ESO Science Data Product Standard for 1D Spectral Products

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ABSTRACT

The ESO Phase 3 process allows the upload, validation, storage, and publication of reduced data through the ESO Science Archive Facility. Since its introduction, ~2 million data products have been archived and published; 80% of them are one-dimensional extracted and calibrated spectra. Central to Phase3 is the ESO science data product standard that defines metadata and data format of any product. This contribution describes the ESO data standard for 1d-spectra, its adoption by the reduction pipelines of selected instrument modes for in-house generation of reduced spectra, the enhanced archive legacy value. Archive usage statistics are provided.

Keywords: data management, archive operations, data flow, data standard, spectral format, Phase 3, science archive, science data products

1. INTRODUCTION

As part of the effort to build an ESO scientific data heritage [Pirenne & Quinn¹] to maximize the scientific return of its observing facilities, ESO on one side receives and publishes scientific data processed by the astronomical community, on the other side supports the generation of science-grade data products for selected La Silla-Paranal instruments. The ESO Science Archive Facility (SAF) is both the collection and publication point of all science products. It guarantees preservation and long-term access of these important datasets to the ESO user community.

In order to provide smooth operations while handling the incoming flow of data, and allowing a user-friendly exploitation of its scientific value, the backend operations department of ESO has come up with a reliable operational system called Phase 3.

1.1 Receiving scientific data by the ESO astronomical community

The ESO observing policy foresees that the observing teams who are granted large amounts of telescope time, either via the ESO Public Surveys or via so-called Large observing Programmes, need to provide to ESO their calibrated data. Other guest observers can also opt for delivering their calibrated data to ESO, on a voluntary basis.

In particular, the ESO Public Surveys deliver their products with annual cadence, according to agreed survey management plans [Arnaboldi^{2,13}]. Principal Investigators of Large Programmes must finalise their delivery and publication within two years of the completion of the data acquisition for the programme [Romaniello³].

Table 1. Number of science data products received by the community as of May 2016

Product category	Number of products received by the astronomical community
Images	270,000
Source Tables	267,000
1D Spectra	73,000
Catalogs	31
Catalogs Records	> 4 billions
Catalogs Columns	> 1,600
Catalogs Tiles	~12,000

So far, SAF has received and published science data products generated by 11 Public Surveys, and by 11 large or guest observing programs. Table 1 shows the amount of products handled and published.

1.2 Generating science-grade data products

Parallel to the publication of science-driven data products received by the community, ESO supports the generation of data-driven science products [Romaniello³]. Dedicated instrument reduction and calibration pipelines are executed using standard sets of processing parameters (one per instrument mode) in order to generate uniform science-grade data products, with instrumental signature removed, and, if possible, flux calibrated. Error estimates and any quality issue are clearly spelt out in the release description that accompanies any data release. The published data products are considered to be ready for scientific analysis.

The pipeline processing uses the archived, closest in time, quality-controlled, and certified master calibrations. It is important to note that the reduction process itself is automatic, while the quality assessment and certification of the master calibrations is human-supervised.

The data processing is either taking place in-house, at ESO, via the supervision of the ESO Quality Control group, or by dedicated teams under the coordination of ESO (e.g., the so called UK in-kind¹ for the backlog of HAWK-I and VIMOS imaging products, or the PIONIER data products generated by the Institut de Planétologie et d'Astrophysique de Grenoble).

Typically on a monthly basis (but within 48 hours in the HARPS case), newly received observations are processed and the products published, also during proprietary period, so to facilitate the immediate exploitation of the data by the principal investigators, and the later re-use of the same data by the community.

So far, ESO has generated and published, starting September 2013, more than 1.6 million science-grade 1d extracted spectra, from selected instruments, as shown in Table 2.

Instrument	Mode	Qty	Available since	Covering observations starting
UVES	ECHELLE, point sources	110,000	Sep 2013	03/2000 beginning of UVES operations
XSHOOTER	ECHELLE, as point sources	50,000	May 2014	10/2009 " of XSHOOTER "
HARPS	ECHELLE w/out polarimetry	242,000	Sep 2014	10/2003 " of HARPS "
GIRAFFE	MEDUSA multi-object-spect.	1,222,000	Mar 2015	04/2003 " of GIRAFFE "

Table 2. Number of 1d spectral science data products generated in-house as of May 2016.

