatted as an array structure, and both objects can be stored in the same data file).

When multiple objects are contained in a file, objects must be stored sequentially (i.e. one object shall be stored after the other, objects cannot be interleaved).

4.2. Data Structures

The following section provides the list of the data structures that are allowed in observational products and supplementary products. These data structures are extensions of the four *basic data structures* (also known as "*PDS4 base classes*", see Table 8). The basic data structures only define how to read the bytes from a file. They contain no interpretation beyond that. For the interpretation, PDS4 defines extensions (see Table 9) to expand and restrict the associated metadata for more specific types.

Basic Structure	*Encoding Type*	*Description*	*Usage and notes*

Table Base	Binary or Character (ASCII)	Fixed-length records (i.e. fixed width rows) of heterogeneous elements (different data type or size). Only 2-dimensional tables are permitted. Fields (i.e. columns) within each record are of fixed width and begin at fixed locations. Grouped fields are allowed (i.e. set of repeating fixed-width elements within one field) - these can be thought of as "sub-tables". See section 4B in the PDS4 Std. Reference [AD.01]. Note that ASCII character tables ***must*** use carriage-return-line-feed (<cr><lf>) line endings.	Suitable for tabular data. Note that variable-width tables are described in PDS4 as a subclass of the “Parsable Byte Stream” (see Table_Delimited in Table 7).
Array Base	Binary or Character (ASCII)	Fixed-width rows of homogeneous elements (same data type and size) in any number of dimensions. See section 4A in the PDS4 Std. Reference [AD.01].	Suitable for images, spectra, spectral cubes, maps etc.
Parsable Byte Stream	Binary or Character (ASCII)	Byte stream that can be parsed with standard rules (comma separated fields, standard punctuation). See section 4C in the PDS4 Std. Reference [AD.01].	Suitable for ASCII text, HTML, XML, tabular data with variable length fields and records (delimited text, e.g. CSV).
Encoded Byte Stream	Binary or Character (ASCII)	Byte stream that must be decoded by software before use. The use of this type of structure is restricted by PDS to a limited set of PDS approved external standards (e.g. PDF/A, JPEG, GIF). See section 4D in the PDS4 Std. Reference [AD.01].	Suitable for documents, thumbnails. ***This structure must not be used for observational products.***

Table 8: PDS4 Basic Data Structures

4.2.1. Data Structure Extensions

The PDS4 Information Model (IM) [AD.03] is the fundamental reference for the PDS4 data structures. Its requirements are specified in the form of PDS4 schemas. The following table shows the data structures that are permitted per product type, along with some additional hints about using each one.

Product Type	***PDS4 Product Class***	***Allowed PDS4 Extensions*** *(a.k.a. data structures or objects)*	***Derived from*** *(See Table 8)*	***Usage and notes***
Observational	Product_Observational (1)	Array_1D (Deprecated)	Array Base	
		Array_2D_Image		
		Array_2D_Map		
		Array_2D_Spectrum		
		Array_3D		
		Array_3D_Image		
		Array_3D_Movie		
		Array_3D_Spectrum		

		Table_Binary	Table Base	Fixed width. Each field must be defined by a record offset and length. Note that not all fields must use binary data-types, and ASCII data types can be included also.
		Table_Character		Fixed width. Each field must be defined by a record offset and length Note: A field delimiter can be used **outside** of the defined fields to allow a fixed-width ASCII table to be read as e.g. as CSV as well, **but** this does not work with group fields, so be aware! Note: In ASCII tables a header line can be included, if the relevant byte offset is used to skip this. If this is done, the field names listed in the ASCII header *must* match those in the PDS4 label. Note: Field_Character includes a field_format attribute which can be used to describe the type, width etc. of the data. This is very useful for validation and should be included if possible.
		Table_Delimited	Parsable Byte Stream	Delimited (e.g by tab or comma). Fields can have variable lengths. Note: In ASCII tables a header line can be included, if the relevant byte offset is used to skip this. If this is done, the field names listed in the ASCII header *must* match those in the PDS4 label. Note: Field_Delimited includes a field_format attribute which can be used to describe the type, width etc. of the data. This is very

				useful for validation and should be included if possible.
		Stream_Text		
		Header		Note that headers can be declared, but are essentially ignored by PDS4 and any information in the header needed to interpret the data must also be stored in the label or an allowed PDS4 data structure.
		Encoded_Header	Encoded Byte Stream	
Supplementary	Product_Browse	Any of the objects listed for Product_Observational, see above		
		Encoded_Image	Encoded Byte Stream	
	Product_Thumbnail	Encoded_Image		
	Product_Document	--	Encoded Byte Stream	
	Product_File_Text	Stream_Text	Parsable Byte Stream	
	Product_Context	Agency, Facility, Instrument, Instrument_Host, Investigation, Resource, Target		
	Product_SPICE_Kernel	SPICE_Kernel	Parsable Byte Stream	
	Product_XML_Schema	XML_Schema	Parsable Byte Stream	

(1) Observational products (Product_Observational) can include, in addition to the observational data, additional data files useful for the interpretation and analysis of the data. These additional files can use, in addition the objects listed under Product_Observational, the Encoded_Image data structure.

(2) Product_Bundle and Product_Collection (aggregate products) have not been included in this table. These products use the Stream_Text data structure.

Table 9: PDS4 Extensions allowed for each product type

IMPORTANT: Instrument Teams for each mission should consult with their SGS representatives to choose the most appropriate data structure(s) (see column "Allowed PDS4 Extensions" in Table 9) for their products. A combination of several data structures might be needed in some cases. Note also that it is possible to archive an existing standard file format **if** the relevant data in the file complies with the PDS4 standards. Some common examples include FITS, CDF and GeoTIFF (all with caveats) and these are described further in the section External Standards.

The appropriate PDS documentation should be consulted on how to design and label a product to these standards, or ask your Archive Scientist to provide templates or examples.

4.3. Data Types

Detailed information of the allowed data types can be found in the PDS4 Standards Reference [AD.01]. These data types are used to describe the format of the individual fields/elements of the data structures described in section 5.2.1.

Character data types (used in ASCII tables): see PDS4 Standards Reference [AD.01], section 5B.

Binary data types (used in binary tables and arrays): see PDS4 Standards Reference [AD.01], section 5C.

4.3.1. Date and Time Types

4.3.2. Date and Time Formats

For a complete list of PDS4 Date and Time Types and applicable rules, see PDS4 Standards Reference [AD.01]. The summary provided below includes additional requirements for PSA.

PDS date and time formats are based on the extended format of cardinal and ordinal date/time strings as defined in ISO 8601:2004. Specifically, all dates and/or times must be represented using one of the two formats below:

YYYY-MM-DDThh:mm:ss.ffffffZ (calendar format)

or

YYYY-DOYThh:mm:ss.ffffffZ (ordinal format)

Where:

YYYY is the 4-digit year

MM is the 2-digit month (possible values 01-12)

DD is the 2-digit day of month (possible values (01-31)

DOY is the 3-digit day of year (possible values 01-365, or 366 in a leap year)

hh is the 2-digit hour (possible values 00-23)

mm is the 2-digit minute (possible values (00-59)

ss is the 2-digit second (possible values 00-59, or 60 if needed for a leap second)

ffffff is decimal seconds (number of digits commensurate with precision)

Z denotes UTC (***required*** when the time is given in UTC)

4.3.3. Spacecraft Clock Formats

The Spacecraft Clock format is a native time format specific to each mission and is therefore defined in each mission-specific dictionary (see relevant mission annex). The Spacecraft Clock (SCLK) values represent the on-board time (OBT) counters of the spacecraft and instrument computers. The SCLK counter is given in the headers of the telemetry packets.

The SCLK typically contains the time as 32 bits of unit seconds followed by 16 bits of fractional seconds. Typically it is represented as a decimal real number in floating point notation with 5 digits after the decimal point. An integer number followed by a slash represents a reset of the spacecraft clock (e.g., “1/” or “2/”). Thus SCLK count values have the form:

```
n/dddddddddd.ddddd
```

where n is an integer number, up to 10 digits after the slash, and 5 digits after the decimal point.

4.3.4. OBT to UTC Time Conversion

UTC time is a function of the Time Correlation Packets and the on-board time (OBT). The Time Correlation Packets contains linear segments that map the on-board time to UTC time. The linear segment is represented by a time offset and a time gradient.

The conversion function is:

Time in UTC = offset + (OBT(seconds) + (OBT(fractional part) * 2-16)) * gradient

Time Correlation Packets are converted to a SPICE spacecraft clock kernel (SCLK) and distributed in the SPICE bundle. The SPICE spacecraft clock kernel (SCLK) can be used to convert the time stamps in the telemetry data (OBT in spacecraft clock format) to the corresponding UTC time.

The relevant mission-specific annex to this document will describe the specifics of OBT to UTC conversion as they apply to a given mission.

IMPORTANT: without applying the correction via time correlation (i.e. simply adding the clock ticks to the epoch), the time will NOT be in UTC and should not be used in archival products unless agreed with the mission archive scientist.

5. PSA POLICIES REGARDING DATA PROVISION

5.1. General Policies

Data Providers should always be aware that archival products have the purpose of serving the entire community therefore should be as user friendly as possible. The following statement is from the PDS Data Providers Handbook: "The general philosophy is that in order to preserve data for the long term, formats must be as simple as possible, well- described, and not reliant on specific software, because that software may be unavailable in the future."
The following is the PDS Standard Policies:

"All data must be provided in one or more of the following formats:

1. *Fixed-width binary or ASCII tables that are composed of identically structured records*
2. *N-dimensional homogeneous arrays of binary elements (N<=16)*
3. *Variable-width ASCII tables composed of identically defined records, where the individual, variable-width fields in the record are delimited and the variable length records are also delimited*
4. *NAIF / SPICE kernel files."*

Furthermore the PSA recommends that:

- products are constructed as simply as possible, generally for each label there should only be a single product, any other implementation will require prior agreement.
- where possible Table data products should use ASCII_Real or ASCII_Integer with fixed width and comma as delimiter, this ensures the data can be viewed easily.

Note for each processing stage more than one product may be supplied. Housekeeping data which have been converted into physical units can be considered either Partially_Processed or Calibrated data, according to the mission in question and the corresponding Annex should be consulted to see which applies.

5.2. Raw Data

- The provision of raw data to the PSA is mandatory.
- Raw data should respect the general policy, hence the TM needs to be parsed and re-formatted into readable tables, images, or other formats as appropriate.
- In some rare cases a data provider may wish to supply a product which is essentially the TM still in the original Hex byte format but re-packaged into a PDS4 product. Such products will be allowed by the PSA but **only** if also accompanied by more easily parsable raw products.

5.3. Partially Processed Data

- The provision of Partially_Processed science data to the PSA is optional.
- If instrument science data requires a conversion to physical units before further processing, the PSA strongly encourages archiving data at this level.
- Furthermore for instruments where part of the processing is strongly dependent on an algorithm selected by the operator, archival of data from this stage of processing is also strongly encouraged. Examples of this would be the storage of interferograms from a Fourier Transform Spectrometer, and images from a camera before geometric calibration.
- Generally there is the expectation that calibration data will only be processed to this level.

5.4. Calibrated Data

- The provision of Calibrated data to the PSA is mandatory.
- As per the PDS standard Calibrated Products should have all instrument aspects removed, therefore typical examples of Calibrated Products would include spectra and non-mosaiced images.

5.5. Derived Data

- The provision of Derived data is optional, but strongly encouraged to enhance the scientific usability of the archive.
- Where clearly different derived products are supplied for an instrument, the possibility exists to create different derived collections. For example a spectrometer studying the atmosphere of a planet may supply both temperature profiles and maps of a particular species. Similarly a camera team may wish to supply stereo images, DTM and mosaics.

5.6. Browse Products

Browse products are considered essential by both the PSA and end-users. These are typically graphical representations of the data in a form that allows the user to quickly asses if the product is of interest or use. The PSA website and other PDS4 compatible software can use these to help the user make a product selection. Such products can be provided for science, or even housekeeping data.

The additional recommendations are given for the creation of browse products:

- The recommended formats for the browse images in PSA are JPEG and PNG.
    - JPEG is recommended for pictures and PNG for plots.
- The browse image size is flexible and must ensure that enough details are visible.
    - anything with a size of less than 128 pixels should be considered as insufficient

  - no maximum size is given, but if the file size exceeds one or two megabytes the PSA should be consulted

- Note that browse images in JPEG format should use the file extension ".jpg".

Each Browse image must be accompanied by a label file. Browse products should link to science products and observational products must also link to browse products using Internal_References, the types are:

- data_to_browse
- browse_to_data

It is possible to use just the LID or the LIDVID (including version) in these references. The PSA recommendation is to use LID only, since this allows new versions of products to be ingested and linked to the latest browse image without any risk of broken links, or indeed for a re-processed browse image to be added without having to supply new data products. However, linking to specific versions is possible if necessary. Please contact your mission archive scientist if this is the case.

When more than one browse product applies, by PSA convention, the first reference to a browse product will become the primary browse product. This convention is necessary because no way of specifying a primary browse product is yet available in the PDS4 standard.

