DOI report following the IVOA conference

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Abstract

The IVOA Data Curation and Preservation Interest Group (DCP) aims at sharing best practices and engaging IVOA member projects in the long-term curation and preservation of astronomical data. A DOI (Digital Object Identifier) is a permanent identifier including metadata. DOI metadata are integrated in the FAIR perspective allowing their indexation and resulting in a PID (Persistent Identifier) network. The Metadata schema used by DOIs includes the ability to link resources that have a persistent identifier. These links establish dependency relationships between resources of different nature and granularity.

A survey about experiments in this area was also conducted within the IVOA community. We will give an overview of this effort by referring to the State of the Art, to examples in astronomy and to the discussions we had during the last IVOA meetings and in the Note editorial team. This document aims at providing information and best practices to the astronomical community on the use of DOIs to cite datasets.

Status of this document

This is an IVOA Working Draft for review by IVOA members and other interested parties. It is a draft document and may be updated, replaced, or obsoleted by other documents at any time. It is inappropriate to use IVOA Working Drafts as reference materials or to cite them as other than "work in progress".

A list of current IVOA Recommendations and other technical documents can be found at https://www.ivoa.net/documents/.

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1 Introduction

The online availability of data and the development of associated services are an opportunity to increase the return on investment of major projects of this domain. Publications must now be able to cite datasets, queries, workflows, and more. This poses problems, particularly in terms of the persistence of the resources thus mentioned, not only in the long term archiving but also in terms of technological evolution (such as change of location, change of domain names). It has become essential to create mechanisms to address these issues. Unique and perennial identifiers (independent of technological developments) are a solution. Their management must also be provided by independent and international organizations, and supported by the world of research (universities, organizations, etc.). The Digital Object Identifier (DOI) system was created with this in mind. A DCP Session was dedicated to DOIs during the College Park IVOA meeting in November 2018 and we decided to work on an IVOA Note to provide the community with a clear snapshot of DOI usage and to extract the best practices (about assignment, granularity, metadata, etc.) and the lessons learned. In this note we present this system, first in a general context and then with relevance to astronomy. We also place it in the more general context of Persistent Identifiers (PID) and we provide an overview of related work by the Research Data Alliance (RDA).

2 State of the art for PID & DOI

The amount of extremely important astronomical data available online is growing quickly. Astronomy has been in the era of "Big Data" for many years [4]. The citation of data is becoming as important as that of the publications themselves. This poses a major problem since access to these data is subject to many hazards including the disappearance of a research organization or a data center, change of domain names or simply rearranging a file system or deleting old files when someone leaves an institution.[5,6]

Moreover, the identifiers must not be seen as isolated, they are part of an ecosystem in which they can be linked, for example tying datasets to their associated papers and software into a global research network, or linking different versions or copies of datasets together.

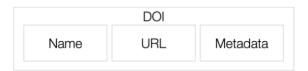


Figure 1: DOI content

It is therefore not possible to consider a URL as a perennial identifier. The unique identifiers that we evoke later are a solution to this problem.

2.1 Persistent Identifier

When a Persistent Identifier (PID) is used to identify a digital object (data set, journal article, document, etc.) accessible over the Internet, its aim is to provide a long-term reference to that object. This persistence, however, is dependent on organizational structures designed to persist longer than any single curator of a digital object.

A PID aims at:

- improving of search and access to data and ultimately their visibility and citation by researchers
- the ability to interact with other services that can easily be referred to by a permanent link
- an added value for the data provider that enhances usefulness in the research process

A PID must be guaranteed to be universally unique.

2.2 Digital Object Identifier

2.2.1 DOI System

A DOI has a Name which is resolved to a Landing Page and a set of Metadata.

The Name has a prefix starting with "10." and followed by a number identifying an organization (example: 26093 for INIST which is the contractor for the Research community in France) and a suffix which is unique within the organization and whose syntaxe is the responsibility of the DOI creator.

eg: vizier catalogue DOI: 10.26093/cds/vizier.34330717 10.26093: prefix attributed to the INIST organization (France) cds/vizier.34330717: suffix created by CDS to provide a unique identifier.

The syntaxe chosen is semi-opaque giving CDS provenance but not the resource itself. Datacite recommends an opaque suffix to be independent of any information that could evolve with the time.

The URL is the path to the Landing Page and is the page which is displayed after the resolution. This URL should not be a direct link to download the dataset.