At the time of writing, more than 80% of the published data products are 1D-extracted spectra. The overly large amount of data products in this format is due to the fact that all spectra from a multi-object spectroscopic observation are extracted and published individually.

2. THE OPERATIONAL APPROACH OF PHASE 3

The task of receiving, archiving, and publishing astronomical data generated by the varied ESO user community has called for a robust approach that could allow the different users to perform their reduction and calibration of the science data adopting their preferred reduction techniques, software, data models, and procedures, while allowing the SAF to perform the task of archiving and publishing the data with minimal effort.

The ESO process that supervises the reception, archiving, and publication of the data products is called Phase 3, as it follows, and closes the loop with, the Phase 1 (proposal submission) and Phase 2 (preparation of the observations) part of the ESO operational data flow [Quinn⁴].

¹ As part of the UK's accession to membership of ESO, this work is on-going by the Cambridge Astronomical Survey Unit, part of the Institute of Astronomy, Cambridge, UK.

The Phase 3 process requires users to submit (via FTP) their data products prepared according to the data formats specified in the *ESO Science Data Products Standard* (SDPS) [Retzlaff & Delmotte⁵] and its addenda [SDPS^{6,7,8,9}], and to submit a release description, a PDF document that describes the scientific goals, and provides quantitative and qualitative description of the release content, of its originating observations, of the calibration and reduction procedures, of the data quality, and of other data format aspects that are left free to the user.

Freedom is left to the data providers to process their data using the procedures they prefer: they can design a pipeline that internally adopts the SDP standard, from the start, or they could instead opt for adding to their pipeline a final step that maps their data to the ESO format standard.

The received data are formally and automatically validated against the SDP standard [Mascetti¹⁰, these proceedings].

If the data are found to be compliant to the standard, a human-supervised step called *content verification* takes place [Delmotte¹¹, these proceedings]. The consistency between the delivered data and the associated documentation ("release description") is checked, as well as the consistency of the metadata of the data products with the metadata of the originating files. Typically, after a few iterations with the submitter, the content verification is successful, and the ingestion and publication of the data takes place.

3. ESO SCIENCE DATA PRODUCT STANDARD

Central to the Phase 3 process is the compliance of the data to the Science Data Product standard. The SDP data format standard was defined with the goals:

- To ensure that all received data have a common data structure and data format;
- To ensure each product is fully characterised using standard descriptors, in common units, permitting swift harvesting, archiving, and publication of its metadata
- To make the publication of new products into the ESO data discovery services fully automatic
- To ease usability to the archival astronomers that can identify data of interest using unified scientific query parameters and that can download data in common formats and units
- To track provenance, for propagation of proprietary rights, and for the purpose of monitoring surveys progress.

The SDP standard is subdivided into different sections for the different types of data. Currently², it covers the following data types:

- Images [Retzlaff & Delmotte⁵]: either simple, or multi-extension FITS format
- Source tables⁵ listing sources detected onto an image
- One dimensional spectra⁵
- Catalogs⁵
- sub-millimeter Flux Maps [SDPS⁶], in particular for the APEX bolometer arrays
- Data Cubes [SDPS⁷] for integral field spectroscopy (first data cubes should be published during summer 2016)
- ESO/GTC (Gran Telescopio de Canarias)[SDPS⁸] fully reduced images and spectra, especially the ones taken as ESO Large Programmes

The standard drives the user in the data preparation part of the submission, from the high level requirements, to the details of the FITS serialization (data structure, required/optional FITS keywords, their formats, units, etc).

To be able to quickly resolve any doubt that the community of Phase 3 data providers could have when preparing their data delivery, a dedicated web page has been setup and forms integral part of the standard: the Phase 3 Questions and Answer web page [SDPS⁹].

² At the time of writing, the VLTI data format standard to support PIONIER data is being prepared.