Browse Product PDS4 templates will be made available in the PSA bundle, but the snippet below gives a complete example:

```xml
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<?xml-model href="http://pds.nasa.gov/pds4/pds/v1/PDS4_PDS_1B00.sch"
schematypens="http://purl.oclc.org/dsdl/schematron"?>
<Product_Browse
    xsi:schemaLocation="http://pds.nasa.gov/pds4/pds/v1
http://pds.nasa.gov/pds4/pds/v1/PDS4_PDS_1B00.xsd
    http://psa.esa.int/psa/v1 http://psa.esa.int/psa/v1/PDS4_PSA_1000.xsd"
    xmlns="http://pds.nasa.gov/pds4/pds/v1"
    xmlns:psa="http://psa.esa.int/psa/v1"
    xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">

    <Identification_Area>

<logical_identifier>urn:esa:psa:bc_mpo_mag:browse_raw:mag_raw_sc_browse_20160413t213630
</logical_identifier>
        <version_id>1.0</version_id>
        <title>MPO-MAG PDS raw science data browse product</title>
        <information_model_version>1.11.0.0</information_model_version>
        <product_class>Product_Browse</product_class>
        <Modification_History>
            <Modification_Detail>
                <modification_date>2018-07-11</modification_date>
                <version_id>1.0</version_id>
                <description>First Version</description>
            </Modification_Detail>
        </Modification_History>
    </Identification_Area>

    <Reference_List>
        <Internal_Reference>

<lid_reference>urn:esa:psa:bc_mpo_mag:data_raw:mag_raw_sc_20160413t213630</lid_referenc
e>
            <reference_type>browse_to_data</reference_type>
        </Internal_Reference>
    </Reference_List>

    <File_Area_Browse>
        <File>
            <file_name>mag_raw_sc_browse_20160413T213630.png</file_name>
            <creation_date_time>2018-07-11T12:47:52.942Z</creation_date_time>
            <file_size unit="byte">334940</file_size>
            <md5_checksum>a0cdad54d3840fd9dd4e5a92fe2b4f9d</md5_checksum>
        </File>
        <Encoded_Image>
            <offset unit="byte">0</offset>
            <encoding_standard_id>PNG</encoding_standard_id>
        </Encoded_Image>
    </File_Area_Browse>

</Product_Browse>
```

Table 1 Example of Browse Product label

The following reference should be added to the applicable science product:

```
<Reference_List>
    <Internal_Reference>

<lid_reference>urn:esa:psa:bc_mpo_mag:browse_raw:mpo_raw_sc_browse_20160413t213630</lid
_reference>
        <reference_type>data_to_browse</reference_type>
    </Internal_Reference>
</Reference_List>
```

Table 2 Example of Browse Product label

These examples are minimal, but missions may require additional meta-data. For example browse product labels can include a Context_Area which may be necessary to include meta-data to help classify the product, rather than relying on resolving the link to the data products first.

5.7. Calibration Data Products

Calibration data may be data files of derived parameters used as inputs to data processing, e.g. pixel number to wavelength, bias value vs gain etc. Calibration data may also be data taken periodically in-flight and used in a time based way for data processing. Examples of these data may be internal or external darks or flat fields, reference spectra of the Sun or other celestial objects etc.

For storage in the PSA three collections are allowed:

- calibration_files (for 'static' data processing files)
- calibration_raw
- calibration_partially_processed

Data taken via in-flight measurements must use the Product_Observational PDS class. Data files used for data processing, taken from ground-based measurements or derived from in-flight data should use the Product_Ancillary.Any calibration observational product or file used as part of a data processing system for processing a particular calibrated data product must be referenced by that data product with the Internal references discussed previous, in particular Source_Product_Internal. For any PDS version prior to 1.11, the Processing_Inputs class from PSA schema 1.0 should be used. **IMPORTANT**: Note that only observational data from the calibration_raw and calibration_partially_processed collections will be visible in the PSA Filter Menu/Table View interface. The other data (coefficients, look up tables etc.) will be available through the FTP interface and via the download manager which will shortly be implemented, providing they are linked from appropriate products.

5.8. Geometry Products

Geometry information may be provided via products in the Geometry collection or as part of observational data products. A minimum set of geometry data to be included with all observational products is currently under consideration and specific policies regarding this will appear in future versions of this document.

6. PRODUCT LABELS

PDS labels are required for describing the contents and format of each individual product. In PDS4, all labels are detached (i.e. separate file) from the files containing the actual data. PDS4 labels are written in XML format. There is one PDS4 label (with file extension "xml") for every product.

The following sections refer to the PDS4 standard from version 1.8 onward and are valid for all PDS4 data currently in the PSA. However as PDS4 is still a relatively new standard, some aspects are still undergoing change. At the time of this issue (2.1) the current version of PDS is 1.10. Where there have been changes since 1.8 or where changes are expected for the next version, the different cases will be treated separately in the appropriate section below. A full description of the changes between each version of the PDS4 standard can be found in the release notes of each Information Model release (see https://pds.jpl.nasa.gov/datastandards/documents/im/).

Figure 3 shows the general structure of a label, simplified to top-level classes that appear in a typical label of an observational product. Most of the top-level classes shown in this figure have nested classes. For detailed information in the structure and content of the PDS4 labels, see section 3 in the PDS4 Standards Reference [AD.01].

XML Declaration and Schema Reference Information

```
<Product Type>
<Identification_Area>
          <Alias_List>
          <Citation_Information>
          <Modification_History >
<Observation_Area>
          <Time_Coordinates>
          <Primary_Result_Summary>
          <Investigation_Area>
          <Observing_System>
          <Target_Identification>
          <Mission_Area>
          <Discipline_Area>
<Reference_List>
              <External_Reference>
              <Internal_Reference>
              <Source_Product_Internal>
              <Source_Product_External>
```

```
<File_Area_Observational>
               <File>
               <Data Structure(s)>
<File_Area_Observational_Supplemental>
               <File>
               <Data Structure(s)>
</Product Type>
```

Figure 3: Simplified PDS4 label example

Product Type	***Top-level Classes***	***Reference***
Product_Observational	Identification_Area Observation_Area Reference_List File_Area_Observational File_Area_Observational_Supplemental	See Product_Observational in the PDS4 Schema (XSD).
Product_Ancillary	Identification_Area Context_Area Reference_List File_Area_Ancillary	
Product_Browse	Identification_Area Reference_List File_Area_Browse	See Product_Browse in the PDS4 Schema (XSD).
Product_Thumbnail	Identification_Area Reference_List File_Area_Encoded_Image	See Product_Thumbnail in the PDS4 Schema (XSD).
Product_Document	Identification_Area Context_Area Reference_List Document	See Product_Document in the PDS4 Schema (XSD).
Product_File_Text	Identification_Area Reference_List File_Area_Text	See Product_File_Text in the PDS4 Schema (XSD).
Product_SPICE_Kernel	Identification_Area Context_Area Reference_List File_Area_SPICE_Kernel	See Product_SPICE_Kernel in the PDS4 Schema (XSD).

Table 10: Top-level classes in PDS4 labels valid for PDS version 1.8 onwards

PDS4 labels must be compliant with:

- The class and attribute structures defined by the PDS, PSA and by the relevant mission in their respective XML Schemas (XSD files).
- The rules governing specific attributes and their values as set by the PDS, PSA and relevant mission in their respective XML Schematron files (SCH files).

6.1. Label Structure Requirements

Label structure requirements specific to the Planetary Science Archive and any mission archiving within the PSA (i.e. mandatory and optional attributes and classes, and rules restricting their values) are provided in the form of XML schemas (PSA PDS4 Schemas or <*Mission*> PDS4 Schemas).

A summary of the requirements will be provided below classified by product type. This is under definition, to be completed in the next version of the document.

6.1.1. XML Declaration

Each label starts with the XML Declaration and a declaration of the schematrons to be used. The statement beginning with <?xml is an XML declaration. It means that the label is an XML versioned document. The statement beginning with <?xml-model is a processing instruction. It identifies the Schematron file against which the label is validated. The Schematron forms part of the dictionary, and each mission will specify the applicable version, which may change over the mission. A label must have at least one such statement (pointing to the Schematron for the PDS version in use) but will typically have several. Note the xml-model statement does not allow multiple instances of the “href” statement. A separate statement should be used for each schematron specified e.g.

```
<?xml version="1.0" encoding="UTF-8"?>
<?xml-model href="http://pds.nasa.gov/pds4/pds/v1/PDS4_PDS_1A00.sch"
schematypens="http://purl.oclc.org/dsdl/schematron"?>
<?xml-model href="http://pds.nasa.gov/pds4/geom/v1/PDS4_GEOM_1900_1510.sch"
schematypens="http://purl.oclc.org/dsdl/schematron"?>
```

Figure 4: Example XML declaration and declaration of schematrons

Each mission archive scientist will be able to supply a template file upon request.

Schema Reference Information

Next the Product class is opened and the schema locations and namespaces are declared.

```
<Product_Observational
  xsi:schemaLocation ="http://pds.nasa.gov/pds4/pds/v1
http://pds.nasa.gov/pds4/pds/v1/PDS4_PDS_1800.xsd
  http://psa.esa.int/psa/v1 http://psa.esa.int/psa/v1/PDS4_PSA_1000.xsd
  http://psa.esa.int/psa/em16/cas/v1
http://psa.esa.int/psa/em16/cas/v1/PDS4_PSA_EM16_CAS_1000.xsd
  http://pds.nasa.gov/pds4/geom/v1
http://pds.nasa.gov/pds4/geom/v1/PDS4_GEOM_1800_1401.xsd"
  xmlns = "http://pds.nasa.gov/pds4/pds/v1"  xmlns:cas =
"http://psa.esa.int/psa/em16/cas/v1"  xmlns:geom =
"http://pds.nasa.gov/pds4/geom/v1"  xmlns:psa =
"http://psa.esa.int/psa/v1"  xmlns:xsi = "http://www.w3.org/2001/XMLSchema-
instance">
```

Figure 5: Example of declaring schema locations and namespaces from an ExoMars 2016 CaSSIS Instrument data product.

These namespaces are used as a shorthand method to include classes and attributes from other dictionaries without having to include the entire URI. So, for example, the PSA dictionary is linked to the psa namespace, so that classes within it can be referred to with this prefix. For example psa:Observation_Context. In this example the PDS core dictionary is declared as the default namespace - all classes and attributes that are not prefixed by a namespace reference are assumed to come from this dictionary.

All dictionaries used in the label must be declared, typically this will be the core PDS dictionary, any relevant discipline dictionaries such as the Geometry dictionary in the example above and any mission or instrument specific dictionaries.

Note that the versions of the schema and schematron files used must be the same. Missions will upgrade the core PDS information model and dictionary versions over time; consult the mission archive scientist or check in the relevant mission Annex for the correct version.

6.1.2. Identification_Area

All labels must include the Identification_Area, which includes the logical_identifier and version_id (forming the LIDVID, and uniquely identifying this product). The information_model_version must also be specified - this will be controlled by the SGS for the appropriate mission, and should match the version of the PDS schema and Schematron. Similarly, the value product_class should match the root class for this product (e.g. a Product_Observational product should have product_class equal to Product_Observational).All PDS products submitted to the PSA must include the Modification_History class, including one Modification_Detail entry for each version of the product. If a software pipeline is used to generate the label, it must either keep a version history of these changes, or append and increment the version, as necessary. An example Identification_Area is shown here:

```
<Identification_Area>


<logical_identifier>urn:esa:psa:bc_mpo_isa:calibration_files:isa_calib_coefficients</lo
gical_identifier>
    <version_id>0.2</version_id>
    <title>ISA calibration data</title>
    <information_model_version>1.11.0.0</information_model_version>
    <product_class>Product_Ancillary</product_class>

    <Modification_History>
        <Modification_Detail>
            <modification_date>2019-02-05</modification_date>
            <version_id>0.1</version_id>
            <description>First entry</description>
        </Modification_Detail>
    </Modification_History>

    <Modification_History>
        <Modification_Detail>
            <modification_date>2019-02-07</modification_date>
            <version_id>0.2</version_id>
            <description>Fixed errors</description>
        </Modification_Detail>
    </Modification_History>

</Identification_Area>
```

Table 3 Identification_Area

6.1.3. Product Observational

The following table provides a list of the label requirements for an observational product produced directly from instrument data - this typically means products in the following collections:

- data_raw
- data_partially_processed
- data_calibrated
- calibration_raw
- calibration_partially_processed

For higher level products the requirements should be discussed with the mission archive scientist.

Class	*Parent Class*	*Required*	*Remarks*
Observation_Area			
Time_Coordinates	Observation_Area	**Required**	start_date_time and stop_date_time are **mandatory**, the class also allows some additional optional time coordinates.
Primary_Result_Summary	Observation_Area	**Required**	See next section
Investigation_Area	Observation_Area	**Required**	Mission information (investigation) shall follow the conventions in the corresponding mission appendix
Observing_System	Observation_Area	**Required**	Spacecraft and Instrument information (type and name) shall follow the conventions in the corresponding mission annex (Mission annexes PDS4)
Mission_Area	Observation_Area	**Required**	See section 7.2.3
Discipline_Area	Observation_Area	Required	See section 7.2.4

Table 11: Requirements for PDS4 labels of observational products

6.1.4. Primary_Result_Summary

This class is used to provide a high-level description of the type of product.

Element	*Type*	*Required*	*No. Occurrences*	*Remarks*
purpose	Attribute	Required	1	See allowed values here.
processing_level	Attribute	Required	1	Indication of the level of processing that has been applied to the data. See allowed values here.
description	Attribute	Required	1	Brief description of the product.
Science_Facets	Class	Optional	0..n	See definition and structure here.

Table 12: Required attributes and classes in Primary Result Summary

6.2. Use of Classes and Attributes

6.2.1. The Mission Area

Mission specific classes and attributes must be included in the <Mission_Area> class of a PDS4 label, which is only available in the following product types:

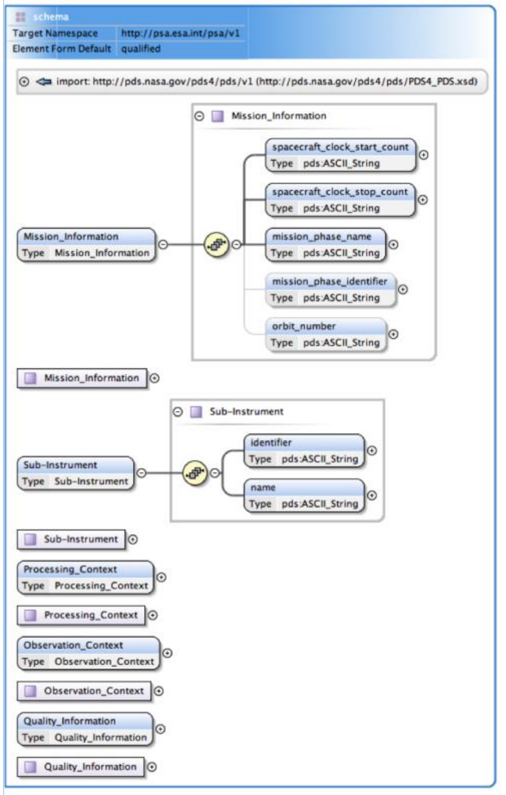
- Product_Observational
- Product_Ancillary
- Product_Bundle
- Product_Collection
- Product_Document

- Product_Native
- Product_SPICE_Kernel
- Product_XML_Schema

It is generally excluded from other Product types such as Product_Browse as there is an expectation that internal references back to observational or other appropriate products will be used.