3 DOI structure

3.1 DOI providers

Ten Registration agencies are providing DOIs, Crossref and DataCite are the best known in astronomy. To create DOIs you have to contract with a registration agency. In general it is often an agency that contracts for all research organizations in the country (examples: INIST in France, DANS in Australia,...)).

3.1.1 Crossref

Crossref (https://www.crossref.org/) is an international non-for-profit organization launched in 2000 as a DOI registration Agency of the IDF. Crossref provides DOI according to a scholix schema adapted for scientific articles.

3.1.2 Datacite

DataCite (https://datacite.org/) is an international non-for-profit organization founded in 2009 as a DOI Registration Agency of the IDF for research data. It can be seen as more domain-specific than Crossref. Its members are Universities, Research libraries, and similar organizations.

DataCite aims at:

- implementing easy access to research data on the Internet
- contributing to the verification of research results and their reuse for future research
- participating in the development of the citation of research data as an integral part of research activity

3.2 Landing page

When a user clicks on a link corresponding to a persistent ID, a resolution occurs at the DOI provider (DataCite for example) level generating a Web page called Landing Page. The resolution of the identifier should not lead to the direct downloading of the dataset. This page displays all relevant

information about the dataset and a valid link to the dataset. It may also include metadata, links to documentation, publications that cite this dataset, usage policy, and so on. The Landing Page must be maintained so that there is always a valid Web page resolved from the unique identifier.

3.3 Resource contents

DOI applies to stable resources that are not modified. However, DOI architecture allows versioning (eg: Zeonodo does). Versioning as well as evolving data is not treated in this document (see example in RDA) see Datacite policy: https://support.datacite.org/docs/datacite-data-file-use-policy

Datacite proposes a list of resource type like Image, Dataset, Model, Service, etc.

see https://doi.org/10.14454/3w3z-sa82

3.4 Metadata (general overview)

Metadata are associated with a DOI when the DOI is created, and maintained by the DOI curator. The DOI documentation provided by Datacite explains the different items and sets a level of relevance.

The DOI metadata are public and can be harvested by API provided by the DOI registration agencies. For instance Datacite provides several API: REST API, OAI-PMH API.

The metadata can be updated after publication and it is the DOI creator who is responsible for their maintenance. For instance the URL linked in DOI must be accessible. It is the responsibility of the creator to update URLS in DOI (for instance: change of domain). The metadata are public and subject to be CC0 compatible.

The latest version is now 4.4, released in March 2021 https://schema.datacite.org/meta/kernel-4.4/

4 Existing DOIs in astronomy

We give a list (not exhaustive) of existing DOIs in astronomy and we enter into more details for a few of them.

4.1 Introduction

A number of data centers and producers already provide resources having a DOI. The resources are diverse: article, pre-print, service, software, product, query result... The resources listed here cover different topics. The metadata provided depends on the nature of the resources and on the DOI registered organization. For instance Datacite and Crossref have

Institute	Туре	Title	Purpose	Example
A&A	article	A&A publishers	Published articles	10.1051/0004-6361/201834931
AAS	article	AAS publishers	Published articles	10.1086/505647
MNRAS	article	MNRAS publishers	Published articles	10.1093/mnras/stv1761
STSCi	observation	MAST	custom collection of MAST observation	10.17909/T9J59Q
CDS	service	vizier service	the CDS catalogue web service (vizier)	10.26093/cds/vizier
CDS	Dataset	vizier catalogues	VizieR catalogues - collection including tables, associated data and their access services	
CADC	Dataset	CANFAR's Data Publication service	researchers can publish data that is associated with a journal paper	10.11570/15.0002
ObsParis	instruments			
ObsParis	service	VESPA	web service	
CSIRO	service/tools	CASDA Virtual Observatory Tools	web service	10.4225/08/5728108951f27
CSIRO	Dataset	CSIRO Data Access Portal	Example: Parkes Observation Data Release(s)	10.25919/5cac1dcf84756 ivo://au.csiro.atnf/P858-2015APRS18
Leibniz/AIP	Dataset	MUSE-Wide survey project pages	spectrum FITS resources access (MUSE)	10.17876/musewide/dr.1/12828
Johns Hopkins University	service	Sciserver – SLOAN DIGITAL SKY SURVEY SkyServer	SDSS DR13 web access	10.7281/t1610xhg
Harvard IQSS Dataverse	documents	Unified Astronomy Thesaurus	Harvard Dataverse (doc pdf)	10.7910/dvn/fhmutt
Harvard IQSS Dataverse	Datasets	Example: Per-Cloud Pixelated Map Result Tables	store FITS/tabular data related to astronomy and/or astronomy papers	10.7910/DVN/74Y5KU
GAVO Data Center Team	Datasets	Example: The HSOY Catalog	Store Astronomical Data	10.21938/hp1aspbywelyxb6qdqyolg ivo://org.gavo.dc/hsoy/q/q
PDS				
ResearchGate	documents	ResearchGate	documents put by authors	10.13140/rg.2.2.35828.65928
ESO	documents	The metadata repository for the European Southern Observatory's DOIs.	articles,pdf	10.18727/0722-6691/5071
FAIRsharing	documents, services	Faisharing- standards,databases, policies	IVOA standards (https://fairsharing.org/collection/IVOA)	10.25504/fairsharing.5subhk
INAF	softwares	INAF-DOI	softwares	10.20371/INAF/PUB/2018_00009