4. ESO SCIENCE DATA PRODUCT STANDARD FOR 1D SPECTRA

The following considerations were instrumental in choosing/setting the standard for 1d spectra described in this section:

- Each product contains a single, extracted, calibrated, and scientifically characterised spectrum; archive users can easily search and download the individual spectra
- The SDP standard does not require resampling of the wavelength axis (non-uniform sampling is supported)
- The SDP standard allows full error propagation, each spectral point having its own error (1d spectrum error array)
- The SDP standard is derived from recommended IVOA standard: ability for the community to use exiting tools³ to handle these data, potential for interoperability.

The science data product standard for 1d spectra implements:

- A FITS binary table format, derived from the Virtual Observatory Spectrum Data Model standard [McDowell¹²]
- A primary header unit with no data (NAXIS=0)
 - The primary header unit [Figure 1] contains header keywords to describe:
 - processing provenance,
 - data axes and spectral characterisation, (spectral coverage, resolving power, signal-to-noise ratio, etc)
 - o instrument setup,
 - o data links (provenance, ancillary files, bibliographic reference, sibling data, see below)
- One single FITS extension must be present
- The FITS extension carries the 1d extracted spectrum
- The extension contains a FITS binary table with a single record (NAXIS=2 and NAXIS2=1)
- The header of the extension contains keywords necessary to describe the data axes, plus some keywords that must be present to ensure VO compliance [Figure 2]
- Each column must specify the standard FITS binary keywords TTYPEn, TUNITn, and TFORMn
- Each column should specify the Virtual Observatory descriptors TUCDn and TUTYPn⁴,
- Spectral coordinate, flux, and error arrays must all be present and supplied one per column
- Other columns/arrays can be present
- All data arrays within the same spectrum file must have the same size (length)
- Variable length arrays are not permitted, hence PCOUNT = 0, GCOUNT = 1
- Spectral coordinate could be either wavelength, frequency, or energy (TTYPE1 = WAVE | FREQ | ENER)
- Spectral coordinate array values must be increasing monotonically, form TDMIN1 to TDMAX1
- If available, a quality, sky background, and continuum arrays can be added with the TTYPEn values of QUAL, SKYBACK, and CONTINUUM
- If the spectrum is normalized to the continuum, the CONTNORM keyword must be set to T (true), and the TUCD2 must be contain (not as primary token) the token: arith.ratio (e.g. phot.flux.density;em.wl;arith.ratio)

By default the TUTYPn convention to be used is the one specified by Spectrum Data Model standard v1.1, though in some more complex cases the adoption of the TUTYPn convention set by the Spectral Data Model v2.0 could be suggested by ESO personnel at the time of data preparation.

4.1 Data linking: associating ancillary files

It is possible to provide ancillary files associated to a spectrum, for example to associate a PNG preview image of the spectrum, or a wavelength-calibrated and distorsion-corrected 2D image of the original dispersed 2D spectrum (lambda, angle), etc.

For ancillary files, which are associated to science products without being directly searchable, any file format including the FITS format is accepted. An ancillary file must be associated to at least one science data product.

³ For example, the popular IRAF ONEDSPEC package can be used to display and process the Phase 3 spectra.

⁴ By default the TUTYPn convention to be used is the one specified by Spectrum Data Model standard v1.1, though in those cases the adoption of the TUTYPn convention set by the Spectral Data Model v2.0 is allowed

⁽http://www.ivoa.net/documents/SpectralDM/20150528/PR-SpectralDM-2.0-20150528.pdf).

The mechanism to associate files requires the following FITS keywords to be present in the primary header unit of the science data product:

- the ASSONn keywords containing the list (1 to n) of the names of the ancillary files to be associated
- the ASSOMn keywords reporting for each associated file its checksum (md5sum), i.e., the digital fingerprint of the file used to verify that its integrity has not been compromised in transmission or storage.

Furthermore, if the associated file is not in FITS format, the following keywords must be present:

• the ASSOCn keywords reporting the category of the associated file (e.g. ANCILLARY.PREVIEW, ANCILLARY.2DSPECTRUM, etc.)

If the associated file is in FITS format, then the ASSOCn keyword must **not** be present, while the associated ancillary FITS file must report its category using the PRODCATG keyword.