6.2.2. Use of the PSA Dictionary in the Mission Area

The PSA Dictionary hosts classes and attributes which are common to all missions. Therefore it is considered useful in a multi-mission archive to have these overriding set of attributes applied uniformly in the archive, simplifying the architecture.



```xml
<!-- ================================================================================ -->
<!-- Mission Area: Attributes specific to PSA & BepiColombo (from their Local Data Dictionary)   -->
<!-- ================================================================================ -->

<!-- IMPORTANT: PSA and Mission Local Data Dictionaries are under construction -->
<Mission_Area>

    <psa:Mission_Information>
        <psa:spacecraft_clock_start_count>0/1.0</psa:spacecraft_clock_start_count>
        <psa:spacecraft_clock_stop_count>0/2.0</psa:spacecraft_clock_stop_count>
        <psa:mission_phase_name>cruise</psa:mission_phase_name>
        <psa:mission_phase_identifier>NECP</psa:mission_phase_identifier>
        <psa:orbit_number>1</psa:orbit_number>
    </psa:Mission_Information>

    <psa:Sub-Instrument>
        <psa:identifier>id</psa:identifier>
        <psa:name>name</psa:name>
    </psa:Sub-Instrument>

    <psa:Quality_Information>
        <psa:quality_flag>flags</psa:quality_flag>
    </psa:Quality_Information>

    <psa:Observation_Context>
        <psa:observation_identifier>obsid</psa:observation_identifier>
        <psa:pointing_mode>pointing_mode</psa:pointing_mode>
    </psa:Observation_Context>

    <psa:Processing_Context>
        <psa:processing_software_title>calibration_sw</psa:processing_software_title>
        <psa:processing_software_version>1.0</psa:processing_software_version>
    </psa:Processing_Context>

</Mission_Area>
```

Figure 6: PSA PDS4 dictionary (Mission Area) and an example of a <Mission_Area> section in a PDS4 label

The following policies apply to the use of the PSA dictionary:

The Mission_Area is **required** for all for Product Observational products

Mission_Information:

mission_phase_name is mandatory. "Not Applicable" may be used with agreement of the mission Archive Scientist e.g. ground based supporting data obtained in parallel with flight data. Validation rules are be added by each mission under the responsibility of the Archive Scientist.

spacecraft_clock_start/stop_count Both the UTC time and spacecraft clock count should be included in the labels. UTC is entered in the Observation_Area/Time_Coordinates class as above, and spacecraft clock count is in the PSA Mission Information class. It is useful to store the original spacecraft clock count in case the conversion to UTC is done incorrectly. This is mandatory for observational products in the data and calibration collections (e.g. data_raw, calibration_partially_processed), but may not be appropriate in, for example, aggregated products in the data_derived collection.

Sub-Instrument: (a sub-instrument here can be a sub-unit of an instrument (e.g. a UV or VIS detector) or an instrument which is part of an instrument suite)

identifier is the short name/acroynm of the sub-instrument or sub-unit

name is the full name of the sub-instrument or sub-unit

type The PSA has adopted the IPDA instrument type list and the value will be validated against the list below. Note the instrument_type attribute in the PDS instrument class must adhere to the PDS validation rule (see below). This attribute is optional but its use is strongly encouraged where applicable, and may be enforced at the mission level.

subtype is a free-text attribute in which more information can be given about the instrument type. For example is type is Magnetometer, subtype could add "dual fluxgate" or similar.

Observation_Context (not mandatory for PSA but may be enforced at mission level)

instrument_pointing_mode

the following values are allowed: Surface, Atmosphere, Limb, No pointing, Space

if you feel these values do not adequately describe your data, contact the relevant mission archive scientist

instrument_pointing_description

mandatory if instrument_pointing_mode is included

observation_identifier

this field is used to record the identifier of the planned observation generating the labelled data

consult the mission archive scientist for the format and source of this ID.

6.2.3. Use of Mission Dictionaries

Mission specific classes and attributes are defined by the by the relevant Science Ground Segment, according to the mission needs, in XML Schema files that are referred to as Mission dictionaries. The Mission specific needs are defined in the appendices of this document. Mission specific classes will include e.g. spacecraft clock start/stop time stamps, mission phase, orbit number, observation context information, data quality flags, processing context information (including processing SW version, input files/parameters, any other relevant processing information).

6.2.4. Use of Discipline Specific Classes and Attributes

The Discipline Area of a label is used to add attributes from the various PDS discipline dictionaries, which can be downloaded from here.

Product_Observational

Product_Context

Product_Ancillary

Product_Bundle

Product_Collection

Product_Document

Product_Native

Product_SPICE_Kernel

Product_XML_Schema

6.2.5. Upcoming Changes to PDS and impact on the PSA

The success of the PSA dictionary had led to PDS creating the MSN (Mission) dictionary at discipline level and we aim to have data providers transitioning to using this dictionary shortly. This will depend on whether the MSN LDD is stable by then and contains all PSA needed attributes.

PDS is currently undergoing a study on a change to instrument_type, currently this is validated against a core list but may move to implementing a new attribute instrument_type_list where a discipline level list may be used. If this goes ahead in the PSA will adopt the IPDA list and make it's use mandatory

Also currently under study is the LID formation rules for Targets, specifically within Target Context files. These changes mostly affect targets with primary/secondary bodies.

PDS Version 1.8, 1.9 and 1.10:

Labels must use PSA schema version 1.0

Data must reference the Mission_Information class in the PSA dictionary

PDS Version 1.11 onwards:

Labels must reference PSA schema version 1.1

Data should reference the Mission_Information class in the MSN dictionary provided that the MSN rules do not conflict with PSA or mission specific rules (e.g. mission phases)

with agreement of the mission archive scientist

Instrument_type may be replaced by instrument_type_list, if this is implemented the IPDA list must be used

References to Target LIDs may need to be updated

A PSA validation rule will be added to PSA schema version 1.1 which will check that the PDS attribute target_name matches the Target LID referenced, for example if the target_name attribute is "Mars" the referenced context file should not be the one for the Sun

Add note to mention that as of PSA LDD 1.1 (compatible with PDS4 IM 1.10.1.0), Processing_Context:Processing_Inputs will be moved to the PDS4 IM (see applicable issue, CCB-177)

Reference_List was updated by adding two new associated classes Source_Product_Internal and Source_Product_External.

6.3. Attributes Used For the PSA Filter Menu

6.3.1. Instrument_Type

The instrument_type attribute does not appear in Product Observational as it can only be referenced from the Context_Area class. Therefore each Product Observational produced by an instrument must have an Observing _System_Component:Instrument with a LID reference back to the appropriate instrument context file. The PSA will then use this to reference link the instrument type to the observational data. For other products, which have a Context_Area, the instrument_type attribute can be used directly. Note as stated above the use of the PDS instrument_type attribute may change in version 1.11.

For non-Instrument data such as spacecraft HK the observing system component = Instrument should be omitted and only the mission, and if appropriate, host should be used.

The IPDA instrument type list, currently only available to the PSA Sub-Instrument class, has been agreed by the IPDA members but has yet not been adopted by PDS. Therefore this list can only be used for a "mission level" attribute. The PSA uses this list to validate sub-instrument_type and this attribute must conform to one of these values:

In-Situ and Radio	Remote sensing-like	Laboratory-like	Others
Radio science	Imager	Microscope	Seismometer
Radar	Imaging spectrometer	Surface tool	Interferometer
Magnetometer	Spectrometer	Sub-surface tool	Gravimeter
Radiometer	Mass spectrometer	Biology experiment	Spectrograph
Particle analyser	Neutron detector	Weather station	SPICE kernels
Dust analyser	Gamma ray detector	Gas analyser	Compilation
Relaxation sounder	Altimeter	Sensor suite	Accelerometer
Mutual impedance probe	Polarimeter	Chemistry laboratory	Spacecraft sensors
Radio receiver		Temperature sensor	Microphone
Spectrum analyser			Not applicable
Electric field instrument			
Langmuir probe			

6.3.2. Wavelength and the Science Facets Class

Although the use of wavelength_range in the Observation_Area:Primary_Result_Summary:Science_Facets is optional in PDS, it is mandatory for observational data in the PSA. Currently, as of PDS version 1.10 the following values are allowed:

Far Infrared

Gamma Ray

Infrared

Microwave

Millimeter

Near Infrared

Radio

Submillimeter

Ultraviolet

Visible

X-ray

Although this is mandatory, the check is not enforced by the PSA dictionary since there is no way to specify "not applicable" for those instruments for which wavelength range is not appropriate. This attribute will be made "nillable" in a future version of the PDS Information Model. In this way it can still be included, but the user and the GUI will know that "Not Applicable" or similar should be displayed. The mandatory use of the wavelength attribute implies the mandatory use of the Science_Facets class in the Primary_Result_Summary. When this class is instantiated the discipline_name attribute must also appear. The allowed list for this attribute is currently:

Atmospheres

Fields

Flux Measurements

Geosciences

Imaging

Particles

Radio Science

Ring-Moon

Systems

Small Bodies

Spectroscopy

Given that this list is a combination of names of actual disciplines with names of PDS nodes the PSA does not consider this a useful attribute and it is not used. Data Providers are free to put the disciple that best matches the data. Note the domain_name, which is optional is Science_Facets, is also not yet being used by PSA. Data providers are, however, encouraged to populate this attribute as it is under consideration for future use. The current list of domain names are:

Atmosphere

Dynamics

Heliosphere

Interior

Interstellar

Ionosphere

Magnetosphere

Rings

Surface

7. GEOMETRY

Geometry information may be provided via products in the Geometry collection or as part of observational data products. A minimum set of Geometry data to be included with all observational products is currently under consideration. Below a preliminary list of the requirements and recommendations, to be consolidated in future versions of this document.

Required : The source data and methods used for generating the geometry data must be documented in the corresponding Experiment-to-Archive ICD (EAICD), along with documenting the coordinate/reference system used for the geometry data. The information should include a description of the quality (i.e., accuracy) of the geometry values.

7.1. Geometry Metadata expected in PDS labels

The rules on the layout and content of the geometry metadata in the PDS labels are defined in the PDS Geometry dictionary. Additional mission-specific guidelines can be found in the appropriate mission annex to this document.

The latest version of the PDS Geometry dictionary can be downloaded from the PDS4 website: https://pds.nasa.gov/pds4/schema/released/

As of PDS version 1.10, no official documentation (user guide) is available for the PDS Geometry dictionary. However, some guidelines can be found in the PDS Small Bodies Node (SBN) PDS4 Wiki, see relevant links below.

Quick Introduction to the Geometry Dictionary

Filling Out the Geometry Dictionary Classes

The table in section 8.1.3 includes a list of geometry attributes to be included in the label of the PDS products to be archived in the PSA, indicating whether the attribute is required, recommended or optional.

```
<!-- ============================================================================== -->
<!-- Discipline Area: Attributes specific to a given discipline e.g. geometry      -->
<!-- ============================================================================== -->

<Discipline_Area>

    <geom:Geometry>

        <!-- <geom:SPICE_Kernel_Files/> -->
        <!-- <geom:Image_Display_Geometry/> -->


        <geom:Geometry_Orbiter>
            <geom:geometry_reference_time>2015-10-04T00:00:00Z</geom:geometry_reference_time>
            <geom:Reference_Frame_Identification/>

            <geom:Coordinate_System>
                <geom:coordinate_system_type>type</geom:coordinate_system_type>
                <geom:coordinate_system_time>2015-10-04T00:00:00Z</geom:coordinate_system_time>
                <geom:Coordinate_System_Origin_Identification></geom:Coordinate_System_Origin_Identification>
                <geom:Reference_Frame_Identification></geom:Reference_Frame_Identification>
            </geom:Coordinate_System>

            <geom:Target_Identification/>

            <geom:Distances>
                <geom:spacecraft_heliocentric_distance unit="AU">0</geom:spacecraft_heliocentric_distance>
            </geom:Distances>

            <geom:Illumination_Geometry>
                <geom:Illumination_Single_Values>
                    <geom:emission_angle unit="deg">0</geom:emission_angle>
                    <geom:incidence_angle unit="deg">0</geom:incidence_angle>
                    <geom:phase_angle unit="deg">0</geom:phase_angle>
                </geom:Illumination_Single_Values>
                <geom:Illumination_FOV_Range_Values>
                    <geom:illumination_range_designation>0</geom:illumination_range_designation>
                </geom:Illumination_FOV_Range_Values>
            </geom:Illumination_Geometry>


        </geom:Geometry_Orbiter>
    </geom:Geometry>

</Discipline_Area>
```

Figure 7: Example of geometry metadata in a PDS4 label

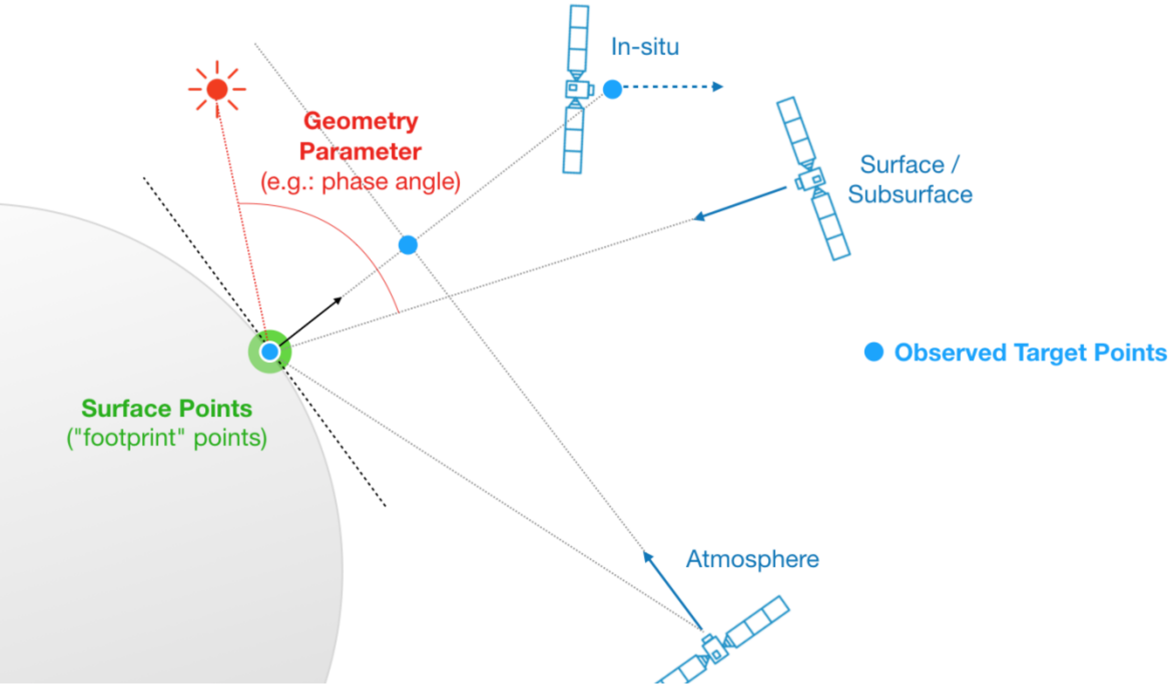
7.1.1. Surface point

As shown on the following figure, geometry parameters are computed at the *surface point* corresponding to the observed target point. Depending on the type of observation, the surface point would be:

for surface observations, the surface point is the intersection between the line-of-sight and the target body surface;

for atmosphere observations, the surface point is the nearest on the target body surface and the line-of-sight;

for in-situ observations, the surface point is the sub-spacecraft point;



7.1.2. Coordinate system and units

Longitudes and latitudes are expressed in planetocentric coordinate system.