Figure 2: Examples of DOIs in astronomy

their own schema which are both based on the Scholix Metadata Schema (https://doi.org/10.5281/zenodo.1120265)

Examples of DOI:

- authors using Zenodo, FAIRsharing, or Paper data
- publishers for articles (e.g. A&A, AAS, MNRAS, ..)
- data producers (Chandra, ESO,..)
- data centers (CADC, CDS).
- software (VESPA Paris Observatory, ...)

A not limited list of DOIs in astronomy.

4.2 DOI initiative at the Chandra Data Archive

Chandra interests :

The Chandra Data Archive has built a full bibliography for the mission, containing all articles using Chandra data, with full high-granularity linking to the observations. It is used as a research tool and to calculate metrics of scientific impact of the observatory.

CDA has used/is using a provisional Persistent ID specification

- agreed upon 17 years ago by NASA data centers (ADEC) and the ADS
- journals and data archives are pushing towards adoption of DOIs across the board for datasets

The CDA has recognized that the growing interest of the astronomical community towards (Datacite) DOIs is an opportunity to improve over the current PID specification and cater to new use cases that have emerged with the growth of the archive. The switch to DataCite DOIs is ongoing.

Why give data objects identifiers?

Three very good reasons:

- provide scientists a tool to credit the data provider
- document accurately what data was used to produce specific scientific results
- provide enduring access to the data objects

To achieve this, we need to:

- label data objects with PIDs
- encourage or enforce insertion of the PIDs in the manuscript
- kee up-to-date record of connections/relations among different types of identifiers
- keep pace with the historical evolution of the archive
- growth of the usage and importance of "advanced data products"

A secondary but no less important goal of the use of PIDs within the Chandra Data Archive is to create, by means of the metadata and relational identifiers that can be attached to PIDs encoded according to a DOI schema, a formal and abstract description of the internal structure of the Chandra data archive holdings, which is missing at this time. In detail, the goals are to:

• represent different levels and types of aggregation of datasets

- provide visibility to "value-added", merged datasets to increase scientific return
- leave a blueprint of the complexity of the archive (and its growth over time) as a part of the scientific legacy of the mission

DOIs for data in the archive

Dataset-based DOIs:

- single observations (L2 observations)
- aggregates
- merged aggregates (catalog-style stacks)
- "unintentional" spatial aggregates (collections of multiple L2 observations)
- User-contributed aggregates
- heterogenous types of data
- sets of single L2 observations (not merged) that have been scientifically selected, analyzed, reprocessed and/or augmented by users (not to be confused with the CCDP as described below, which are associated to publication by definition).
- Chandra Source Catalog DOI(s)
- one DOI for each version of the CSC, associated to a landing page that can resolve fragments to achieve the required granularity

Chandra paper collections

Chandra paper collections DOIs (a.k.a. Consolidated Chandra Data Page - CCDP) are DOIs minted for the collection of data used, cited or referenced by papers that are classified as "Chandra Science Papers" and listed in the CDA bibliographic database. This class of CDA DOIs acts as a nexus between existing DOIs of different nature by providing:

- basic bibliographic metadata about each Chandra science paper and linkage to the DOI(s) of the paper
- intermediate landing page linking landing pages to each CDA dataset used in the paper

Metadata

Requirements on metadata assignment/definition

- accurate enough to allow unequivocal identification of object
- need to express relationships with other associated objects
- literature objects
- other related data objects
- include versioning information
- including path (landing page) to the data objects

Requirements on upkeep of metadata

- "one-and-done" metadata
 - observational/data objects metadata that won't change over time \dots
 - ...or change seldom
- continuously updated metadata
 - literature objects that keep using the same data products
 - new types/level of aggregations of basic data products

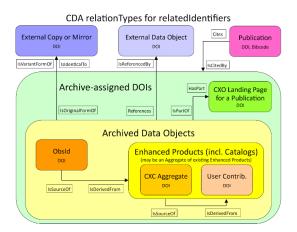


Figure 3: Chandra DOI

Practical considerations

DataCite metadata schema 4.1 provides flexibility to define (a very basic set of) properties of Chandra observations.