4.2 Data linking: associating bibliographic reference

The REFERENC keyword must be present in the primary header unit of the science data product and must contain a digital reference to the primary scientific publication describing the content, coverage, process of creation, scientific quality of the data product. The digital reference can either be a BIBCODE (19-digit bibliographic identifier⁵ adopted by the CDS, NED, and ADS) or a DOI⁶ (Digital Object Identifier). If no reference can yet be provided, the keyword must be present, and its value left empty.

4.3 Data linking: associating other spectra or catalog records of the same object

Within a data collection, all 1d spectra of the same object must carry the same value (identical spelling) of the OBJECT FITS keyword.

It is possible to link a catalog record to the spectrum its measurements were derived from, by storing in a dedicated catalog column the original file name of the pertaining 1d spectrum, and using the TXLNKi keyword mechanism explained in §5.2.2.1 of the SDP standard.

When a catalog record refers to multiple spectra of the same object, it is possible to link the record to those spectra by storing the OBJECT value in a dedicated catalog column, identified by the Uniform Content Descriptor [Preite Martinez¹⁵]: meta.id;meta.main.

4.4 Data linking: provenance information

A full section of the SDP standard is dedicated to the FITS representation of the processing provenance, which must be present in all science data products, hence also in 1d spectra. In the 1d spectral case the processing provenance is serialized in the primary header unit of the science data product using the keywords PROVn listing the science files originating the data product at hand.

⁵ BIBCODE, see: http://simbad.u-strasbg.fr/guide/refcode/refcode-paper.html

⁶ Digital Object Identifier (DOI®) System: https://www.doi.org/overview/DOI_article_ELIS3.pdf

Comprehensive list of primary header keywords for the single object 1D spectrum in the binary table format

SIMPLE =	т	1 :	Standard FITS format (NOST-100-2.0)
BITPIX =			Number of bits per data pixel
NAXIS =			Number of data axes
EXTEND =			Extensions may be present
ORIGIN =			European Southern Observatory
DATE =			Date this file was written
TELESCOP=			ESO Telescope designation
INSTRUME=			Instrument name
DISPELEM=			Dispersive element name
SPECSYS =			Reference frame for spectral coordinates
OBJECT =			Target designation
EXT_OBJ =			TRUE if extended
RA =			[deg] Spectroscopic target position (J2000.0)
DEC =			[deg] Spectroscopic target position (J2000.0)
EQUINOX =			Standard FK5 (years)
RADECSYS=			Coordinate reference frame
EXPTIME =			Total integration time per pixel (s)
MJD-OBS =			<pre>[d] Start of observations (days)</pre>
MJD-END =			<pre>[d] End of observations (days)</pre>
TIMESYS =			Time system used
PROG_ID =			ESO programme identification
OBID1 =			Observation block ID
M_EPOCH =			TRUE if resulting from multiple epochs
PROV1 =			Originating science file
PROCSOFT=			Data reduction software/system with version no.
			Mashaimus of chasemustica
OBSTECH =			Technique of observation
PRODCATG=	'SCIENCE.SPECTRUM'	/ 1	Data product category
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Figure 1 The primary header unit for 1d spectral products (mandatory keywords in bold)

Comprehensive list of extension header keywords for the single object 1D spectrum in the binary table format