All angles are expressed in degrees.

All distance are expressed in kilometres.

7.1.3. List of Geometry Attributes

The following table provides a set of geometry parameters currently being considered as guidelines for PDS4 labels. This list is provided as a guide only and the appropriate mission annex or the mission Archive Scientist should be consulted in case the use of a given parameter is unclear.

Names in bold are parameters used as inputs in the PSA user interface filter menu and entries in italics should be considered as "TBC".

Name	PSA Requirement	Description	Comments	PDS4 attribute
SPICE Kernels	required	This class is used to cite the SPICE kernel files used in calculating the associated geometric values.		Product_Observational: Observation_Area: Discipline_Area: Geometry: SPICE_Kernel_Files
Expanded Geometry	optional	Required when geometry is supplied as a separate geometry product.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Expanded_Geometry

start_time		Earliest UTC time corresponding to the observation footprint	Different from product label START/STOP_TIME keywords values when there are several footprints for an observation (due to limb observation, not currently the case with geogen).	
stop_time		Latest UTC time corresponding to the observation footprint		
reference_time	required	Reference UTC time at which the geometry parameters are computed.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: geometry_reference_time
center_latitude		Latitude of the observation footprint center point.	Planetocentric latitude of the pixel projected onto the target, in the range ±90°	Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Surface_Geometry_Specific: Pixel_Intercept: pixel_latitude with reference_pixel_location = Center
center_longitude		Longitude of the observation footprint center point.	Planetocentric longitude of the pixel projected onto the target, in the range 0-360°	Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Surface_Geometry_Specific: Pixel_Intercept: pixel_longitude with reference_pixel_location = Center
westernmost_longitude		Westernmost observation longitude of the footprint.	These give the extend / boundary box of a footprint and	Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Surface_Geometry_Min_Max: minimum_longitude

			can be used to perform first-order geometry search, without using the actual footprint geometry.	
easternmost_longitude		Easternmost observation longitude of the footprint.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Surface_Geometry_Min_Max: maximum_longitude
minimum_latitude		Minimum observation latitude of the footprint.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Surface_Geometry_Min_Max: minimum_latitude
maximum_latitude		Maximum observation latitude of the footprint.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Surface_Geometry_Min_Max: maximum_latitude
local_true_solar_time		Local solar time for the surface point, evaluated at the reference time. The local solar time is the angle between the planetocentric longitude of the Sun, as viewed from the center of the target body, and the planetocentric	spice.et2lst()	Product_Observational: Observation_Area: Time_Coordinates: local_true_solar_time

		longitude of the surface point, expressed on a “24 hour” clock.		
solar_longitude		Planetocentric longitude (Ls) of the sun for the target body at the reference time. The planetocentric longitude is the angle between the body-sun vector at the time of interest and the body-sun vector at the vernal equinox. This provides a measure of season on a target body, with values of 0 to 90 degrees representing northern spring, 90 to 180 degrees representing northern summer, 180 to 270 degrees representing northern autumn and 270 to 360 degrees representing northern winter.	spice.lspcn(), corrected for light time and stellar aberration ('LT+S').	Product_Observational: Observation_Area: Time_Coordinates: solar_longitude
sub_solar_latitude		Latitude of the sub-solar point on the target body at the reference time. The sub-solar point is the point on a body's reference surface where a line from the body center to the sun center intersects that surface.	spice.subslr() + spice.reclat(), correct ed for light time and stellar aberration.	Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Surface_Geometry_Specific: subsolar_latitude

sub_solar_longitude		Longitude of the sub-solar point on the target body at the reference time . The sub-solar point is the point on a body's reference surface where a line from the body center to the sun center intersects that surface.	spice.subslr() + spice.reclat() , corrected for light time and stellar aberration.	Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Surface_Geometry_Specific: subsolar_longitude
solar_distance		Distance from the center of the sun to the center of the target body at the reference time.	spice.spkpos() + spice.vnorm(sunpos)	Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Distances_Specific: target_heliocentric_distance
spacecraft_solar_distance		Distance from the spacecraft to the center of the sun at the reference time.	spice.spkpos() + spice.vnorm(sunpos-scpos)	Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Distances_Specific: spacecraft_heliocentric_distance
spacecraft_altitude		Distance from the spacecraft to the sub-spacecraft point on the target body at the reference time.	spice.subpnt() + spice.vnorm(srfvec=vector from observer to sub-observer point) Candidate for min/max parameter	Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Distances_Specific: spacecraft_target_subspacecraft_distance
target_center_distance		Distance from the spacecraft to the center of the target body at the reference time.	spice.spkpos() + spice.vnorm(scpos) Candidate for min/max parameter	Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Distances_Specific: spacecraft_target_center_distance
sub_spacecraft_latitude		Latitude of the sub-spacecraft point on the target body at the reference time .	spice.subpnt()+ spice.reclat() When using a triaxial ellipsoid to model the	Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Surface_Geometry_Specific: subspacecraft_latitude

			surface of the target body, the sub-spacecraft point is defined as the nearest point on the target relative to the spacecraft. The sub-spacecraft point is defined as the intercept, on the surface represented by the DSK data, of the line containing the spacecraft and the nearest point on the target's reference ellipsoid. If multiple such intercepts exist, the one closest to the observer is selected.	
sub_spacecraft_longitude		Longitude of the sub-spacecraft point on the target body at the reference time.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Surface_Geometry_Specific: subspacecraft_longitude
sub_spacecraft_solar_zenith_angle		Solar zenith angle at the sub-spacecraft point on the target body surface at the reference time. The solar zenith angle is the angle subtended between the		

		direction towards the Sun and the local normal at the surface.		
target_right_ascension		Right ascension of the position vector of the target body center as seen from the spacecraft in the Earth mean equator and equinox frame (J2000).	spice.spkezr(target, et, 'J2000', 'LT+S', obsrvr) spice.recrac()	Product_Observational: Observation_Area: Discipline_Area: Geometry: Image_Display_Geometry: Object_Orientation_RA_Dec: right_ascension_angle If used, the Reference_Frame_Identification and the Geometry_Target_Identification classes should be included.
target_declination		Declination of the position vector of the target body center as seen from the spacecraft in the Earth mean equator and equinox frame (J2000).		Product_Observational: Observation_Area: Discipline_Area: Geometry: Image_Display_Geometry: Object_Orientation_RA_Dec: declination_angle If used, the Reference_Frame_Identification and the Geometry_Target_Identification classes should be included.
sun_right_ascension		Right ascension of the position vector of the Sun as seen from the spacecraft in the Earth mean equator and equinox frame (J2000).	spice.spkezr('SUN', et, 'J2000', 'LT+S', obsrvr) spice.recrac()	Product_Observational: Observation_Area: Discipline_Area: Geometry: Image_Display_Geometry: Object_Orientation_RA_Dec: right_ascension_angle If used, the Reference_Frame_Identification and the Geometry_Target_Identification classes should be included.
sun_declination		Declination of the position vector of the Sun as seen from the spacecraft in the Earth mean equator and equinox frame (J2000).		Product_Observational: Observation_Area: Discipline_Area: Geometry: Image_Display_Geometry: Object_Orientation_RA_Dec: declination_angle If used, the Reference_Frame_Identification and the

				Geometry_Target_Identification classes should be included.
x_sc_sun_position		X component of the position vector from spacecraft to Sun, expressed in J2000 coordinates, and corrected for light time and stellar aberration, evaluated at the reference time.	spice.spkezr('SUN', et, 'J2000', 'LT+S', obsrvr)	Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Vectors: Vectors_Cartesian_Specific: Vector_Cartesian_Position_Sun_To_Spacecraft
y_sc_sun_position		Y component of the position vector from spacecraft to Sun, expressed in J2000 coordinates, and corrected for light time and stellar aberration, evaluated at the reference time.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Vectors: Vectors_Cartesian_Specific: Vector_Cartesian_Position_Sun_To_Spacecraft
z_sc_sun_position		Z component of the position vector from spacecraft to Sun, expressed in J2000 coordinates, and corrected for light time and stellar aberration, evaluated at the reference time.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Vectors: Vectors_Cartesian_Specific: Vector_Cartesian_Position_Sun_To_Spacecraft
x_sc_sun_velocity		X component of the velocity vector of Sun relative to the spacecraft, expressed in J2000 coordinates, and corrected for light time and stellar aberration, evaluated at the reference time.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Vectors: Vectors_Cartesian_Specific: Vector_Cartesian_Velocity_Spacecraft_Relative_To_Sun
y_sc_sun_velocity		Y component of the velocity vector of Sun relative to the		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter:

		spacecraft, expressed in J2000 coordinates, and corrected for light time and stellar aberration , evaluated at the reference time.		Vectors: Vectors_Cartesian_Specific: Vector_Cartesian_Velocity_Spacecraft_Relative_To_Sun
z_sc_sun_velocity		Z component of the velocity vector of Sun relative to the spacecraft, expressed in J2000 coordinates, and corrected for light time and stellar aberration , evaluated at the reference time.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Vectors: Vectors_Cartesian_Specific: Vector_Cartesian_Velocity_Spacecraft_Relative_To_Sun
x_sc_target_position		X component of the position vector from the spacecraft to target body center, expressed in J2000 coordinates, and corrected for light time and stellar aberration, evaluated at the reference time.	spice.spkezr(target, et, 'J2000', 'LT+S', obsrvr)	Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Vectors: Vectors_Cartesian_Specific: Vector_Cartesian_Position_Spacecraft_To_Target
y_sc_target_position		Y component of the position vector from the spacecraft to target body center expressed in J2000 coordinates, and corrected for light time and stellar aberration, evaluated at the reference time.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Vectors: Vectors_Cartesian_Specific: Vector_Cartesian_Position_Spacecraft_To_Target
z_sc_target_position		Z component of the position vector from the spacecraft to target body center expressed in J2000 coordinates, and		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Vectors: Vectors_Cartesian_Specific: Vector_Cartesian_Position_Spacecraft_To_Target

		corrected for light time and stellar aberration, evaluated at the reference time.		
x_sc_target_velocity		X component of the velocity vector of the target body center relative to the spacecraft, expressed in J2000 coordinates, and corrected for light time and stellar aberration, evaluated at the reference time.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Vectors: Vectors_Cartesian_Specific: Vector_Cartesian_Velocity_Spacecraft_Relative_To_Target
y_sc_target_velocity		Y component of the velocity vector of the target body center relative to the spacecraft, expressed in J2000 coordinates, and corrected for light time and stellar aberration , evaluated at the reference time .		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Vectors: Vectors_Cartesian_Specific: Vector_Cartesian_Velocity_Spacecraft_Relative_To_Target
z_sc_target_velocity		Z component of the velocity vector of the target body center relative to the spacecraft, expressed in J2000 coordinates, and corrected for light time and stellar aberration , evaluated at the reference time .		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Vectors: Vectors_Cartesian_Specific: Vector_Cartesian_Velocity_Spacecraft_Relative_To_Target
min_incidence_angle		Minimum incidence angle. The incidence angle is the angle between the local vertical at a given surface point and the	spice.ilumin() When using a DSK as surface model for an atmosphere	Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Illumination_Geometry: minimum_incidence_angle

		vector from the surface point to the sun.	observation (line-of-sight not intersecting the surface), illumination angles are computed with respect to the DSK. Shouldn't it be computed with respect to the ellpsoid?	
max_incidence_angle		Maximum incidence angle. The incidence angle is the angle between the local vertical at a given surface point and the vector from that the surface point to the sun.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Illumination_Geometry: Illumination_Min_Max: maximum_incidence_angle
min_emission_angle		Minimum emission angle. The emission angle is the angle between the surface normal at a given surface point and the vector from the surface point to the spacecraft.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Illumination_Geometry: Illumination_Min_Max: minimum_emission_angle
max_emission_angle		Maximum emission angle. The emission angle is the angle between the surface normal at a given surface point and the vector from the surface point to the spacecraft.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Illumination_Geometry: Illumination_Min_Max: maximum_emission_angle