The Smithsonian Institution (SI) is a DataCite member and has anointed the CDA as a DataCite "provides". CDA will mint DOIs with the prefix 10.0344. Main CDA efforts focus on:

- backfilling of the archive: 40,000 DOIs
- average number of new DOIs: 3,000/year
- creating mechanism to generate landing pages for all classes of data products

DOIs will replace the ivo identifiers currently used by CDA. The dependencies on existing internal/external usage of the old-style PIDs that will need to be replaced are:

- the ivo identifiers populate the DS IDENT keyword in FITS headers
- DS_IDENT= 'ADS/Sa.CXO#obs/22056' / dataset identifier -> DS_IDENT= '10.0344/SAO.CXO.obs.22056'
- CIAO tool list_datasetid reads, creates and lists PIDs for Chandra observations

4.3 VizieR DOI assignment

VizieR assigns DOIs on catalogs. The DOI with its metadata is built by the CDS when the catalog is ingested into VizieR.

The VizieR DOI definition given by the CDS:

- A VizieR DOI is assigned to one VizieR catalog made from tables and associated data (spectra, images, ..), carefully preserved by the CDS and related to an article coming from a trusted scientific journal.
- The dataset is available in open-access through CDS services.
- The DOI identifies the data with metadata assigned by CDS and authors, and the services to access the dataset.

Currently, VizieR DOIs are assigned only for catalogs coming from authors publications in A&A and AAS.



Figure 4: The landing page for doi:10.26093/cds/vizier.35880108

4.4 CADC Self-Serve DOI Service

The CADC has recently deployed a Self-Serve DOI Service in CADC/CAN-FAR built with IVOA Services. The motivation was to respond to the express needs of its user community. The CADC has been manually minting DOIs since 2013 and Self-Serve DOI Service was deployed in March 2019.

Overview

Guiding principles:

- Data organisation completely in the hands of the user
- No metadata other than the DOI to the paper itself
- Re-using the user storage service and group management service of CANFAR

The Canadian Advanced Network For Astronomical Research (CAN-FAR)

- A science platform for Canadian astronomy
- In operation since 2011
- A set of cloud-hosted services: user storage, interactive processing, batch processing, group management and DOI hosting
- Integrated with CADC data collections

The Canadian Astronomy Data Centre (CADC)

- The operations centre for CANFAR
- Authorized by the DataCite Canada Consortium (member of DataCite) to issue DOI's

The workflow:

- 1. Authentication: The user authenticates in the CANFAR portal.
- 2. Request: The user requests a DOI. The service then
 - generates a DOI
 - creates the directory structure and DataCite XML
 - creates the RW group and adds the user to it
 - creates a DOI-reviewer user account and a read group for that account
- 3. Upload and organize data
- 4. Give publisher the DOI-reviewer account and password
- 5. Publish
 - step 1: Lock data directory and make it publicly readable
 - step 2: Publish to DataCite
- 6. Augment with Publication DOI

Summary

An authenticated self-serve service with a data organisation completely in the hands of the user and built on top of VO services: SSO, CDP, GMS and VOSpace.

The service dynamically generates landing pages from the DataCite XML document meaning there is no duplication of metadata.

4.5 China-VO and NADC PaperData

PaperData is a Persistent Data Repository for Journal Papers and powered by China-VO and China National Astronomical Data Center (NADC). It is recommended by AAS Journals (AJ/ApJ/ApJL/ApJS/RNAAS) and Research in Astronomy and Astrophysics (RAA).

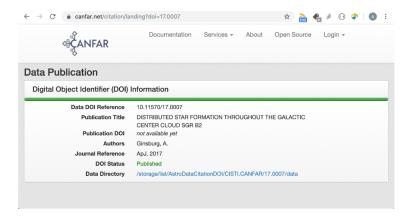


Figure 5: The Landing Page for doi:10.11570/17.0007

PID syntax and Metadata

Example of syntax: doi://10.12149/10000

10.12149 is the suffix for China National Astronomical Data Center (NADC)

10000 serial number starting

The Metadata is based on VOResource Schema and CrossRef DOI Metadata Schema.