		'BINTABLE'		FITS Extension first keyword
BITPIX :	=			Number of bits per data pixel
NAXIS :	=		2 /	Number of data axes
NAXIS1 :	=	:	%d /	Length of data axis 1
NAXIS2 :	=		%d /	Length of data axis 2
PCOUNT	-		0 /	Parameter count
GCOUNT				Group count
		SPECTRUM V1.0'		VO Data Model
		'ESO/SAF'		VO Publishing Authority
TITLE				Dataset title
OBJECT :				Target designation
RA :				[deg] Spectroscopic target position (J2000.0)
220	=			[deg] Spectroscopic target position (J2000.0)
APERTURE:	=			[deg] Aperture diameter
TELAPSE :	=			[s] Total elapsed time
TMID :	=	:	%f /	[d] MJD mid exposure
SPEC VAL:	=		%f /	[nm] Mean Wavelength
SPEC BW :	=		%f /	[nm] Bandpass Width Wmax - Wmin
TFIELDS :	=			Number of fields in each row
NELEM :				Length of the data arrays
TTYPE1 :				Label for field 1
		Spectrum.Data.Spe	•	
TFORM1		-		Data format of field1
TUNIT1 :				Physical unit of field1
TUCD1 :				UCD of field 1
TDMIN1 :	=			Start in spectral coord.
TDMAX1 :	=		%f /	Stop in spectral coord.
TTYPE2 :				Label for field 2
TUTYP2 :	=	'Spectrum.Data.Flu:	xAxi	s.Value'
TFORM2 :	=	:	%s /	Data format of field 2
TUNIT2 :	=		%s /	Physical unit of field 2
TUCD2 :	-			UCD of field 2
			35 /	
TTYPE3 :	=	'ERR'	1	Label for field 3
TTYPE3 : TUTYP3 :	=	'ERR' 'Spectrum.Data.Flu:	×Axi	Label for field 3 Ls.Accuracy.StatError'
TTYPE3 : TUTYP3 : TFORM3 :	=	'ERR' 'Spectrum.Data.Flu	×Axi %s /	'Label for field 3 Ls.Accuracy.StatError' 'Data format of field 3
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TTYPE3 : TUTYP3 : TFORM3 : TUNIT3 : TUCD3 : TTYPE4 : TUTYP4 :		'ERR' 'Spectrum.Data.Flu: 'QUAL'	xAxi %s / %s / %s / %s /	<pre>/ Label for field 3 / Label for field 3 / Data format of field 3 / Physical unit of field 3 / UCD of field 3 / Content of field 4 / UType of field 4</pre>
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Figure 2 The header of the FITS binary table extension for 1d spectral products (mandatory keywords in bold)

5. ARCHIVE USAGE STATISTICS

5.1 Data Holdings

Via Phase 3, as of May 2016 about 2 million of science data products have been made available to the user community. Figure 3 shows the incoming flow of data by the different product categories. Initially, the ESO Public Survey teams uploaded images and source-tables. September 2013 marks the beginning of the in-house generation and publishing of 1d spectra. The VISTA public survey teams then started providing photometric tile catalogs for each of the VIRCAM tiles observed. Along the way, a SAF in-house porting of previously (before Phase 3) generated advanced science products took place (GOODS, zCOSMOS, ESSENCE, etc.). Then came the data of the ESO spectroscopic public surveys (PESSTO and GaiaESO), and of the VST/OMEGACAM public surveys.

As can be seen, the 1d spectra (plotted divided by 10 to ease comparison) outnumber all other product categories, constituting about 80% of all products.

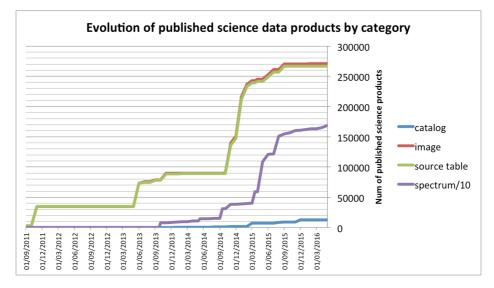


Figure 3 Evolution of Phase 3 data holdings by science product category (spectrum divided by 10)

The generation of in-house data products continued with the production of XSHOOTER ECHELLE 1d spectra (May 2014), HARPS non-polarimetric 1d spectra (Sep 2014), and GIRAFFE MEDUSA (Mar 2015). As shown in Figure 4, the main contributor to the number of published spectra is the GIRAFFE MEDUSA mode (plotted divided by 10), whereby up to 130 targets spectra of intermediate resolution could be acquired in a single observation.

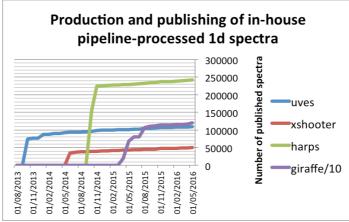


Figure 4 In-house generation of pipeline-processed science grade data products

5.2 Interest by the astronomical community

All plots in this section show both the evolution with time of (blue) the number of published⁷ products available for download, and (red) the number of products successfully downloaded by unprivileged users external to ESO. Access by the principal investigators and their teams is therefore not included in these plots.