min_phase_angle		Minimum phase angle. The phase angle is the angle between the vectors from the surface point to the spacecraft and from the surface point to the Sun.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Illumination_Geometry: Illumination_Min_Max: minimum_phase_angle
max_phase_angle		Maximum phase angle. The phase angle is the angle between the vectors from the surface point to the spacecraft and from the surface point to the Sun.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Illumination_Geometry: Illumination_Min_Max: maximum_phase_angle
min_slant_distance		Minimum slant distance. The slant distance is the distance from the spacecraft to the nearest point on the detector line-of-sight to the target body surface.	Surface: spoint, trgepc, srfvec, found = spice.sincpt(method, target, et, fixref, abcorr, obsrvr, dref, dvec) spice.vnorm(srfvec) Atmosphere: trg_pnear, dist = spice.npedln(trg_radii[0], trg_radii[1], trg_radii[2], scpos, dvec) los_pnear, dist = spice.nplnpt(scpos, dvec, trg_pnear)	Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Distances_Min_Max: minimum_spacecraft_target_boresight_intercept_distance

			slant = spice.vnorm(los_pnear-scpos) In-Situ: Should always be 0.	
max_slant_distance		Maximum slant distance. The slant distance is the distance from the spacecraft to the nearest point on the detector line-of-sight to the target body surface.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Distances_Min_Max: maximum_spacecraft_target_boresight_intercept_distance
min_tangent_altitude		Minimum tangent altitude. The tangent altitude is the distance from the target body surface nearest point to the detector line-of-sight.	spice.npedln() When using DSK as surface model, the ellipsoid is used anyway as surface model to derive the nearest point on the surface from the line-of-sight (no existing SPICE function to derive this, conversation with Nat Bachman). However, the tangent altitude and slant distance are computed based on the DSK.	Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Distances_Min_Max: minimum_spacecraft_target_boresight_intercept_distance

max_tangent_altitude		Maximum tangent altitude. The tangent altitude is the distance from the target body surface nearest point to the detector line-of-sight.		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Distances_Min_Max: maximum_spacecraft_target_boresight_intercept_distance
horizontal_pixel_scale		horizontal/vertical picture scale. Alternative: distance per horizontal/vertical resolution unit at the center of the observation (LoS).		Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Pixel_Dimensions: horizontal_pixel_field_of_view with pixel_field_of_view_method = central pixel
vertical_pixel_scale				Product_Observational: Observation_Area: Discipline_Area: Geometry: Geometry_Orbiter: Pixel_Dimensions: vertical_pixel_field_of_view with pixel_field_of_view_method = central pixel
boresight_right_ascension		Right ascension of the detector boresight vector, in the Earth mean equator and equinox frame (J2000), at the reference time.	mat_detec_j2000 = spice.pxform(self.detector.frame, 'J2000', et) pvec = spice.mxv(mat_detec_j2000, dvec) spice.recrad()	TBC
boresight_declination		Declination of the detector boresight vector, in the Earth mean equator and equinox		TBC

		frame (J2000), at the reference time.		
boresight_target_angle		The separation angle between the detector line-of-sight (boresight) and the target body center as seen from the spacecraft, at the reference time.		TBC
boresight_solar_elongation		Separation angle between the detector line-of-sight and the position vector of the Sun as seen from the spacecraft, at the reference time.		TBC

7.2. Geometry Products

Geometry products can be generated, and should be included in the Geometry collection.

Some observations may need to include separate geometry products including pointing, orientation and positioning information (e.g. pixel-by-pixel information for high-resolution cameras or hyper-spectral qubes), typically provided as tables or arrays of calculated values.

GIS shape files with the observation footprints (and some additional geometry information) can also be considered for this collection, but discussions on an appropriate format are ongoing.

Specific guidelines will be added in a future version of this document.

8. PERMISSIBLE VALUES

The permissible values described in this section are only those applicable to all data being delivered for archiving within the PSA. The more specific values that are applicable to each mission are included as appendices to this document. Each mission shall have their own appendix listing the specific values defined for attributes at the mission, instrument host, instrument and target level, plus any additional criteria applicable only to that mission. The PDS Small Bodies Node (SBN) provides a useful wiki page giving a quick reference for standard values in PDS labels - although this is not definitive, it is a useful reference. For a definitive list of allowed values, consult the Data Dictionary for the release of PDS4, or check the relevant Schema and Schematron files.

8.1. Data Processing Levels

Data processing levels to be used are defined in the table below, and are based on the PDS Policy on Data Processing Levels (see PDS4 Standards Reference [AD.01], section 10B).

PDS4 Level Identifier	Definition
Telemetry	Original stream from an instrument encoded in telemetry packets.
Raw	Original data from an instrument. If compression, reformatting, packetization, or other translation has been applied to facilitate data transmission or storage, those processes will be reversed so that the archived data are in a PDS approved archive format.

Partially Processed	Data that have been processed beyond the raw stage but which have not yet reached calibrated status.
Calibrated	Data converted to physical units where all of the calibration based on the instrument has been done.
Derived	Results that have been distilled from one or more calibrated data products (for example, maps, gravity or magnetic fields, or ring particle size distributions). Supplementary data, such as calibration tables or tables of viewing geometry, used to interpret observational data should also be classified as 'derived' data if not easily matched to one of the other three categories. Geometry products and SPICE kernels will be classified as Derived.

Table 13: Data processing levels

9. SPICE KERNELS

The SPICE (Spacecraft Planets Instrument C- Matrix Events) information system uses *ancillary data* to provide Solar System geometry information to scientists and engineers for planetary missions in order to plan and analyze scientific observations from space-born instruments . SPICE is used on all PSA supported missions to assist the science data processing, analysis and archiving activities. SPICE is developed by the NASA´s Navigation and Ancillary Information Facility (NAIF) and is implemented for the PSA supported missions by the ESA SPICE Service (ESS). More information is available at the ESS home page:

http://spice.esac.esa.int

The SPICE toolkit is available in FORTRAN, C at the NAIF web site (http://naif.jpl.nasa.gov). Interfaces to higher-level data analysis software in the Interactive Data Language (IDL), Matlab and JAVA are also provided. A Python wrapper approved by NAIF (SpiceyPy), is also available.

SPICE data is known as "kernels". SPICE kernels are composed of navigation, orientation and other ancillary information structured and formatted for easy access. All SPICE kernels needed to compute the UTC time and geometric quantities for a mission must be archived along with the science data. Mission related SPICE kernels are generated mainly by the ESS (with the information provided by Flight Dynamics, the Science Ground Segment and by the Instrument Teams).

The archived SPICE kernels are peer-reviewed versions of the SPICE operational kernels datasets which are used in the study, development and operations of ESA Missions and which are available at the ESA SPICE FTP area:

ftp://spiftp.esac.esa.int/data/SPICE/ftp://spiftp.esac.esa.int/data/SPICE/<mission_name>/kernels/

In addition, both the SPICE operational kernels datasets and the archived SPICE bundles are mirrored in the NAIF server (https://naif.jpl.nasa.gov/pub/naif/).

A mission level bundle must be created containing all mission related SPICE kernels. The following SPICE kernel files might be included in each SPICE bundle:

SPK: Spacecraft and natural bodies ephemeris files, also known as the planetary spacecraft ephemeris kernel file, including the spacecraft trajectory of reconstructed and predicted positions.

DSK: Digital shape diles, include information of the digital shape of extended bodies (not always present)

CK: Spacecraft orientation file, also known as the attitude c-kernel (CK) file.

SCLK: Spacecraft clock file which contains the time correlation data to convert OBT to UTC.

FK: Mission Reference frames file, also known as the frame kernel.

IK: Instrument kernels.

PCK: Planetary constants file (*.tpc), also known as the planetary constants kernel (PCK) file.

LSK: NAIF leap seconds kernel.

MK: Meta-kernel files, which include a list of the relevant kernels to setup a unique and unambiguous mission scenario.

Due to its unique nature the SPICE bundles have some particularities with respect to the rest of the bundles of a given mission. These particularities are described in the following sections.

9.1. Product types

SPICE Bundles will include products only of these types:

Product_Bundle

Product_Collection

Product_SPICE_Kernel (under the "spice_kernels" directory)

Product_Document (under the "document" directory)

Product_Ancillary (under the "miscellaneous" directory)

Product_Zipped (under the "miscellaneous directory, if needed")

9.2. Directory structure and File naming

SPICE_Kernels products follow a particular directory structure and file naming convention. The SPICE_kernel collection is composed by a series of directories that contain kernels of each kernel type. This replicates the directory structure of the ESA SPICE FTP and the canonical SPICE kernel dataset structure.

The products in the SPICE_kernels collection filename is, except for the meta-kernel files, composed by:

<ker_name>.<kernel_extension>

where:

<ker_name>: is the kernel filename, in most cases very similar to the one which can be found in the ESA SPICE FTP area.

<kernel_extension>: is the kernel extension. Typically, it consists of a first letter describing the kernel format: “b” for binary and “t” for text, followed by one or two letters that reference the kernel tye e.g.: “sp” for SPK, “c” for CK, “sc” for SCLK.

Note that the kernel filename <ker_name> always contains a version number which identifies the kernel as a unique file and that is considered part of the filename and not a version number *per se*. Hence in an archive it is common to find products with filename - LIDVID pair such as:

em16_tgo_v01.tf - urn:esa:psa:em16_spice:spice_kernels: fk_em16_tgo_v0**1**.tf::**1**.0

em16_tgo_v02.tf - urn:esa:psa:em16_spice:spice_kernels: fk_em16_tgo_v0**2**.tf::**1**.0

The directory structure and the products contained in each directory –including LIDVIDs – are described in the following table:

Data Organisation (bold) and File name (italics)	N [1]	Product Type LIDVID
<mission_acronym>_spice/	1	
bundle_<sc>_spice_v<ver>.xml	1..n	Product_Bundle urn:esa:psa:<sc>_spice::<n>.0
readme.txt	1	fixed
document	1	fixed
collection_document_v<ver>.xml collection_document_inventory_v<ver>.csv	1..n	Product_Collection urn:esa:psa:<sc>_spice:document::<n>.0
spiceds_v<ver>.xml/.html	1..n	Product_Document urn:esa:psa:<sc>_spice:document:spiceds::<n>.0
miscellaneous	1	fixed
collection_miscellaneous_v<ver>.xml collection_miscellaneous_inventory_v<ver>.csv	1..n	Product_Collection urn:esa:psa:<sc>_spice:miscellaneous::<n>.0
spice_kernels	1	fixed
collection_spice_kernels_v<ver>.xml/.csv collection_spice_kernels_inventory_v<ver>.csv	1..n	Product_Collection urn:esa:psa:<sc>_spice:spice_kernels::<n>.0
ck	1	
<ker_name>.xml/.bc	1	Product_SPICE_Kernel urn:esa:psa:<sc>_spice:spice_kernels:ck_<filename.ext>::1.0
dsk	0,1	
<ker_name>.xml/.bds	1	Product_SPICE_Kernel urn:esa:psa:<sc>_spice:spice_kernels:dsk_<filename.ext>::1.0
fk	1	
<ker_name>.xml/.tf	1	Product_SPICE_Kernel

		urn:esa:psa:<sc>_spice:spice_kernels:fk_<filename.ext>::1.0
ik	1	
<ker_name>.xml/.ti	1	Product_SPICE_Kernel urn:esa:psa:<sc>_spice:spice_kernels:ik_<filename.ext>::1.0
lsk	1	
<ker_name>.xml/.tls	1	Product_SPICE_Kernel urn:esa:psa:<sc>_spice:spice_kernels:lsk_<filename.ext>::1.0
mk	1	
<sc>_v<ver>.xml/.tm	1..n	Product_SPICE_Kernel urn:esa:psa:<sc>_spice:spice_kernels:mk_<sc>_<ver>::<n>.0
pck	1	
<ker_name>.xml/.tpc/.bpc	1	Product_SPICE_Kernel urn:esa:psa:<sc>_spice:spice_kernels:pck_<filename.ext>::1.0
sclk	1	
<ker_name>.xml/.tsc	1	Product_SPICE_Kernel urn:esa:psa:<sc>_spice:spice_kernels:sclk_<filename.ext>::1.0
spk	1	
<ker_name>.xml/.bsp	1	Product_SPICE_Kernel urn:esa:psa:<sc>_spice:spice_kernels:spk_<filename.ext>::1.0

[1] Number of Occurrences

Table 14: Directory structure and products contained in each directory for SPICE archives

where:

<sc> is the short mission name or acronym (e.g. em16, bc, etc.).

<des> is a short description of the scope of a particular meta-kernel (scenario, mission phase, data type, instrument of applicability, etc.).

<ver> is a three-digit incremental version number present in the file name.

<n> is a one or multiple digit incremental version number present in the VID, if the product filename includes <ver> then this is a one or multiple digit version of <ver>.

Note that the miscellaneous collection can have other collections as needed containing Product_Ancillary described as Stream_Text, Table_Character of Encoded_Images. The document collection might contain other collections with Product_Document products. In addition a potential inclusion in the miscellaneous collection would be the checksum and orbnum data files for which the N and LIDVID would tentatively be as indicated in the table hereafter.

Data Organisation (bold) and File name (italics)	**N [1]**	Product Type LIDVID
checksum	0,1	
checksum_v<ver>.xml/.tab	1..n	Product_Ancillary (described as Checksum_Manifest) urn:esa:psa:<sc>_spice:miscellaneous:checksum_checksum::<n>.0

orbnum	0,1	fixed
<ker_name>.xml/.orb	1	Product_Ancillary (described as Table_Character) urn:esa:psa:<sc>_spice:miscellaneous: orbnum_<filename.ext>::1.0

9.3. LID/LIDVID Construction Rules

The LID/LIDVID construction rules, as it can be derived from the previous section are also particular for the SPICE bundles. The initial part of the LIDs for ESA missions will be “urn:esa:psa:<sc>_spice:" where <sc> is the mission acronym (e.g. em16, bc, etc.), e.g.:

urn:esa:psa:em16_spice:

There are four methods of constructing LIDVIDs depending on the product.