Quality Audit and Data Security

Requirements:

- Paper has been accepted
- Metadata is complete and true

Check by NADC administrators.

Once a DOI is issued, no change of content/deletion is allowed.

4.6 MAST

MAST is currently using DOIs to allow authors to link to MAST data in publications. MAST has a number of fixed DOIs that have been created for catalogs and other large datasets.

MAST has also built a "DOI Portal" that allows users to make DOIs for ad hoc datasets downloaded from the CAOM collections in the MAST Data Discovery portal (e.g., http://doi.org/10.17909/T9P41K). MAST DOIs use

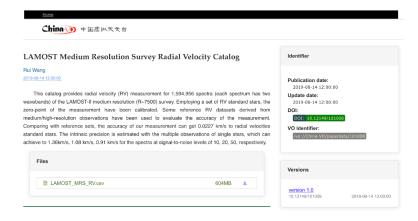


Figure 6: Example of Landing Page for doi:10.12149/101008

CAOM observation IDs to create these ad hoc data sets. Users can find the right DOI for their purposes by visiting the DOI search page at MAST: https://archive.stsci.edu/doi/search/. Behind the scenes we have a DOI API: https://mast.stsci.edu/portal/doi. MAST gets its DOIs from DataCite and uses the DataCite metadata schema.

MAST has built DOI creation into the process used for user-contributed data products (HLSPs), and encourages authors to include the DOI for their HLSP in their accompanying paper(s). MAST also publishes DOIs for all of its HLSPs so that other authors using HLSP data can reference those DOIs. https://archive.stsci.edu/hlsp/

Over the past couple of years MAST has worked with AAS Journals on a pilot project to get authors using MAST data to include MAST DOIs in their publications by building it into the electronic submission process. MAST is also currently working on integrating DOIs more closely into its bibliographic tracking processes and improving its DOI metrics.

Novacescu, J. et al. A Model for Data Citation in Astronomical Research Using Digital Object Identifiers (DOIs). ApJS 236, 20 (2018). https://doi.org/10.3847/1538-4365/aab76a

5 DOIs and IVOA standards and protocols

5.1 IVOA identifiers

The IVOA hasn't the authority to generate DOIs, each data center has to manage it locally. Resources available in the Virtual Observatory framework are searchable through the VO-registries that have their own identification: the IVOA Identifiers (IVOID). The IVOID is used in some VO-DataModels

(like ObsCore).

However, data producers and the VO community could benefit from joining the effort by linking IVOIDs with DOIs to improve VO citation and to make DOIs more visible in the VO-framework.

5.2 Registry

We recommend data centers that publish in VO-registries add the DOI as altidentifier.

Example:

```
<metadata>
  <ri:Resource ....>
        <title>.....</title>
        <identifier>ivo://CDS.VizieR/J/A+A/171/261</identifier>
        <altidentifier>doi:10.26093/cds/vizier.31710261</altidentifier>
        </ri:Resource ....>
</metadata>
```

Example of input already in the Registry and having DOI: http://dc.zah.uni-heidelberg.de/tap/sync?lang=ADQL&phase=RUN&format=html &request=doQuery&query=select+*+from+rr.alt identifier

5.3 ObsCore

Obscore metadata includes different identifiers at different granularities:

- Identifiers defined with ivoid (https://doi.org/10.25504/FAIRsharing.L4Q3H9) : obs_publisher_did, publisher_id, obs_creator_did
- bib reference is dedicated for bibliography
- obsid is dedicated to observation. the obsid can be repeated for each record coming from the same observation. This Identification is free and could be used for DOI.

6 Providing DOI with metadata

6.1 Attribute proposal

We list several attributes useful to facilitate cross references in the VO but also/almost between data producers.

Note: each metadata is followed by the reference in parentheses to link to the schema of the DOI documentation:

https://schema.datacite.org/meta/kernel-4.2/

Creators (Ref1) add ORCID if exists

Contributors (Ref2) add ORCID if exists

Alternate identifier (Ref4) Please add "ivoid" if exists in order to link the virtual Observatory.

When existing, bibcode, ISSN can also be useful..