Figure 5 shows that the Phase 3 system is continuously active in receiving and publishing science data products (blue curve); at the same time, the user community has been as active in downloading the available data products (red curve).

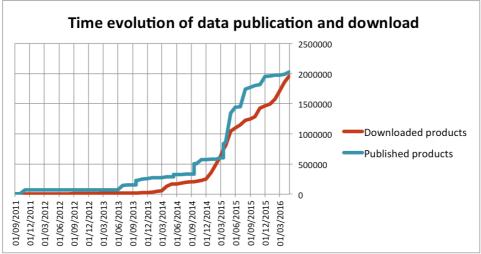


Figure 5 In average every science data product has been downloaded at least once

Figure 6 splits the same data of figure 5 by the science data product category. The interest for the \sim 12,000 published tile catalogs is very high: in average each of the tile catalog FITS files has been retrieved more than 6 times (ratio=6). Spectra are also quite popular, with each of the 1.6 million spectra downloaded at least once in average (ratio=1). In average, one every 4 source tables and one every 2 images have not been downloaded (ratio=0.75 and 0.5 respectively).

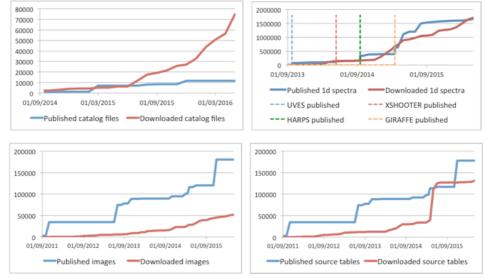


Figure 6 Popularity of science data products by category

⁷ While Phase 3 can handle different versions of the same product uploaded at different times by the public survey teams, the plots in this section consider only the latest version of any data product. As of May 2016, about 10% of the data have been declared obsolete and superseded by a newer version.

Highlighted in the top right panel of fig. 6 are the moments in time when the UVES, XSHOOTER, HARPS, and GIRAFFE in-house production and publication started. After the publishing of the initial backlog, new products are generated and published about once a month. Despite the considerable effort of ESO in publishing more and more products, the community is always catching up quickly.

Figure 7 shows the growth of archive users, external to ESO, downloading Phase 3 science data products. The number of distinct accounts currently is about 1400, and is still linearly growing with time. Also shown, the number of users that have downloaded at least one spectrum, and the number of users that never retrieved any spectrum. There are 687 users (out of 1442, i.e. 47%) who have used the Phase 3 archive exclusively to download spectra.

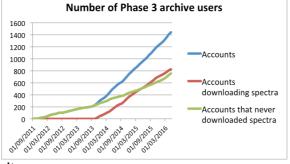


Figure 7 Growth of user community

6. CONCLUSIONS

Phase 3 is successful in both handling and publishing the incoming flow of science data products, and in attracting a growing community of archive researchers. Currently, spectra constitute the 80% of the science data products in the Phase 3 data holdings. In 2015, almost 1,000,000 spectral data products were downloaded from the ESO Science Archive Facility.

The data format chosen for the 1d spectral products has been described, along with the reasons why certain choices were made. In particular, important has been the choice of moving away from the typical format for 1d spectra adopted by ground-based astronomical observatories (a 1d FITS image, equally-sampled on the spectral axis) in favour of a richer FITS binary table that does not require resampling of the data, and permits full error propagation. The chosen 1d spectral data format is used both for data received from the community (e.g. ESO spectroscopic public surveys, or other large programmes), and for science-grade data products generated in-house. The format is compliant with International Virtual Observatory Alliance standards, and hence supported by many software analysis packages and tools.

Phase 3, in its fifth year of operations, is still evolving [Retzlaff¹⁴]. The number and types of science-ready data published by the Science Archive Facility is growing. Soon, new types of science data products will be ingested and served to the astronomical community through the SAF, starting from the pipeline-processed VLT/MUSE spectral data cubes. Many other new science data products are expected, like the pipeline-processed VIMOS and HAWK-I imaging data, the science data from various large ESO observing programmes, the VLTI/PIONIER interferometric data, etc. The ESO Science Archive Facility, with its growing legacy value, is well on its way to becoming an essential science tool for the astronomical community at large.

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