9.3.1. Path and full filename in LID

The first method ignores the version number referenced in the data filename (LID) for the VID construction and applies to following products:

SPICE kernels under **spice_kernels** except data in **mk**;

ancillary products under **miscellaneous**;

documents under **document**;

The LIDs will include the directory path and the full file name with extension and VIDs will always be set to 1, e.g.:

spice_kernels/fk/bc_mpo_v01.tf	urn:esa:psa:bc_spice:spice_kernels:fk_bc_mpo_v01.tls::1.0
spice_kernels/fk/bc_mpo_v02.tf	urn:esa:psa:bc_spice:spice_kernels:fk_bc_mpo_v02.tls::1.0
spice_kernels/spk/de430.bsp	urn:esa:psa:bc_spice:spice_kernels:spk_de430.bsp::1.0
spice_kernels/spk/de431.bsp	urn:esa:psa:bc_spice:spice_kernels:spk_de431.bsp::1.0

Table 15: Example of LIDVID as compared to the data filename for the "first method".

9.3.2. Path and filename without version in LID

The second method will include the directory path and the file name up to the version part and VIDs will always be set to the version part from the file name. This method applies to the following products:

mk SPICE kernels under the spice_kernels;

checksum tables;

primary SPICE archive description documents (spiceds_v<ver>.html)

spice_kernels/mk/bc_v001.tm	urn:esa:psa:bc_spice:spice_kernels:mk_bc::1.0
spice_kernels/mk/bc_v002.tm	urn:esa:psa:bc_spice:spice_kernels:mk_bc::2.0

document/spiceds_v001.html	urn:esa:psa:bc_spice:document:spiceds::1.0
document/spiceds_v002.html	urn:esa:psa:bc_spice:document:spiceds::2.0

Table 16: Example of LIDVID as compared to the data filename for the "second method".

9.3.3. Subdirectory name only in LID

The third method includes only the subdirectory name and VIDs will always be set to the version part from the file name. This schema applies to:

SPICE **document** collection products;

SPICE **miscellaneous** collection products.

SPICE_kernels collection top level directory products;

document/collection_document_v001.xml	urn:esa:psa:bc_spice:document::1.0
miscellaneous/collection_miscellaneous_v002.xml	urn:esa:psa:bc_spice:miscellaneous::2.0
spice_kernels/collection_spice_kernels_v010.xml	urn:esa:psa:bc_spice:spice_kernels::10.0

Table 17: Example of LIDVID as compared to the data filename for the "third method".

9.3.4. No filename in LID

The last method includes only the initial part of the LID and VIDs will always be set to the version part from the file name. It applies to:

all **SPICE bundle** products;

bundle_em16_spice_v001.xml	urn:esa:psa:em16_spice::1.0
bundle_em16_spice_v002.xml	urn:esa:psa:em16_spice::2.0

Table 16: Example of LIDVID as compared to the data filename for the "fourth method".

9.4. Product Reference and Collection Inventory Construction Rules

What follows is a set of rules provided by NAIF that the PSA implements to construct Product references and collection inventories:

All products' Context_Area includes only Mission (*_to_investigation), Spacecraft (is_instrument_host), and one primary Target (*_to_target) LID references. These LIDs should be obtained from the PSA.

All products' Reference_List includes the latest primary SPICE archive description document LID reference (*_to_document) (*except the primary SPICE archive description documents (spiceds_v<ver>.html) which can't reference themselves).

Each MK's Reference_List also includes LIDVID references for all kernels (data_to_associate) listed in the MK.

Each collection inventory lists LIDVIDs of *all* non-collection products provided under collection's directory at the time when collection product was created. In a particular collection inventory, ***P*** -for primary- is used only for newly added products (that don't appear in any of the collections with earlier versions) and ***S*** **–** for secondary - is used for products that have already been registered in a collection with an earlier version.

Each Bundle label includes Bundle_Member_Entry'es only for the latest SPICE kernel collection LIDVID (bundle_has_spice_kernel_collection), the latest document collection LIDVID (bundle_has_document_collection) and the latest miscellaneous collection LIDVID (bundle_has_miscellaneous_collection). These collections have Primary statuses if they have not been registered in any earlier bundle versions. Otherwise they have Secondary statuses.

9.5. Start and Stop Date Time Assignment Rules

What follows is a set of rules provided by NAIF that the PSA implements to assign start and stop date time to products:

start_date_time and *stop_date_time* appear in *Context_Area/Time_Coordinates* only in bundle, SPICE kernel collection, and SPICE kernel labels;

for kernels for which time boundaries can determined from the data (SPK, CK, etc) *start_date_time* and *stop_date_time* set to those boundaries;

for kernels for which time boundaries cannot be determined from the data (LSK, SCLK, PCK, etc) *start_date_time* and *stop_date_time* set to the default mission time range (from launch to an arbitrary date many decades into the future, e.g. 2050-01-01);

for meta-kernels *start_date_time* and *stop_date_time* are set to the coverage provided by spacecraft SPK or CKs;

for a SPICE collection the coverage is set to the boundaries of the combined coverage of the latest MKs that are part of this collection

for a SPICE bundle the coverage is set to the boundaries of the coverage of the SPICE collection that is its member.

9.6. PDS4 XML/Schema

All the PDS4 SPICE Bundles must use the PDS4 XML/Schema Version 1.11.0.0 (Sun Sep 23 16:29:35 PDT 2018). PSA and mission specific dictionaries are not to be used.

When using the PDS validate tool, version 1.15.0 is recommended. The command to validate a SPICE Bundle is as follows:

```
validate -t em16_spice/ -m 1B00
```

9.7. DOIs for SPICE Kernel Datasets

The ESA SPICE Service has incorporated the usage of DOIs in order to facilitate the citation of SPICE data. The DOI reference needs to be included in the SPICE Bundle label (*bundle_<sc>_spice_v<ver>.xml*). The DOI is referenced in the Citation Information field of the label:

```
<Citation_Information>
   <publication_year>$CURRENT_YEAR</publication_year>
   <doi>$DOI</doi>
   <keyword>Observation Geometry</keyword>
   <description>This bundle contains $PDS4_MISSION_NAME SPICE kernels and related
documentation </description>
</Citation_Information>
```

The DOIs for the ESA missions that incorporate SPICE are available from: https://www.cosmos.esa.int/web/spice/data

Please note that the version of the Archive Bundle release is not recorded by the DOI; there is only one DOI for all the versions of the SPICE Bundle. Using the archive access time should be enough to determine which version of the Bundle has been used.

An example on the guidelines to cite a SPICE Bundle is provided hereby:

ESA SPICE Service, ExoMars 2016 SPICE Bundle, https://doi.org/10.5270/esa-kfjsoi9

9.8. ESA SPICE Service SPICE Bundle generation pipeline

The ESA SPICE Service (ESS) has developed a pipeline to generate PDS4 SPICE Bundles: **arcgen**. This pipeline is available under request at: https://repos.cosmos.esa.int/socci/projects/SPICE/repos/arcgen/

This pipeline requires the set of peer-reviewed kernels to be archived (or incremented), the previous version of the Bundle (if available) a grammar to generate the appropriate meta-kernel and the update of a simple configuration file.

The pipeline includes templates for all the labels of all the products of the Bundle as well, these can be made available under request as well.

Please contact ESS (esa_spice@sciops.esa.int) if you wish to have more information of the arcgen pipeline.

9.9. SPICE_kernel product label example

What follows is a preliminary example of a SPICE_kernel product label for:

spice_kernels/fk/em16_tgo_v16.tf

```
<?xml-model href="http://pds.nasa.gov/pds4/pds/v1/PDS4_PDS_1B00.sch"
    schematypens="http://purl.oclc.org/dsdl/schematron"?>


<Product_SPICE_Kernel xmlns="http://pds.nasa.gov/pds4/pds/v1"
 xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
 xsi:schemaLocation="http://pds.nasa.gov/pds4/pds/v1
http://pds.nasa.gov/pds4/pds/v1/PDS4_PDS_1B00.xsd">

    <Identification_Area>

<logical_identifier>urn:esa:psa:em16_spice:spice_kernels:fk_em16_tgo_v16.tf</logical_id
entifier>
        <version_id>1.0</version_id>
        <title>em16_tgo_v16.tf</title>
        <information_model_version>1.11.0.0</information_model_version>
        <product_class>Product_SPICE_Kernel</product_class>
        <Citation_Information>
            <publication_year>2018</publication_year>
            <keyword>Observation Geometry</keyword>
            <description>SPICE FK file that provides TGO spacecraft, structures,
instruments and sensors frames. Created by the ESA SPICE Service.</description>
        </Citation_Information>
    </Identification_Area>
    <Context_Area>
        <Time_Coordinates>
            <start_date_time>2016-03-14T08:13:00Z</start_date_time>
            <stop_date_time>2050-01-01T00:00:00Z</stop_date_time>
        </Time_Coordinates>
        <Primary_Result_Summary>
            <purpose>Observation Geometry</purpose>
            <processing_level>Derived</processing_level>
        </Primary_Result_Summary>
        <Investigation_Area>
            <name>ExoMars 2016</name>
            <type>Mission</type>
            <Internal_Reference>

<lid_reference>urn:esa:psa:context:investigation:mission.em16</lid_reference>
                <reference_type>data_to_investigation</reference_type>
            </Internal_Reference>
        </Investigation_Area>
        <Observing_System>
            <Observing_System_Component>
                <name>TGO</name>
                <type>Spacecraft</type>
                <Internal_Reference>

<lid_reference>urn:esa:psa:context:instrument_host:spacecraft.tgo</lid_reference>
                    <reference_type>is_instrument_host</reference_type>
                </Internal_Reference>
            </Observing_System_Component>
        </Observing_System>
        <Target_Identification>
            <name>Mars</name>
            <type>Planet</type>
            <Internal_Reference>
                <lid_reference>urn:nasa:pds:context:target.mars</lid_reference>
```

```
                <reference_type>data_to_target</reference_type>
            </Internal_Reference>
        </Target_Identification>
    </Context_Area>
    <Reference_List>
        <Internal_Reference>
            <lid_reference>urn:esa:psa:em16_spice:document:spiceds</lid_reference>
            <reference_type>data_to_document</reference_type>
        </Internal_Reference>
    </Reference_List>
    <File_Area_SPICE_Kernel>
        <File>
            <file_name>em16_tgo_v16.tf</file_name>
            <creation_date_time>2018-09-25T11:02:40</creation_date_time>
            <file_size unit="byte">159097</file_size>
            <md5_checksum>2bfd4c686e92c159ae50560dd0422d08</md5_checksum>
        </File>
        <SPICE_Kernel>
            <offset unit="byte">0</offset>
            <object_length unit="byte">159097</object_length>
            <parsing_standard_id>SPICE</parsing_standard_id>
            <description>SPICE FK file that provides TGO spacecraft, structures,
instruments and sensors frames. Created by the ESA SPICE Service.</description>
            <kernel_type>FK</kernel_type>
            <encoding_type>Character</encoding_type>
        </SPICE_Kernel>
    </File_Area_SPICE_Kernel>
</Product_SPICE_Kernel>
```


10. EXTERNAL STANDARDS

Many PDS4 products are created from scratch from one of the 4 allowed base data types, but products following external standards or formats may also be archived if the data within them also follow the PDS4 rules. Such files typically contain additional data or meta-data which do not, or cannot, be described by PDS4. If these meta-data are important for use of the product, they should be replicated in a PDS4 format (e.g. as attributes in the label, or in a separate table in the data product).

If the file format has a header this can be declared in the file area using the Header or Encoded_Header classes. In this case the the attribute <parsing_standard_id> is mandatory to indicate the encoding standard in which the header is formatted. For a complete list of the allowed header encodings in observational products, see allowed values of this attribute in the PDS4 Information Model (IM) [AD.03]. If the file format is not on this list, the header can simply be ignored; it will not appear in the label and will be transparent to any PDS4 application.

This section defines specific requirements and recommendations that should be followed when using one of the following encoding standards to format the data (e.g. FITS, CDF). In addition, PDS hosts a web page containing resources on how to archive various external standards: https://pds.nasa.gov/datastandards/documents/archiving/

IMPORTANT: When using any of these external encoding data standards, it is strongly recommended to design data products that are PDS4-compliant and meet all PSA archiving requirements to avoid any reformatting or conversion of data only for archiving purposes. This will guarantee that the same data formats used and exchanged by the science team during the mission will be archived and preserved.

10.1. Specific Requirements and Recommendations for FITS

FITS stands for **Flexible Image Transport System (FITS)**, and is the standard archival data format for astronomical data sets. Although FITS was originally designed for transporting image data on magnetic tape (which accounts for the ‘I’ and ‘T’ in the name), the capabilities of the FITS format have expanded to accommodate more complex data structures. This standard has been endorsed by the International Astronomical Union (IAU) for the interchange of astronomical data (IAU 1983).

The official reference document that defines the requirements for FITS format data files can be found at FITS Standard.

The FITS format is also commonly used by the planetary community to format and exchange their data, specially for images, tables and spectral data. However, the *de-facto* archiving standard for planetary data is PDS. Due to this, the recommendation is to design FITS data that are PDS4-compliant and meet all PSA archiving requirements to avoid any reformatting or conversion of data only for archiving purposes. This will guarantee that the same data formats used and exchanged by the science teams during the mission will be archived and preserved.

Some caveats on the PDS4 compatibility of FITS data formats and data types can be found in the PDS Small Bodies Node (SBN) PDS4 Wiki, as well as guidelines on how to generate PDS4 labels for FITS files.

The most significant compatibility issues are listed below:

FITS TABLE extension data is structurally compliant with PDS4 fixed-width ASCII table (Table_Character) requirements, but PDS requires that every line of the table data ends with a "carriage-return/linefeed" sequence.

it may also be possible to use a Table_Binary PDS4 structure along with appropriate ASCII data types to avoid having to insert CR/LF into the FITS files

FITS BINTABLE extension data is structurally compliant with PDS4 binary table (Table_Binary) requirements but only if the format is not abused (e.g. attach header values to an observational data array is not allowed in PDS4).