Related identifiers (Ref5):

The DOI XML schema (https://schema.datacite.org/) provides a rich grammar:

IsCitedBy, IsSupplementTo, IsSupplementedBy, IsContinuedBy, IsPartOf, HasPartOf, IsReferencedBy, Cites,

We propose to use:

- **IsVariantFormOf** for a resource provided in another form that original resource
 - e.g.: the original archive of Gaia is ESA, but the data is replicated and accessible also through other services or available with advanced values through other data centers.
- **IsOriginalFormOf**: to link the original resource to another resource that can be in another form
- isIdenticalTo: for mirrored data

- **IsSupplementTo** when a resource is a component of an original resource or when it is associated with a main resource.
- IsPartOf for resources depending on other DOI-resources
- Cites: to cite another external or local resource

Example:

```
<relatedIdentifiers>
  <relatedIdentifier relatedIdentifierType="bibcode" relationType="IsSupplementTo">
    2019A&amp; A...621L...2R
  </relatedIdentifier>
  <relatedIdentifier relatedIdentifierType="DOI" relationType="IsSupplementTo">
    10.1051/0004-6361/201834608
  </relatedIdentifier>
<//relatedIdentifiers>
```

Description (Ref6) The description is an opportunity to add relevant information like the origin of the resource (to complete alternate-identifiers).

```
eg: Description put for CDS catalog entry
```

```
<descriptions>
  <description descriptionType="Other">
    VizieR Catalog in addition to the article published in journal
    Astronomy & Astrophysics with title
    'Hyades tidal tails revealed by Gaia DR2.' (doi: 10.1051/0004-6361/201834608)
  </description>
</descriptions>
```

6.2 DOI framework

DOI proposal to make an interconnected DOI network (see schema 7)

7 Feedbacks recommendations

7.1 DOI naming

DataCite recommends using an opaque syntaxe. To remove any significance in a name avoids bad interpretation and is more sustainable. For example, the data center where the data are deposited may change and therefore should not be used in the syntax.

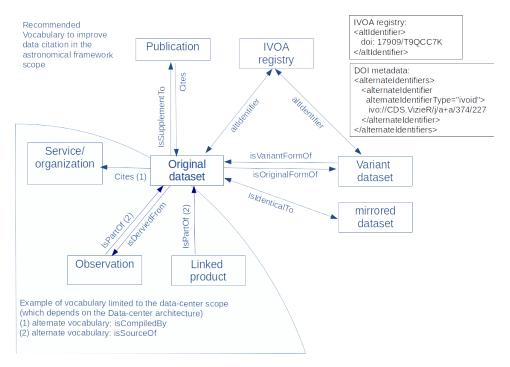


Figure 7: DOI architecture proposal

7.2 DOI sustainability

The data provider must immediately pass on any modification related to maintenance to the registration organization: Landing Page URL, metadata, change of domain name or server name, data location, etc.

If the dataset hosting is transferred to another data center, the DOI will not change, the resolving must connect to the new Landing Page which will give a link to the new dataset location.

7.3 In case of changes in Data

It is possible that the data evolves for various reasons (error detection, generation with a new algorithm, new HPC infrastructure, etc.) In this case it is better to assign a new DOI. These two DOIs will coexist and will be permanent references to different datasets.

7.4 DOI resolving and Landing Page

A DOI is not just a reference but must be clickable and trigger the display of a Landing Page (direct download was banned at the time of writing the note).

The Landing Page does not need to display all of the metadata but a summary of the dataset to give the user additional information to decide whether or not to download the dataset or to use a resource in case of a service. It includes a link to the description of the metadata (see of metadata Schema associated with a DOI provided by DataCite) and a link to download the dataset. These links must always be up to date and not lead to HTTP errors.

The maintenance is the responsibility of the DOI provider. Depending on the relationship the two have, the DOI provider may be able to push this requirement down onto the data provider, but in general its the DOI provider who must agree, as part of their membership in the Registration Agency, to provide direct access to the resources and ensure the metadata they curate is correct.

7.5 License on Data and License on metadata

We distinguish the license applied on the Data and the license applied on the metadata provided by the DOI register agencies.

It is recommended to fill the licenses of the Data in its DOI metadata. URL Link to the license (see list https://spdx.org/licenses/) is preferable to be machine-readable.

```
Example:
```

The metadata provided within the DOI becomes public and subject to be CC0 compatible. For instance, an abstract of an article can be subject to licenses.

8 Miscellaneous links

```
https://wiki.ivoa.net/internal/IVOA/InterOpNov2018DCP/DataCiteDOIsBoF.pdf https://wiki.ivoa.net/twiki/bin/view/IVOA/DataCiteDOIsBoF2017, ADASS Santiago BoF http://adass2018.astro.umd.edu/abstracts/B4-lt.pdf, ADASS College Park, BoF 4 " Data Citation: from Archives to Science Platforms"
```

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