The only integer data types stored in a compliant FITS file are unsigned 8-bit bytes and signed 2-, 4-, and 8-byte integers, although PDS allows more integer data types.

however, unsigned data can be written into a FITS table or array after shifting to use the signed range and using the BZERO or TZERO keywords to specify the offset to be applied on reading

the equivalent PDS4 attribute is value_offset, which can be used e.g. with a signed data type to read the data and correctly apply the offset.

Array Axis Ordering. FITS array data are are stored such that the *NAXIS1* subscript varies fastest, *NAXIS2* next fastest, and so on up to *NAXISn*. So the storage order is first-index-fastest in FITS notation. This is the opposite in PDS.

Padding in Tables. FITS standard requires that the BINTABLE data be padded with null ("\0") from the end of the last record to the end of the containing 2880-byte FITS block and TABLE data be padded with blanks to an even number of FITS 2880-byte blocks following the last record in the table. There is no requirement that these padding characters be included in the PDS4 label, and they are generally ignored.

FITS files comprise of one or more Header and Data Units (HDUs). The first (mandatory) HDU is called the primary HDU and *must* contain a primary header, and optional data. Subsequent HDUs are called FITS extensions and currently include image, ASCII table and binary table data formats, with accompanying headers. Each HDU in a FITS file must be described in the corresponding PDS4 label.

The PSA recommends the use of a **header only primary HDU** which should provide meta-data for the entire product (file), and one or more FITS extensions (additional HDUs) providing the actual data and corresponding meta-data. This is the structure given below.

10.1.1. Recommended FITS keywords for PDS4 archives

The table below includes a list of FITS keywords to be used to describe the data and metadata typically included in PDS4 products in the PSA.

This is an initial proposal, to be consolidated in future versions of this document.

In the Primary Header and Data Unit (HDU), the following structure is expected:

```
SIMPLE   =  T / conforms to FITS standard
BITPIX   =  8 / array data type
NAXIS    =  0 / number of array dimensions - 0 indicates there is no data array for this HDU, only a header
EXTEND   =  T / FITS extensions are permitted here
< INSERT HERE THE METADATA LISTED BELOW AS APPLICABLE >
END
```

This indicates that the primary HDU has a header only, containing keywords in the following list. Any meta-data needed to analyse the data cannot only be in the FITS header (which is ignored by PDS4) and must also be included in the PDS4 label. Where corresponding PDS4 keywords exist they are included in the table.

FITS Keyword	Data Type	Type of FITS Keyword	PSA Requirement	Definition	PDS4 Keyword
Identification Area					
LOGID	string			Logical identifier as per PSA conventions; unique at PDS level.	logical_identifier
VERSION	string			Version of the product, format: M.N (major.minor).	version_id
TITLE	string			Brief title for the product	title
HISTORY	string				

ORIGIN	string	reserved		Organization or institution responsible for creating the FITS file.	not available in PDS4 (TBC)
AUTHOR	string	reserved		The value field shall contain a character string identifying who compiled the information in the data associated with the header. This keyword is appropriate when the data originate in a published paper or are compiled from many sources.	Citation_Information: author_list
REFERENC	string	reserved		The value field shall contain a character string citing a reference where the data associated with the header are published.	Citation_Information: description
Observation Area					
DATE-OBS	string	reserved		The date of the observation, in the format specified in the FITS Standard. The old date format was 'yy/mm/dd' and may be used only for dates from 1900 through 1999. The new Y2K compliant date format is 'yyyy-mm-dd' or 'yyyy-mm-ddTHH:MM:SS[.sss]'.	start_time
DATE-ST	string			Start date (first date of the measurements in the product)	start_time
DATE-END	string			Stop date (last date of the measurements in the product)	stop_time
PROLEVEL	string			Processing level. Allowed values are: Raw, Partially Processed, Calibrated, Derived	processing_level
MISSION	string			Mission Name	Observing_System_Component: name with type = Mission

INSTHOST	string			Instrument Host	Observing_System_Component: name with type = Spacecraft
INSTRU	string	reserved		The value field shall contain a character string identifying the instrument used to acquire the data associated with the header.	Observing_System_Component: name with type = Instrument
INSTTYPE	string			Instrument Type; see allowed values in section	Observing_System_Component: type with type = Instrument
SUBINST	string			Sub-Instrument Identifier (typically an acronym)	Sub-Instrument: identifier
SUBINSTN	string			Sub-Instrument Name	Sub-Instrument: name
SUBINSTT	string			Sub-Instrument Type; see allowed values in section	Sub-Instrument: type
OBJECT	string	reserved		The value field shall contain a character string giving a name for the object observed (see also the NAIF ID list).	Target_Identification: name
Mission Area: Mission Information					
CLK-ST	string			Spacecraft clock elapsed time for the first measurement in the data product	spacecraft_clock_start_count
CLK-END	string			Spacecraft clock elapsed time for the last measurement in the data product	spacecraft_clock_stop_count
PHASENA	string			Mission phase name; allowed values are defined in the corresponding mission dictionary.	mission_phase_name
PHASEID	string			Mission phase identifier (typically an acronym); allowed values are defined in the corresponding mission dictionary.	mission_phase_identifier
ORB-ST	Unsigned Integer			Orbit for the first measurement in the data product.	start_orbit_number

ORB-END	Unsigned Integer			Orbit for the last measurement in the data product.	stop_orbit_number
Mission Area: Observation Context					
OBSID	string			Observation Identifier; allowed values are defined by the mission in the corresponding Annex.	observation_identifier
POINTING (TBC)	string			Spacecraft pointing; allowed values are defined in the PSA dictionary.	spacecraft_pointing
Mission Area: Quality Information					
QUALFLAG	string			Quality flag; allowed values or guidelines are defined by the mission in the corresponding Annex.	quality_flag
Mission Area: Processing Context					
PROCSW	string			Processing Software Title	processing_software_title
PROCSWVE	string			Processing Software Version	processing_software_version
File Area Observational					
DATE	string	reserved		The date on which the file was created, in the format specified in the FITS Standard. The old date format was 'yy/mm/dd' and may be used only for dates from 1900 through 1999. The new Y2K compliant date format is 'yyyy-mm-dd' or 'yyyy-mm-ddTHH:MM:SS[.sss]'.	File_Area_Observational: File: creation_date_time

10.1.2. FITS Keywords for ASCII Table Extensions

See relevant information at the PDS SBN PDS4 Wiki > ASCII Tables.

```
XTENSION = 'TABLE'            / ASCII table extension
BITPIX   = 8                  / 8-bit bytes
NAXIS    = 2                  / 2-dimensional ASCII table
NAXIS1   = <record_length>    / width of table in bytes
NAXIS2   = <records>          / number of rows in table
PCOUNT   = 0                  / size of special data area
GCOUNT   = 1                  / one data group (required keyword)
TFIELDS  = <fields>           / number of fields in each row
```

In PDS4, an ASCII Table is described with the class <*Table_Character*>, where:

NAXIS1 corresponds to the <*record_length*> attribute in the <*Record_Character*> class.

NAXIS2 corresponds to the <*records*> attribute in the <*Table_Character*> class.

TFIELDS corresponds to the <*fields*> attribute in the <*Record_Character*> class. Unlike in *BINTAB* tables, ASCII tables may not have fields that are arrays, vectors, or complex numbers.

The required <*groups*> attribute will always have a value of zero (fields in FITS tables are not allowed to have repetition counters).

For each column (<*Field_Character*> in PDS4), the following keywords are needed for each column, where the 'n' is an integer counter of the field starting from one, and with no padding (e.g. TTYPE1):

FITS	PDS4 Field_Character	Status
TTYPEn	<name>	mandatory
TBCOLn	<field_location>	mandatory
TFORMn	<data_type> (1)	mandatory
TUNITn	<unit>	mandatory (if applicable)
TSCALn	<scaling_factor>	optional
TZEROn	<value_offset>	optional
TNULLn	see below (2)	optional
TDISPn	see below (3)	optional

(1) see table below.

(2) *TNULL* is a string used as a null data flag for the field and corresponds to the value found in the file - before scaling or offset are applied. It can be translated into one of the specific flags in the <*Special_Constants*> class, depending on the circumstances of the data.

(3) *TDISP* is an optional keyword that can be used to contain a more specific display format than that implied by the *TFORM* keyword.

TFORM	PDS4 <data_type>
Iw	ASCII_Integer (4)
Fw.d	ASCII_Real
Ew.d	ASCII_Real

Dw.d	ASCII_Real

(4) Or more specific ASCII_* string type e.g. ASCII_Date_Time for date/time fields conforming to the standard ISO 8601 format.

10.1.3. FITS Keywords for Binary Table Extensions

See relevant information at the PDS SBN PDS4 Wiki > Binary Tables.

10.1.4. FITS Keywords for Array Extensions

See relevant information at the PDS SBN PDS4 Wiki > Arrays.

10.1.5. FITS Keywords for Planetary Surface Data (GeoFITS)

An extension of FITS metadata for planetary surface investigations in under definition by VESPA (Virtual European Solar and Planetary Access) in the frame of Europlanet H2020 , see GeoFITS.

10.1.6. Relevant FITS tools

FITS data is already supported by GDAL via the external library CFITSIO (see the GDAL documentation).

FV: Interactive FITS file editor. FV can be used with the DS9 image display.

fitsverify - A FITS File Format-Verification Tool. A web version of this tool can be found at: https://fits.gsfc.nasa.gov/fits_verify.html

10.2. Specific Requirements and Recommendations for CDF

The Common Data Format (CDF) is widely used in the heliophysics community and by some instruments on planetary missions, typically for those time series data files produced by the in situ instruments. CDF files can be archived in PDS4, provided they are formatted to meet the CDF-A standard (CDF-Archive) and include appropriate meta-data.

The values of the <parsing_standard_id> attribute to be used in PDS4 labels for CDF products is: "CDF 3.4 ISTP/IACG".

As per the guidelines defined by the PDS Plasma Planetary Interactions (PPI) Node, to ensure data in a CDF file will be archivable in PDS4 with no conversion, the following set of requirements should be met:

- The CDF file must be CDF version 3.4 or later.
- All data variables which are part of the CDF file are included in the same file.
- No compression (file or variable).
- No unused records (no superfluous, non-decodable records).
- No fragmented variables (all data for a variable must be contiguous in the file).

- No sparse variables. All data values are physical (data for all dimensions in a variable are written).
- No virtual (calculated) variables.
- Variables are stored in row majority order.
- Use only "zVariables" for data.

In addition, the CDF file should include at least a minimum set of metadata as per the requirements listed in the following section: ISTP/IACG Metadata.

Reference documents are listed below, and can be found in the PDS Plasma Planetary Interactions (PPI) Node documentation page:

CDF-A Specification: The CDF-A Specification describes the types of CDF files which meet basic archiving requirements. The specification includes HPDE and PDS extensions which define additional requirements for each domain.

Guide to Archiving CDF Files in PDS4: Details on how to prepare CDF files for archiving in a PDS4 system with information about available tools.

Since CDF stores all data are zVariables, which are essentially arrays, some extra care must be taken. PDS4 arrays **only** allow for binary formats, and so if an ASCII PDS4 date/time format is written to a CDF file, it cannot be labelled as an array, but instead a single record Table_Character can be used with the appropriate Group_Field definition. If in doubt, please consult your mission archive scientist.

The following sub-sections describe data and metadata conventions for CDF files to be archived as PDS4 products in the PSA.

10.2.1. Expected Time Related Variables in CDF Files

10.2.1.1. CDF Variables:

Name	Description	Data Type	Comment
Epoch	Timetag after time correlation has been performed	CDF_TIME_TT2000	This should always be ZVARIABLE 0 in a CDF file. For details of the CDF_TT000 data type, and conversion to UTC, see https://spdf.gsfc.nasa.gov/istp_guide/variables.html#Epoch
sclk	Spacecraft Clock Time	CDF_CHAR	This should always follow the Epoch variable in a CDF file. Note if the sclk variable is not used the spacecraft clock start and end time should be recorded as global attributes named *P*DS_sclk_start_count and PDS_sclk_stop_count

10.2.1.2. PDS4 Attributes

CDF	PDS4 Label Attribute	Comment
Epoch	<Time_Coordinates> <start_date_time></start_date_time> <stop_date_time></stop_date_time></Time_Coordinates>	The UTC start and end time (following time correlation) of the product extracted from the Epoch variable in the CDF. This goes at the start of the observation area in a PDS4 label.
sclk	<psa:Mission_Information> <psa:spacecraft_clock_start_count></psa:spacecraft_clock_start_count> <psa:spacecraft_clock_stop_count></psa:spacecraft_clock_stop_count>	Either the start and end values of the sclk variable in the CDF or the values of the PDS_sclk_start_count and PDS_sclk_stop_count global attributes. The PSA Mission_Information class is typically the first class specified in the Mission Area and is compulsory for archiving in the PSA.

10.2.2. ISTP/IACG Metadata

Detailed definition of the ISTP/IACG metadata attributes can be found in the following links:

Global Attributes: https://spdf.gsfc.nasa.gov/istp_guide/gattributes.html

Variable Attributes: https://spdf.gsfc.nasa.gov/istp_guide/vattributes.html

All of the global attributes shall be CDF_CHAR data types.

CDF Attribute	PSA Requirement based on ISTP/IACG	ISTP/IACG Definition	Enumerated Values	PDS4 Metadata Use
Global Attributes				
Acknowledgement	recommended		n/a	n/a

ADID_ref	no longer relevant		n/a	n/a
Data_type	required	ISTP defined exchangeable data product type. (enumeration)		
Data_version	required	Project assigned version for the data.	n/a	Product_Observational: Identification_Area: version_id
Descriptor	required	The name of the instrument or sensor that collected the data.	See applicable Mission annex.	long name used in: Product_Observational: Observing_System_Component: name when type = Instrument
Discipline	required	The science discipline and subdiscipline. (enumeration)	Planetary Physics>Atmospheres Planetary Physics>Fields Planetary Physics>Flux Measurements Planetary Physics>Particles Planetary Physics>Spectroscopy	Product_Observational: Observation_Area: Primary_Result_Summary: Science_Facets: discipline_name The value in PDS4 will include only the subdiscipline.
Generated_by	recommended	The generating data center/group.	n/a	n/a
Generated_with_software	recommended		n/a	psa: Processing_Context: processing_software_version
Generation_date	recommended	Date stamp for the creation of the file.	n/a	Product_Observational: Identification_Area: Modification_History: Modification_Detail: modification_date
HTTP_LINK	recommended	The URL for the PI or Co-I web site holding on-line data.	n/a	n/a

Instrument_type	required	The ISTP defined instrument type. Multi-valued. (enumeration)	Electric Fields (space) Engineering Ephemeris Gamma and X-Rays Magnetic Fields (space) Particles (space) Plasma and Solar Wind Radio and Plasma Waves (space)	Product_Observational: Observing_System_Component: type with type = Instrument See section 7.3.1; updates expected in PDS4 version 1.11.
LINK_TEXT	recommended	Text describing on-line data available at PI or Co-I web sites.	n/a	n/a
LINK_TITLE	recommended	The title of the web site holding on-line data available at PI or Co-I web sites.	n/a	n/a
Logical_file_id	required	The name of the CDF file using the ISTP naming convention.	n/a	n/a
Logical_source	required	Combined source_name, data_type, and descriptor information. String containing source_name, data_type and descriptor separated by underscores. *Note: this should be upper case despite the file name being lower case.*	n/a	n/a

Logical_source_description	required	Full words associated with the Logical_source. Value should be ~1 line working/useful title for the data file.	n/a	Product_Observational: Identification_Area: title
Mission_group	required	The assigned name of the mission or project. (enumeration)	See applicable Mission annex.	Product_Observational: Observation_Area: Investigation_Area: name
MODS	recommended	History of modifications made to the CDF data set.	n/a	Product_Observational: Identification_Area: Modification_History: Modification_Detail
Parents	optional	The parent CDF(S) for files of derived and merged data sets.	n/a	Product_Observational: Reference_List: Source_Product_Internal/External
PDS_collection_id	required	Collection identifier portion of the PDS4 logical_identifier of the primary collection with which the data product is a member.	n/a	Collection identifier portion in Product_Observational: Identification_Area: logical_identifier
PDS_sclk_start_count	recommended	Spacecraft clock (or Mission Elapsed Time) start count associated with the first start time of the file.	n/a	msn:spacecraft_clock_start_count
PDS_sclk_stop_count	recommended	Spacecraft clock (or Mission Elapsed Time) stop count associated with	n/a	msn:spacecraft_clock_stop_count

		the last end time of the file.		
PDS_start_time	required	First start time (UTC) of the file in the format: YYYY-MM-DDThh:mm:ss.sssZ. Where YYYY = 4-digit year, MM = month of year, DD = day of month, hh = hour of day, mm= minute of hour, ss.sss = seconds of minute, and "T", and "Z" are literal.	n/a	Product_Observational: Observation_Area: Time_Coordinates: start_date_time
PDS_stop_time	required	Last stop time (UTC) of the file in the format: YYYY-MM-DDThh:mm:ss.sssZ. See PDS_start_time for details.	n/a	Product_Observational: Observation_Area: Time_Coordinates: stop_date_time
PI_affiliation	required	A recognizable abbreviation of the PI affiliation.	n/a	n/a
PI_name	required	First initial and last name of the PI.	n/a	n/a
Planet	recommended		See section 3.3.1 for allowed values.	Target_Identification: name when type = Planet
Project	required	The name of the project i.e. mission full name.	See applicable Mission annex.	Product_Observational: Observing_System_Component: name when type = Mission
Rules_of_use	recommended	Citability and PI access restrictions. This may point to a World Wide Web page specifying the rules of use.	n/a	Some information can be provided in: Product_Observational: Identification_Area: Citation_Information: description

Skeleton_version	optional	The skeleton file version number.	n/a	n/a
Software_version	optional	The version of the software that generated the CDF.	n/a	psa: Processing_Context: processing_software_version
Source_name	required	The mission or investigation that contains the sensors i.e. mission full name.	See applicable Mission annex.	Product_Observational: Observation_Area: Investigation_Area: name
TEXT	required	Description of the experiment. Value should be a full (long) description of the data file.	n/a	Product_Context: Instrument: description
Time_resolution	recommended	The time resolution of the file.	n/a	n/a
TITLE	optional	A title for the data set.	n/a	Product_Observational: Identification_Area: title
Validate	optional	Written by software for automatic validation of features.	n/a	n/a
Variable Attributes				
AVG_TYPE	optional		n/a	n/a
CATDESC	required	Approximately 80-character string which is a textual description of the variable. Brief (~1 line) description of the variable.	n/a	Array_*D/description
DEPEND_0	required		n/a	Axis_Array/axis_name
DEPEND_i	required	Ties a dimensional data variable to a support_data variable. Contains the name of the variable. "i" is	n/a	Axis_Array/axis_name

		replaced with the index of the dimension. For ISTP the DEPEND_0 must be defined and have the value 'Epoch'.		
DICT_KEY	optional			n/a
DISPLAY_TYPE	required	what type of plot to make (e.g. time_series, spectrogram, stack_plot, image) . Enumerated values list may be expanded as needed.	time_series spectrogram stack_plot image	potentially used in Discipline_Area (giving hints for data visualization)
FIELDNAM	required	A description of the variable (up to 30 characters).	n/a	Array_*D/name
FILLVAL	required	The value used for missing or invalid variable values. Should be of same data type as the variable which they are describing.	n/a	potentially used in: Special_Constants/*_constant
FORMAT/ FORMAT_PTR	required	A Fortran format specification that is used when displaying a variable value.	n/a	mapped to: …/field_format
LABLAXIS/ LABL_PTR_i	required	The label for the y-axis of a plot or to provide a heading for a data listing. If labeling a variable with dimensions use the LABL_PTR_i form	n/a	n/a

		with "i" replaced with the index of the dimension.		
MONOTON	optional	The monotonicity of a variable: INCREASE (strictly increasing values), DECREASE (strictly decreasing values), or FALSE (not monotonic).	INCREASE DECREASE FALSE	n/a
UNITS/UNIT_PTR	required	The units of the variable. In the UNIT_PTR form it contains the name of the variable which stores the UNITS string. To be used only if UNITS is not present.	n/a	Element_Array/unit
SCALEMIN	optional	The minimum value for scaling a variable when graphically displaying its values. Should be of same data type as the variable which they are describing. Only mandatory for time-varying variables.	n/a	potentially used in Discipline_Area (giving hints for data visualization)
SCALEMAX	optional	The maximum value for scaling a variable when graphically displaying its values. Should be of same data type	n/a	potentially used in Discipline_Area (giving hints for data visualization)

		as the variable which they are describing. Only mandatory for time-varying variables.		
SCALETYP	recommended	Type of axis for plotting.	linear log	potentially used in Discipline_Area (giving hints for data visualization)
VALIDMIN	required	The minimum valid value for a variable. Should be of same data type as the variable which they are describing.	n/a	use dependent upon variable
VALIDMAX	required	The maximum valid value for a variable. Should be of same data type as the variable which they are describing.	n/a	use dependent upon variable
VAR_NOTES	required	Ancillary information about the variable. Note: While ISTP/IACG classifies VAR_NOTES as optional, please include a complete description here as it will be used for the description in the PDS label file.	n/a	Array_*D/description
VAR_TYPE	required	Identifies a variable as either data,	data support_data	n/a

		support_data, metadata or ignore_data. Value should be a full description of the variable.	metadata ignore_data	

10.2.3. SPASE Metadata Attributes

Under discussion.

CDF Attribute	PSA Requirement	Description	Enumerated Values	PDS4 Metadata Use
Global Attributes				
spase_DatasetResourceID	required	Unique dataset identifier assigned by SPASE, of the form spase://VSPO/"UNIQUE_ID", where "UNIQUE_ID" is the ID assigned to the SPASE resource record for the dataset in the SPASE system. The SPASE resource record provides metadata about the dataset, including pointers to locations holding the data.		TBC
spase_DatasetResource	recommended	The SPASE XML description of the dataset that corresponds to the SPASE ResourceID.		TBC
spase_GranuleResourceID	recommended	The Granule ResourceID assigned to the data file.		TBC
spase_GranuleResource	recommended	The SPASE XML description of the dataset that corresponds to the SPASE Granule ResourceID		TBC

10.2.4. VESPA Metadata Attributes

The following table provides the list of the CDF global attributes derived from the VESPA keywords.

Name	PSA Requirement	Description	Comment	PDS4 Attribute
TARGET_NAME	required	Name of the target	e.g., 'Sun'	Target_Identification: name
TARGET_CLASS	required	Class of the target	e.g., 'Star'	Target_Identification: type
TARGET_REGION	required	Region where the target in the observed	e.g., 'Corona'	n/a

ACCESS_FORMAT	optional	Format of the file	e.g. "CDF 3.4 ISTP/IACG"	<parsing_standard_id>
DATAPRODUCT_TYPE	optional	High level scientific organization of the data		
TIME_MIN	required	The date and time of the beginning of the first acquisition for the data contained in the file		
TIME_MAX	required	The date and time of the end of the last acquisition for the data contained in the file		
REFERENCE	optional	Bibcode, DOI or URL		

10.2.5. Additional Metadata Attributes

Placeholder; under discussion.

10.2.6. Use of PDS4 local data dictionaries (LDD) to describe CDF data products

Variables in CDF files are organised as arrays of various dimensions (1, 2, 3, … N).

The core PDS4 DOES SUPPORT describing individual arrays (dimensions, data types, units, etc.).

The Core PDS4 DOES NOT describe relationships between the arrays i.e.

Array 1 contains TIME(i) or ENERGY(i)

Arrays 2, 3, … N contain something B_VECTOR(x,y,z)(i) at TIME(i)

The "Particle" and "Alt" Local Data Dictionaries (LDDs) are designed to describe relationships between the arrays:

Primary values (flux), axis values (time), and face values (bin variables).

In addition:

The PSA and Mission local data dictionaries should be used to define mission specific keywords (e.g. mission_phase_name, …)

Other useful LDDs (Geometry, Cartography, etc.)

All Local Data Dictionaries (LDDs) registered with PDS are available at: https://pds.nasa.gov/pds4/schema/released/

10.2.7. Relevant CDF tools

Tools to verify ISTP/IACG compliance

SKTEditor/Other tool – verify that the CDFs comply with standards and tools http://spdf.sci.gsfc.nasa.gov/skteditor /

CDFConvert – convert internal structure of existing CDF files

http://cdaweb.sci.gsfc.nasa.gov/pub/software/cdf/dist

this repository contains the complete CDF library, including various tools like cdfconvert

- `> cdfconvert {src.cdf} {dest.cdf} -single -network -sparseness vars:srecords.no -compression vars:none -zmode 2`

This will convert {src.cdf} (which can be a multiple file CDF) and write to {dest.cdf} a copy that is written as a single file with network encodings, no sparseness, no compression and that contains only zVariables.

Tools to verify CDF-A compliance

http://release.igpp.ucla.edu/pds/cdf/

cdfcheck: Scan a CDF file and determine if the content is compliant with archive requirements. Checks include if the CDF files meets requirements specified for CDF tools, ISTP/CDF and PDS archiving.

Example: http://release.igpp.ucla.edu/pds/cdf/example/index.html

Tools to create PDS4 labels for CDF files (Product_Observational)

Data providers can create tools to generate PDS4 labels from CDF files

PPI has created an application (igpp.docgen) which defines a environment that can process Apache Velocity templates into PDS4 labels.

http://release.igpp.ucla.edu/igpp/docgen /

Example: http://release.igpp.ucla.edu/igpp/docgen/example/cdf/generate-pds4.html

Tools to read PDS4-compatible CDF data

PDS4-compatible CDF reader in Python: https://github.com/MAVENSDC/cdflib

10.2.8. How-to Steps

CDF is a complex data format but properly formatted files can be fully described in PDS4. Some simple rules to follow are:

Make sure that the CDFs you build conform to the CDF ISTP/IACG spec: SKTEditor.

Make sure that you create CDF-A compatible files: CDFConvert.

Validate that your CDFs are truly CDF-A compliant: cdfcheck.

Identify which LDDs are required to support your labels.

Create mission specific LDDs if necessary.

If using igpp.docgen to build your labels, create the Velocity template and the run the code.

10.3. Specific Requirements and Recommendations for GeoTIFF

According to Wikipedia, GeoTIFF is "a public domain metadata standard which allows georeferencing information to be embedded within a TIFF file. The potential additional information includes map projection, coordinate systems, ellipsoids, datums, and everything else necessary to establish the exact spatial reference for the file. The GeoTIFF format is fully compliant with TIFF 6.0, so software incapable of reading and interpreting the specialized metadata will still be able to open a GeoTIFF format file." As such, GeoTIFF is a very useful format for producing image data with associated GIS-compliant meta-data.

Under the following conditions, GeoTIFF can be archived as a primary data format (Product_Observational). Note that as always, any meta-data which is contained in the GeoTIFF and is necessary for the interpretation of the data must be replicated in the PDS4 label in the appropriate way

GeoTIFF files can be archived in PDS4 archives with several caveats:

Image data must be **uncompressed**

No tiling is allowed

In case of images with multiple bands, the order should be **band-sequential**

In PDS Information Model >= 1F00:

within the PDS4 label pds:Header the “parsing_standard_id” should be listed as “TIFF 6.0”

The TIFF data type(s) used must match a PDS4 equivalent

and the endianness must be properly defined

All TIFF files are structured into a an Image File Header (IFH) - which is always the first 8 bytes of the file - followed by Image File Directories (IFDs) and bitmapped data objects. There is always one IFD per bitmap image.The location of the first IFD is given in the IFH, and each IFD points to the location of the *next* IFD, if present.

For archiving in PDS4 only the last of these is relevant, and its structure must be mapped to the appropriate PDS4 data type.

Relevant references include:

TIFF standard

GeoTIFF format specification

GeoTIFF OGC standard

11. INTEROPERABILITY

11.1. EPN-TAP Extension and Metadata Requirements

To be included in a future version of this document.